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# Electronic Energy and Local Property Errors at QTAIM Critical Points while Climbing Perdew's Ladder of Density-Functional Approximations

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Supporting information for:  
Electronic-Energy and Local Property Errors  
at QTAIM Critical Points while Climbing  
Perdew's Ladder of Density-Functional  
Approximations

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# S1 Composition of the Large Datasets

## S1.1 The G2 Dataset (also called G2/97)

The G2 dataset counts for a total of 148 reference atomization energies of small molecules. Due to inconsistent QTAIM topologies avoiding a fair and strict comparison between all methods, we had to remove 9 of the systems (out of 148). They are:  $\text{Na}_2$ ,  $\text{Si}_2$ ,  $\text{P}_2$ ,  $\text{Si}_2\text{H}_6$ ,  $\text{C}_4\text{H}_6$  (bicyclo[1.1.0]butane),  $\text{C}_4\text{H}_6$  (cyclobutene),  $\text{C}_4\text{H}_8$  (cyclobutane),  $\text{C}_4\text{H}_8$  (isobutene), CCH. Due to integral storage limitations, we had to also to remove  $(\text{CH}_3)_3\text{C}$  for which we were unable to compute the CCSD/def2-QZVP reference densities. In this investigation, we thus benchmarked the topology of 138 molecules summarized in Table S4.

## S1.2 The DBH24 Dataset

The DBH24 counts for a total of 24 barrier height energies (12 direct and 12 reverse reactions). In this investigation, we thus benchmarked the topology of 12 transition state structures summarized in Table S5.

## S1.3 The NCB31 Dataset

The NCB31 dataset counts for a total of 31 reference weak interaction energies of organic dimers. Due to integral storage limitations, we had to remove 4 systems (out of 31) for which we were unable to compute the CCSD/def2-QZVP reference densities. They are: benzene – neon, benzene – benzene (sandwich), benzene – benzene (T-shaped), benzene – benzene (parallel-displaced). In this investigation, we thus benchmarked the topology of 27 dimers in weak interactions summarized in Table S6.

## **S2 List of the Density-Functional Approximations**

### **S2.1 Nonempirical Density-Functional Approximations**

PBE, PBE0 and PBE-QIDH are here considered as nonempirical density functionals.

### **S2.2 Minimally Parameterized Density Functional Approximations**

BLYP, B3LYP and B2-PLYP are here considered as minimally parameterized density functionals

### **S2.3 Highly Parameterized Density Functional Approximations**

We consider here a list of 20 highly parameterized density functionals. They are: M06-2X, SOGGA11-X,  $\omega$ B97X,  $\omega$ B97XD,  $\omega$ B97, M11, MN15, N12-SX, N12, M05-2X, M05, SOGGA11, BMK, MN15-L, M06-L, MN12-SX, M06, MN12-L, M11-L and M06-HF.

## S3 Density Comparison from a Becke-Lebedev Integration Grid

### S3.1 $S$ Criteria

$$S_{\text{Cosine}}(\rho_1, \rho_2) = \frac{\int \rho_1(\mathbf{r})\rho_2(\mathbf{r})d\mathbf{r}}{\sqrt{\int \rho_1^2(\mathbf{r})d\mathbf{r} \int \rho_2^2(\mathbf{r})d\mathbf{r}}} \quad (1)$$

$$S_{\text{Tanimoto}}(\rho_1, \rho_2) = \frac{\int \rho_1(\mathbf{r})\rho_2(\mathbf{r})d\mathbf{r}}{\int \rho_1^2(\mathbf{r})d\mathbf{r} + \int \rho_2^2(\mathbf{r})d\mathbf{r} - \int \rho_1(\mathbf{r})\rho_2(\mathbf{r})d\mathbf{r}} \quad (2)$$

$$S_{\text{Dice}}(\rho_1, \rho_2) = \frac{2 \int \rho_1(\mathbf{r})\rho_2(\mathbf{r})d\mathbf{r}}{\int \rho_1^2(\mathbf{r})d\mathbf{r} + \int \rho_2^2(\mathbf{r})d\mathbf{r}} \quad (3)$$

### S3.2 Notes

- $\forall(\rho_1, \rho_2), \quad 0 \leq S(\rho_1, \rho_2) \leq 1.$
- if  $\rho_1 = \rho_2$  then  $S(\rho_1, \rho_2) = 1.$
- if  $\rho_1 \perp \rho_2$  then  $S(\rho_1, \rho_2) = 0.$
- All  $S$  criteria are estimated from densities computed on an ‘ultrafine’ Becke-Lebedev integration grid using the release 2.1.1 of the HORTON software.

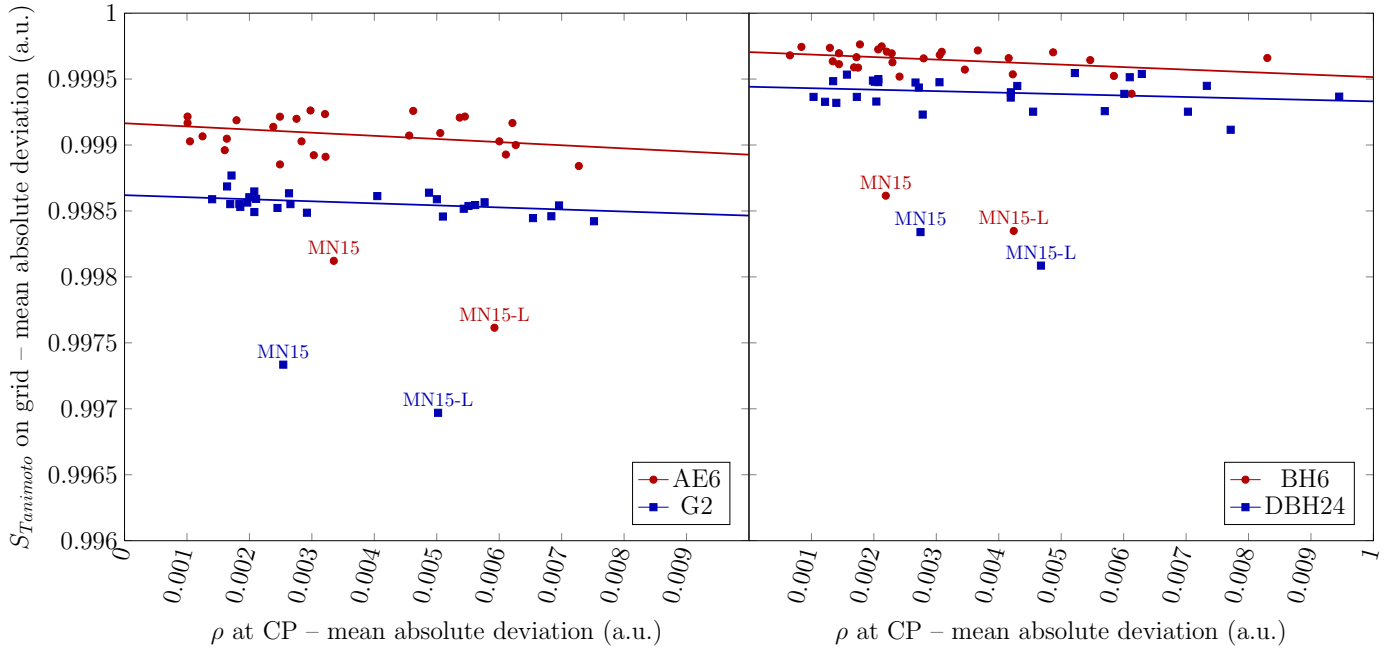


Figure S1: Correlation diagrams between the density errors computed at critical points and the  $S_{\text{Tanimoto}}$  criteria computed on an ‘ultrafine’ Becke-Lebedev integration grid. Except for MN15-L and MN15, the density error at critical points varies linearly with the  $S_{\text{Tanimoto}}$  criteria showing that the density error at bond and ring critical points provide a quantitative picture of the quality of the density derived from a given density functional. Numerical errors at critical points remain also one or two orders of magnitude larger than those computed on an integration grid. MN15-L and MN15 are the only two outliers of this trend. For both density functionals, the quality of the density out of the critical points is in average lower than at the critical point.

# S4 Density and Energy Errors from Large Databases

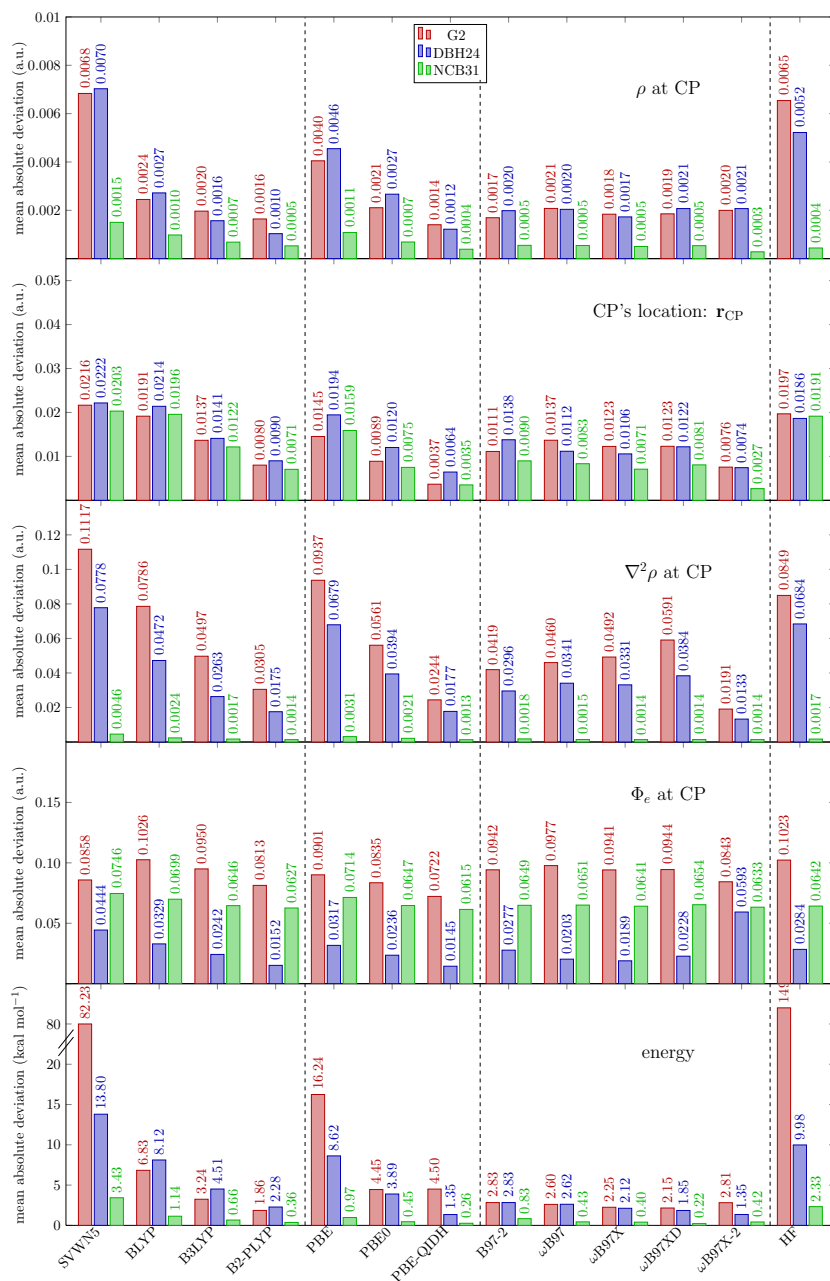


Figure S2: From top to down, mean absolute deviations (MADs) calculated over the density ( $\rho$  in a.u.), position ( $\mathbf{r}_{CP}$  in a.u.), Laplacian of the electron density ( $\nabla^2\rho$  in a.u.), and electrostatic potential from electrons ( $\Phi_e$  in a.u.) errors from the 746 critical points gathered into the G2, DBH24 and NCB31 representative databases for a selection of density functionals. As a matter of comparison, the energy performance (MADs in kcal mol $^{-1}$ ) of each density functional is provided in the down panel. All computations are performed with the def2-QZVP basis set.

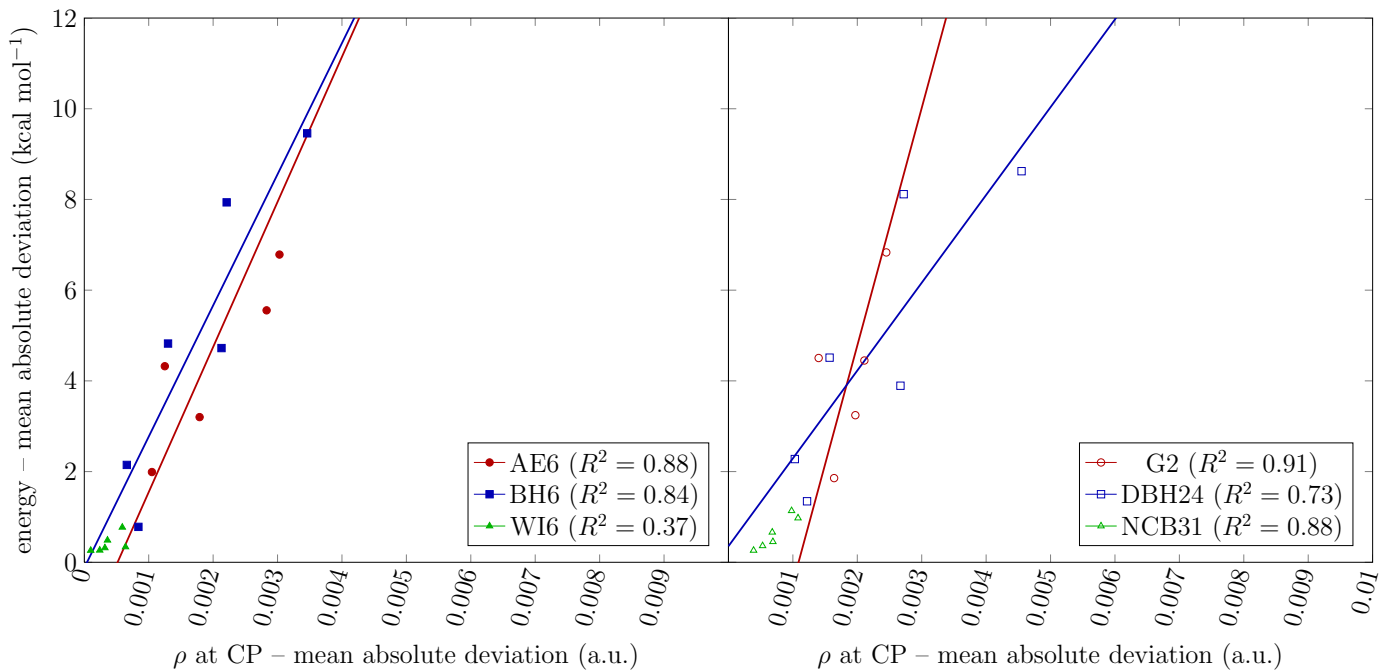


Figure S3: Correlation diagrams between the density and energy mean absolute deviation (MAD) criteria for PBE- (PBE, PBE0, PBE-QIDH) and BLYP-based (BLYP, B3LYP, B2-PLYP) nonempirical and minimally parameterized density functionals on the (red) atomization energy (left) AE6 and (right) G2, (blue) barrier height (left) BH6 and (right) DBH24, and (green) weak interaction (left) WI6 and (right) NCB31 databases. For each database, the coefficients of determination ( $R^2$ ) related to each linear regression are provided in the legend.



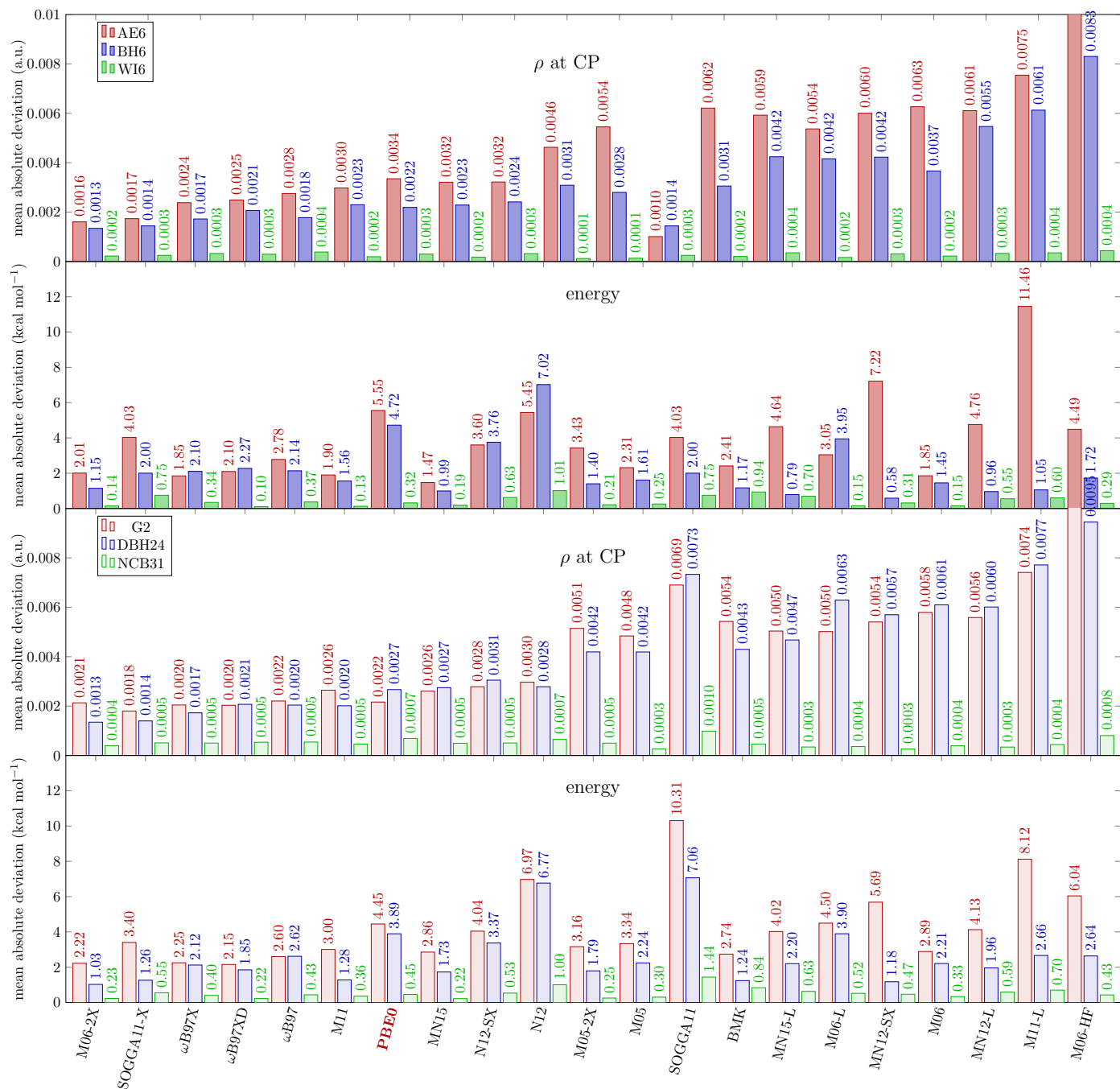


Figure S4: From top to down, for a selection of 20 highly parameterized density functionals (see Section S2), mean absolute deviations (MADs) calculated over the density ( $\rho$  in a.u.) errors from the 46 critical points gathered into the AE6, BH6 and WI6 representative databases, the corresponding energy (kcal mol<sup>-1</sup>) errors, the density errors from the 746 critical points gathered into the G2, DBH24 and NCB31 databases, and the corresponding energy errors. All computations are performed with the def2-QZVP basis set.

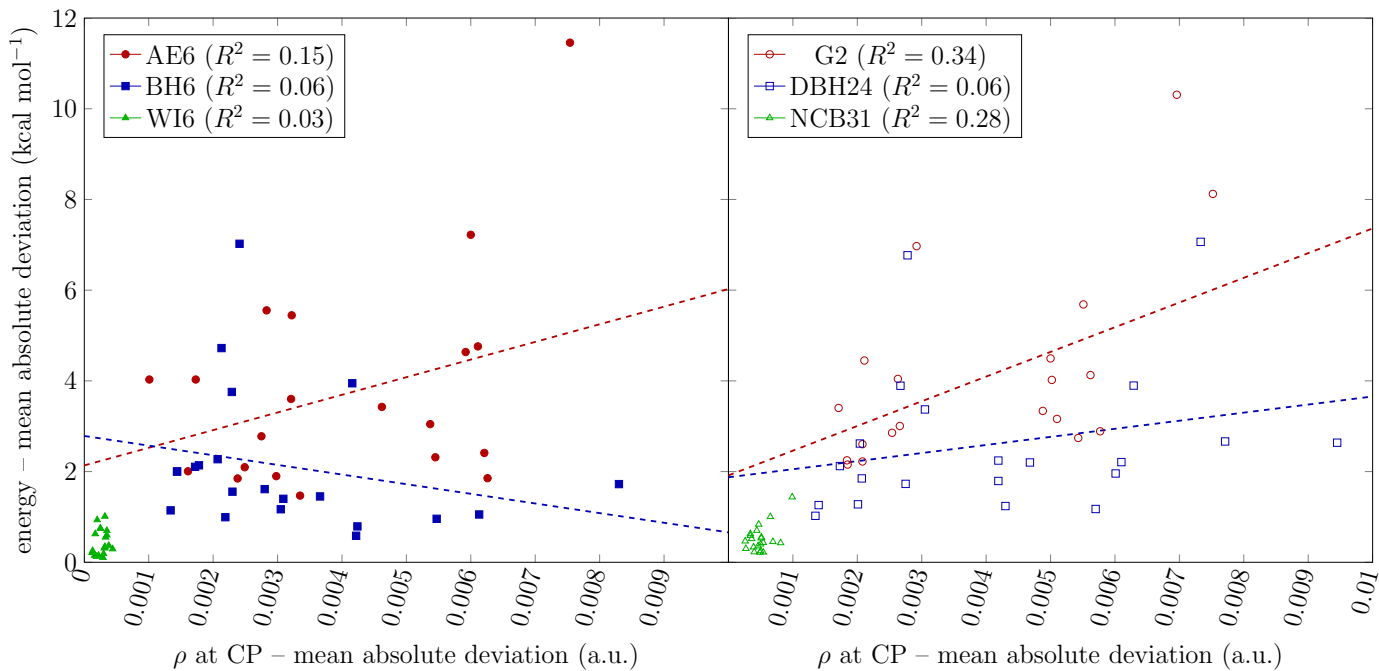


Figure S5: Correlation diagrams between the density and energy mean absolute deviation (MAD) criteria for a selection of 20 highly parameterized density functionals (see Section S2) on the (red) atomization energy (left) AE6 and (right) G2, (blue) barrier height (left) BH6 and (right) DBH24, and (green) weak interaction (left) WI6 and (right) NCB31 databases. For each database, the coefficients of determination ( $R^2$ ) related to each linear regression are provided in the legend.

# S5 Density Computed at Bond and Ring Critical Points

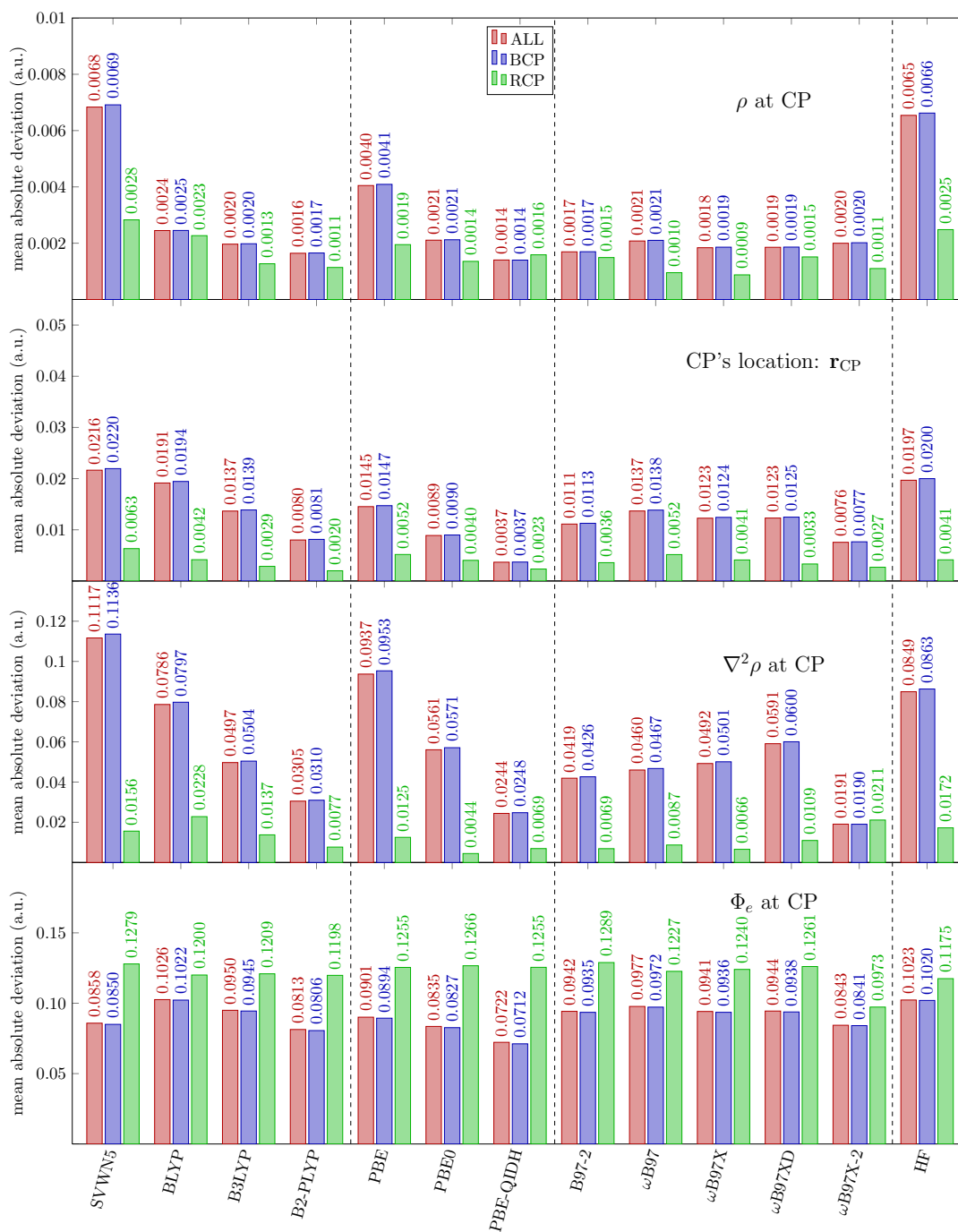


Figure S6: From top to down, mean absolute deviations (MADs) calculated over the density ( $\rho$  in a.u.), position ( $\mathbf{r}_{CP}$  in a.u.), Laplacian of the electron density ( $\nabla^2\rho$  in a.u.), and electrostatic potential from electrons ( $\Phi_e$  in a.u.) errors from the 727 bond and 19 ring critical points gathered into the G2, DBH24 and NCB31 databases for a selection of density functionals. All computations are performed with the def2-QZVP basis set.

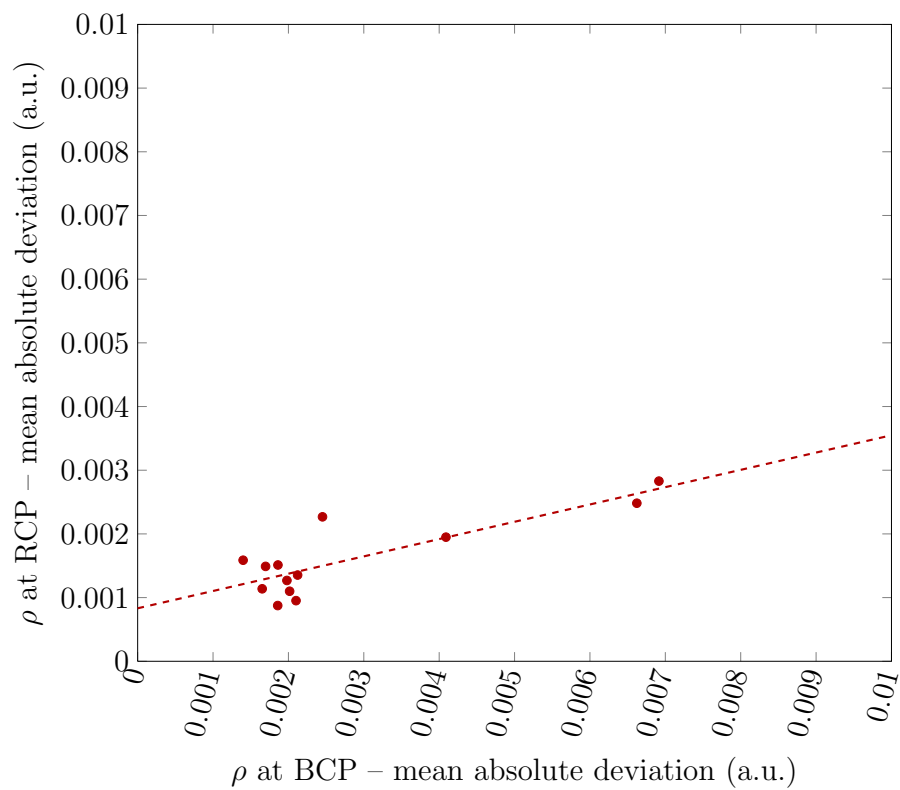


Figure S7: Correlation diagram between the density errors computed at the 727 bond and 19 ring critical points derived from the G2, DBH24, and NCB31 databases for PBE- (PBE, PBE0, PBE-QIDH) and BLYP-based (BLYP, B3LYP, B2-PLYP) nonempirical and minimally parameterized density functionals.

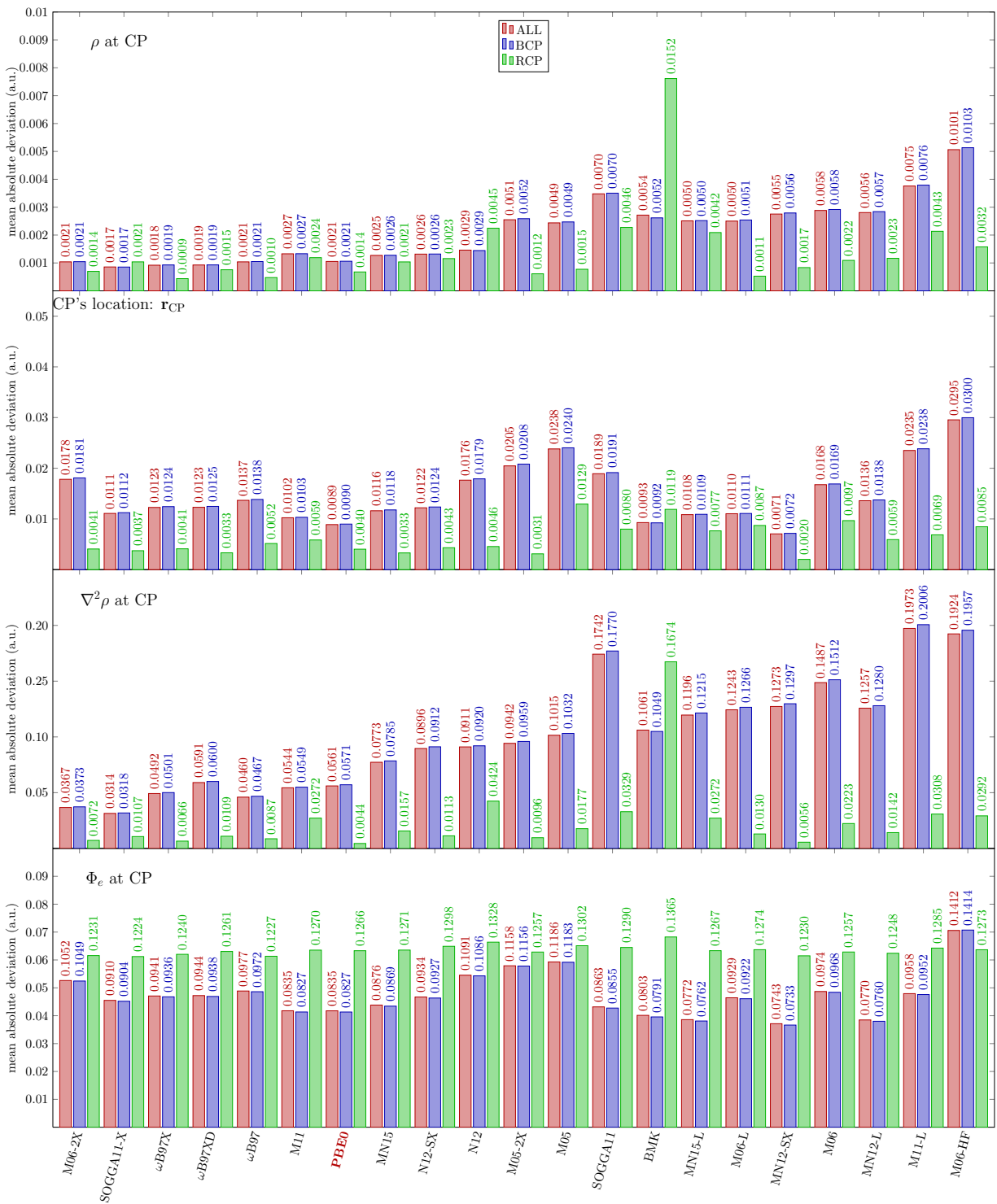


Figure S8: From top to down, mean absolute deviations (MADs) calculated over the density ( $\rho$  in a.u.), position ( $\mathbf{r}_{CP}$  in a.u.), Laplacian of the electron density ( $\nabla^2\rho$  in a.u.), and electrostatic potential from electrons ( $\Phi_e$  in a.u.) errors from the 727 bond and 19 ring critical points gathered into the G2, DBH24 and NCB31 representative databases for a selection of 20 highly parameterized density functionals (see Section S2). All computations are performed with the def2-QZVP basis set.

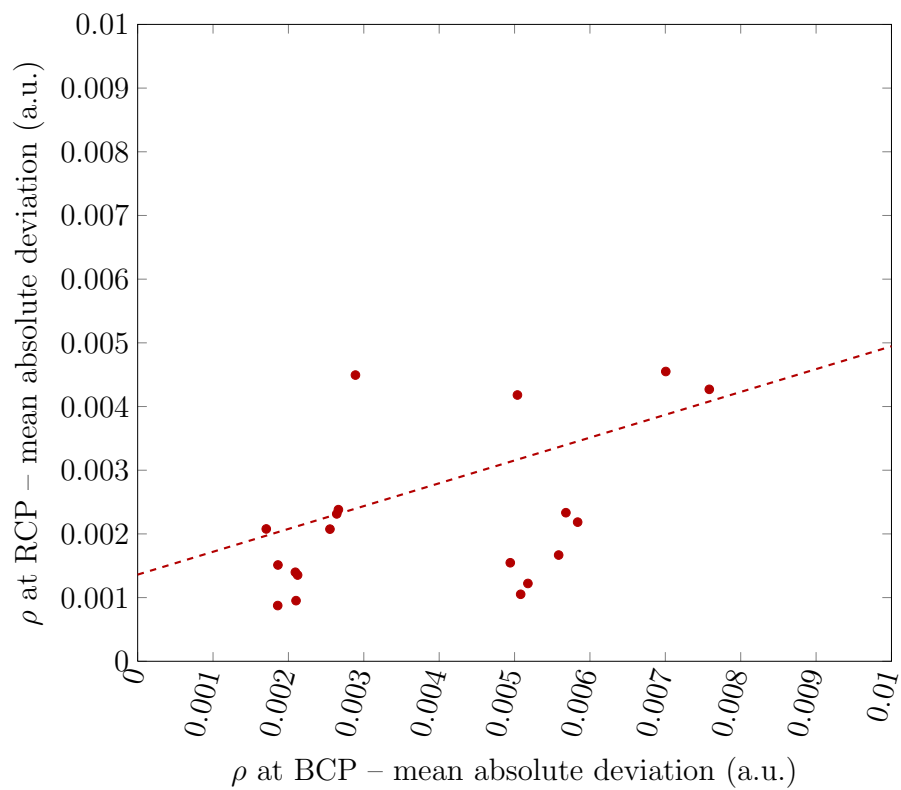


Figure S9: Correlation diagram between the density errors computed at the 727 bond and 19 ring critical points derived from the G2, DBH24, and NCB31 databases for a selection of 20 highly parameterized density functionals (see Section S2).

Table S1: Mean absolute deviations of the  $S$  criteria calculated according to the Cosinus, Tanimoto and Dice formulation calculated over the systems included into the AE6 dataset. All the computations are done at the def2-QZVP level of theory. Reference densities are computed at the CCSD/def2-QZVP level of theory. The definition of the  $S$  criteria is provided in Section S3.

	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
MAD( $S_{\text{Cosine}}$ )	0.999464	0.999474	0.999543	0.999524	0.999615	0.999541	0.999605	0.999522
MAD( $S_{\text{Tanimoto}}$ )	0.998841	0.998923	0.999072	0.999048	0.999216	0.998911	0.999208	0.998757
MAD( $S_{\text{Dice}}$ )	0.999419	0.999461	0.999536	0.999523	0.999607	0.999455	0.999604	0.999378
	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
MAD( $S_{\text{Cosine}}$ )	0.999487	0.999418	0.999598	0.999517	0.999637	0.999510	0.999591	0.999515
MAD( $S_{\text{Tanimoto}}$ )	0.998928	0.997615	0.999188	0.999028	0.999216	0.999000	0.999167	0.998122
MAD( $S_{\text{Dice}}$ )	0.999464	0.998805	0.999594	0.999513	0.999607	0.999499	0.999583	0.999060
	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
MAD( $S_{\text{Cosine}}$ )	0.999602	0.999508	0.999646	0.999493	0.999615	0.999579	0.999612	0.999638
MAD( $S_{\text{Tanimoto}}$ )	0.999167	0.998961	0.999259	0.998903	0.999199	0.999138	0.999215	0.999235
MAD( $S_{\text{Dice}}$ )	0.999583	0.999480	0.999629	0.999451	0.999599	0.999569	0.999607	0.999617
	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
MAD( $S_{\text{Cosine}}$ )	0.999546	0.999644	0.999545	0.999516	0.999533	0.999435		
MAD( $S_{\text{Tanimoto}}$ )	0.999028	0.999262	0.999091	0.999028	0.999066	0.998853		
MAD( $S_{\text{Dice}}$ )	0.999514	0.999631	0.999545	0.999513	0.999532	0.999426		

Table S2: Mean absolute deviations of the  $S$  criteria calculated according to the Cosinus, Tanimoto and Dice formulation calculated over the systems included into the BH6 dataset. All the computations are done at the def2-QZVP level of theory. Reference densities are computed at the CCSD/def2-QZVP level of theory. The definition of the  $S$  criteria is provided in Section S3.

	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
MAD( $S_{\text{Cosine}}$ )	0.999803	0.999863	0.999791	0.999795	0.999855	0.999856	0.999830	0.999811
MAD( $S_{\text{Tanimoto}}$ )	0.999524	0.999708	0.999572	0.999589	0.999696	0.999519	0.999659	0.999389
MAD( $S_{\text{Dice}}$ )	0.999762	0.999854	0.999786	0.999794	0.999848	0.999760	0.999829	0.999694
	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
MAD( $S_{\text{Cosine}}$ )	0.999835	0.999808	0.999872	0.999876	0.999849	0.999868	0.999814	0.999807
MAD( $S_{\text{Tanimoto}}$ )	0.999644	0.998349	0.999737	0.999748	0.999657	0.999717	0.999613	0.998616
MAD( $S_{\text{Dice}}$ )	0.999822	0.999173	0.999868	0.999874	0.999828	0.999859	0.999807	0.999307
	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
MAD( $S_{\text{Cosine}}$ )	0.999859	0.999841	0.999867	0.999863	0.999894	0.999841	0.999866	0.999861
MAD( $S_{\text{Tanimoto}}$ )	0.999683	0.999635	0.999707	0.999660	0.999763	0.999666	0.999725	0.999695
MAD( $S_{\text{Dice}}$ )	0.999841	0.999818	0.999854	0.999830	0.999881	0.999833	0.999862	0.999848
	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
MAD( $S_{\text{Cosine}}$ )	0.999816	0.999825	0.999852	0.999842	0.999872	0.999799		
MAD( $S_{\text{Tanimoto}}$ )	0.999536	0.999627	0.999703	0.999680	0.999744	0.999587		
MAD( $S_{\text{Dice}}$ )	0.999768	0.999814	0.999852	0.999840	0.999872	0.999793		



Table S3: Mean absolute deviations of the  $S$  criteria calculated according to the Cosinus, Tanimoto and Dice formulation calculated over the systems included into the WI6 dataset. All the computations are done at the def2-QZVP level of theory. Reference densities are computed at the CCSD/def2-QZVP level of theory. The definition of the  $S$  criteria is provided in Section S3.

	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
MAD( $S_{\text{Cosine}}$ )	0.999340	0.998996	0.999222	0.999005	0.999330	0.999089	0.999230	0.998929
MAD( $S_{\text{Tanimoto}}$ )	0.998553	0.997949	0.998421	0.998009	0.998646	0.998047	0.998457	0.997393
MAD( $S_{\text{Dice}}$ )	0.999276	0.998972	0.999210	0.999003	0.999322	0.999022	0.999227	0.998694
	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
MAD( $S_{\text{Cosine}}$ )	0.999140	0.999292	0.999160	0.999260	0.999131	0.999233	0.999337	0.998649
MAD( $S_{\text{Tanimoto}}$ )	0.998235	0.996508	0.998307	0.998511	0.998166	0.998432	0.998661	0.995610
MAD( $S_{\text{Dice}}$ )	0.999116	0.998251	0.999152	0.999255	0.999081	0.999215	0.999330	0.997799
	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
MAD( $S_{\text{Cosine}}$ )	0.999220	0.999005	0.999309	0.998956	0.999263	0.999309	0.999013	0.999001
MAD( $S_{\text{Tanimoto}}$ )	0.998377	0.997908	0.998559	0.997765	0.998475	0.998589	0.998011	0.997931
MAD( $S_{\text{Dice}}$ )	0.999187	0.998952	0.999279	0.998880	0.999237	0.999293	0.999004	0.998964
	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
MAD( $S_{\text{Cosine}}$ )	0.999116	0.999306	0.999094	0.999279	0.999362	0.999185		
MAD( $S_{\text{Tanimoto}}$ )	0.998164	0.998578	0.998192	0.998551	0.998724	0.998349		
MAD( $S_{\text{Dice}}$ )	0.999081	0.999288	0.999094	0.999274	0.999361	0.999173		

Table S4: Mean absolute deviations of the  $S$  criteria calculated according to the Cosinus, Tanimoto and Dice formulation calculated over the systems included into the G2 dataset. All the computations are done at the def2-QZVP level of theory. Reference densities are computed at the CCSD/def2-QZVP level of theory. The definition of the  $S$  criteria is provided in Section S3.

	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
MAD( $S_{\text{Cosine}}$ )	0.999249	0.999287	0.999324	0.999277	0.999302	0.999308	0.999302	0.999332
MAD( $S_{\text{Tanimoto}}$ )	0.998460	0.998523	0.998613	0.998552	0.998542	0.998487	0.998589	0.998422
MAD( $S_{\text{Dice}}$ )	0.999209	0.999245	0.999295	0.999259	0.999257	0.999230	0.999281	0.999202
	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
MAD( $S_{\text{Cosine}}$ )	0.999283	0.999245	0.999292	0.999304	0.999373	0.999308	0.999403	0.999270
MAD( $S_{\text{Tanimoto}}$ )	0.998545	0.996970	0.998564	0.998592	0.998639	0.998566	0.998769	0.997335
MAD( $S_{\text{Dice}}$ )	0.999260	0.998469	0.999267	0.999283	0.999310	0.999270	0.999377	0.998654
	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
MAD( $S_{\text{Cosine}}$ )	0.999292	0.999291	0.999260	0.999337	0.999359	0.999295	0.999273	0.999354
MAD( $S_{\text{Tanimoto}}$ )	0.998517	0.998492	0.998458	0.998542	0.998648	0.998553	0.998531	0.998634
MAD( $S_{\text{Dice}}$ )	0.999244	0.999231	0.999212	0.999260	0.999315	0.999261	0.999248	0.999305
	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
MAD( $S_{\text{Cosine}}$ )	0.999323	0.999302	0.999212	0.999353	0.999296	0.999325		
MAD( $S_{\text{Tanimoto}}$ )	0.998538	0.998552	0.998446	0.998686	0.998589	0.998604		
MAD( $S_{\text{Dice}}$ )	0.999257	0.999264	0.999200	0.999332	0.999282	0.999289		

Table S5: Mean absolute deviations of the  $S$  criteria calculated according to the Cosinus, Tanimoto and Dice formulation calculated over the systems included into the DBH24 dataset. All the computations are done at the def2-QZVP level of theory. Reference densities are computed at the CCSD/def2-QZVP level of theory. The definition of the  $S$  criteria is provided in Section S3.

	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
MAD( $S_{\text{Cosine}}$ )	0.999667	0.999729	0.999632	0.999745	0.999734	0.999702	0.999770	0.999686
MAD( $S_{\text{Tanimoto}}$ )	0.999253	0.999436	0.999253	0.999489	0.999449	0.999231	0.999539	0.999116
MAD( $S_{\text{Dice}}$ )	0.999626	0.999718	0.999626	0.999744	0.999724	0.999615	0.999769	0.999558
	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
MAD( $S_{\text{Cosine}}$ )	0.999713	0.999649	0.999770	0.999739	0.999703	0.999766	0.999667	0.999638
MAD( $S_{\text{Tanimoto}}$ )	0.999388	0.998086	0.999534	0.999474	0.999360	0.999514	0.999320	0.998340
MAD( $S_{\text{Dice}}$ )	0.999693	0.999041	0.999767	0.999737	0.999680	0.999757	0.999659	0.999169
	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
MAD( $S_{\text{Cosine}}$ )	0.999741	0.999766	0.999715	0.999719	0.999678	0.999691	0.999754	0.999753
MAD( $S_{\text{Tanimoto}}$ )	0.999448	0.999484	0.999400	0.999367	0.999330	0.999365	0.999500	0.999476
MAD( $S_{\text{Dice}}$ )	0.999724	0.999742	0.999700	0.999683	0.999664	0.999682	0.999750	0.999738
	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
MAD( $S_{\text{Cosine}}$ )	0.999669	0.999751	0.999773	0.999684	0.999664	0.999745		
MAD( $S_{\text{Tanimoto}}$ )	0.999257	0.999480	0.999546	0.999365	0.999328	0.999477		
MAD( $S_{\text{Dice}}$ )	0.999628	0.999739	0.999773	0.999682	0.999664	0.999738		

Table S6: Mean absolute deviations of the  $S$  criteria calculated according to the Cosinus, Tanimoto and Dice formulation calculated over the systems included into the NCB31 dataset. All the computations are done at the def2-QZVP level of theory. Reference densities are computed at the CCSD/def2-QZVP level of theory. The definition of the  $S$  criteria is provided in Section S3.

	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
MAD( $S_{\text{Cosine}}$ )	0.999825	0.999803	0.999834	0.999821	0.999816	0.999791	0.999788	0.999796
MAD( $S_{\text{Tanimoto}}$ )	0.999567	0.999557	0.999638	0.999627	0.999590	0.999378	0.999556	0.999387
MAD( $S_{\text{Dice}}$ )	0.999784	0.999778	0.999819	0.999813	0.999795	0.999689	0.999778	0.999693
	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
MAD( $S_{\text{Cosine}}$ )	0.999828	0.999742	0.999803	0.999837	0.999830	0.999839	0.999802	0.999754
MAD( $S_{\text{Tanimoto}}$ )	0.999611	0.998334	0.999581	0.999656	0.999578	0.999632	0.999574	0.998615
MAD( $S_{\text{Dice}}$ )	0.999805	0.999165	0.999790	0.999828	0.999789	0.999816	0.999787	0.999306
	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
MAD( $S_{\text{Cosine}}$ )	0.999820	0.999791	0.999812	0.999791	0.999791	0.999777	0.999816	0.999794
MAD( $S_{\text{Tanimoto}}$ )	0.999582	0.999509	0.999564	0.999491	0.999531	0.999515	0.999606	0.999530
MAD( $S_{\text{Dice}}$ )	0.999791	0.999754	0.999782	0.999745	0.999765	0.999757	0.999803	0.999765
	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
MAD( $S_{\text{Cosine}}$ )	0.999834	0.999826	0.999809	0.999808	0.999811	0.999785		
MAD( $S_{\text{Tanimoto}}$ )	0.999559	0.999597	0.999608	0.999596	0.999612	0.999539		
MAD( $S_{\text{Dice}}$ )	0.999779	0.999798	0.999804	0.999798	0.999806	0.999769		

Table S7: Atomization energies (kcal mol<sup>-1</sup>) over the 6 systems included into the AE6 dataset. All the computations are done at the def2-QZVP level of theory.

	ref.	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L
SiH <sub>4</sub>	324.95	347.17	318.01	313.52	318.36	320.33	319.77	328.05
S <sub>2</sub>	104.25	135.18	107.33	115.19	109.56	105.42	120.36	110.60
SiO	193.06	223.92	195.34	196.35	188.49	182.59	190.18	188.06
C <sub>3</sub> H <sub>4</sub>	705.06	801.41	701.63	720.74	704.19	702.15	701.07	707.63
HCOCOH	633.99	752.36	640.66	662.94	635.63	629.33	633.65	634.79
C <sub>4</sub> H <sub>8</sub>	1149.37	1303.70	1131.06	1167.06	1145.46	1149.73	1145.19	1148.91
	ref.	M11-L	MN12-L	MN15-L	B3LYP	PBE0	M05	M06
SiH <sub>4</sub>	324.95	326.05	329.65	330.35	324.11	315.62	322.23	328.79
S <sub>2</sub>	104.25	115.92	106.40	107.57	103.42	107.06	106.47	105.62
SiO	193.06	179.91	185.12	187.15	188.00	183.07	187.29	191.36
C <sub>3</sub> H <sub>4</sub>	705.06	692.27	702.27	699.86	702.87	707.85	705.18	706.53
HCOCOH	633.99	622.08	627.51	632.46	630.92	635.32	633.95	636.67
C <sub>4</sub> H <sub>8</sub>	1149.37	1131.26	1144.88	1142.92	1142.16	1156.45	1152.39	1149.44
	ref.	SOGGA11-X	MN15	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97
SiH <sub>4</sub>	324.95	320.33	324.84	323.30	320.81	316.62	316.42	324.55
S <sub>2</sub>	104.25	105.42	104.23	103.45	105.30	108.95	105.03	101.14
SiO	193.06	182.59	193.63	190.24	190.89	192.20	190.03	187.35
C <sub>3</sub> H <sub>4</sub>	705.06	702.15	702.28	703.56	704.17	703.56	707.18	701.22
HCOCOH	633.99	629.33	634.49	637.77	632.89	629.92	627.06	632.50
C <sub>4</sub> H <sub>8</sub>	1149.37	1149.73	1144.53	1153.29	1146.68	1148.28	1154.92	1151.48
	ref.	$\omega$ B97X	$\omega$ B97X-D	N12-SX	MN12-SX	M11	HF	B2-PLYP
SiH <sub>4</sub>	324.95	324.66	324.07	320.30	325.13	324.79	256.84	322.66
S <sub>2</sub>	104.25	103.66	105.43	112.07	108.13	104.52	51.80	103.67
SiO	193.06	187.91	187.49	188.81	185.48	188.02	110.70	191.98
C <sub>3</sub> H <sub>4</sub>	705.06	702.29	702.20	701.65	694.87	703.05	524.69	703.94
HCOCOH	633.99	632.86	632.74	635.11	626.28	632.32	421.97	633.17
C <sub>4</sub> H <sub>8</sub>	1149.37	1150.53	1150.20	1149.00	1135.59	1147.14	870.38	1143.31
	ref.	PBE-QIDH	$\omega$ B97X-2					
SiH <sub>4</sub>	324.95	319.35	323.16					
S <sub>2</sub>	104.25	104.03	103.39					
SiO	193.06	185.17	192.15					
C <sub>3</sub> H <sub>4</sub>	705.06	706.96	699.97					
HCOCOH	633.99	631.31	630.31					
C <sub>4</sub> H <sub>8</sub>	1149.37	1157.00	1141.46					

Table S8: Barrier height energies (kcal mol<sup>-1</sup>) over the 6 reactions included into the BH6 dataset. All the computations are done at the def2-QZVP level of theory.

	ref.	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L
H <sub>3</sub> CH + OH → [H <sub>3</sub> CHOH] <sup>‡</sup>	6.70	-16.76	-2.37	-5.24	2.45	6.00	-2.09	3.91
[H <sub>3</sub> CHOH] <sup>‡</sup> → CH <sub>3</sub> + H <sub>2</sub> O	19.60	2.22	10.54	8.89	13.81	15.20	11.45	12.42
H + HO → [HHO] <sup>‡</sup>	10.70	-1.97	1.42	3.60	8.12	9.41	3.37	6.92
[HHO] <sup>‡</sup> → H <sub>2</sub> + O	13.10	-12.67	1.51	-1.35	8.38	10.01	5.52	7.28
H + HSH → [HHSH] <sup>‡</sup>	3.60	-6.74	-2.12	-1.12	4.48	3.43	1.12	3.70
[HHSH] <sup>‡</sup> → H <sub>2</sub> + SH	17.30	-0.41	14.40	9.46	15.96	14.93	9.49	13.29
	ref.	M11-L	MN12-L	MN15-L	B3LYP	PBE0	M05	M06
H <sub>3</sub> CH + OH → [H <sub>3</sub> CHOH] <sup>‡</sup>	6.70	9.15	9.34	7.58	2.33	2.07	5.44	5.40
[H <sub>3</sub> CHOH] <sup>‡</sup> → CH <sub>3</sub> + H <sub>2</sub> O	19.60	18.72	18.75	19.44	13.97	14.01	17.95	17.42
H + HO → [HHO] <sup>‡</sup>	10.70	9.13	10.10	7.86	4.01	7.04	8.27	8.61
[HHO] <sup>‡</sup> → H <sub>2</sub> + O	13.10	12.47	12.68	12.77	6.32	5.95	11.66	10.45
H + HSH → [HHSH] <sup>‡</sup>	3.60	3.49	3.23	3.92	-0.48	1.18	4.60	3.95
[HHSH] <sup>‡</sup> → H <sub>2</sub> + SH	17.30	16.62	16.42	17.52	15.92	12.41	19.21	17.16
	ref.	SOGGA11-X	MN15	BMK	M06-2X	M05-2X	M06-HF	ωB97
H <sub>3</sub> CH + OH → [H <sub>3</sub> CHOH] <sup>‡</sup>	6.70	6.00	5.84	5.86	5.36	4.87	5.81	4.95
[H <sub>3</sub> CHOH] <sup>‡</sup> → CH <sub>3</sub> + H <sub>2</sub> O	19.60	15.20	18.58	16.61	17.73	17.56	19.29	15.64
H + HO → [HHO] <sup>‡</sup>	10.70	9.41	9.85	10.19	9.87	10.27	10.05	10.57
[HHO] <sup>‡</sup> → H <sub>2</sub> + O	13.10	10.01	11.03	10.98	11.58	11.55	16.13	11.00
H + HSH → [HHSH] <sup>‡</sup>	3.60	3.43	4.30	3.49	4.41	5.45	5.79	6.94
[HHSH] <sup>‡</sup> → H <sub>2</sub> + SH	17.30	14.93	16.83	16.85	17.81	18.01	20.56	18.85
	ref.	ωB97X	ωB97X-D	N12-SX	MN12-SX	M11	HF	B2-PLYP
H <sub>3</sub> CH + OH → [H <sub>3</sub> CHOH] <sup>‡</sup>	6.70	4.42	3.72	1.50	7.77	4.88	26.65	4.39
[H <sub>3</sub> CHOH] <sup>‡</sup> → CH <sub>3</sub> + H <sub>2</sub> O	19.60	15.45	15.23	14.13	19.31	18.74	28.81	17.03
H + HO → [HHO] <sup>‡</sup>	10.70	9.73	8.78	9.77	10.00	8.74	17.36	8.03
[HHO] <sup>‡</sup> → H <sub>2</sub> + O	13.10	10.15	9.80	7.13	13.07	10.24	32.84	10.01
H + HSH → [HHSH] <sup>‡</sup>	3.60	5.60	4.17	4.53	4.24	2.62	11.91	2.04
[HHSH] <sup>‡</sup> → H <sub>2</sub> + SH	17.30	17.59	16.80	13.27	18.08	16.43	27.17	16.62
	ref.	PBE-QIDH	ωB97X-2					
H <sub>3</sub> CH + OH → [H <sub>3</sub> CHOH] <sup>‡</sup>	6.70	6.66	5.60					
[H <sub>3</sub> CHOH] <sup>‡</sup> → CH <sub>3</sub> + H <sub>2</sub> O	19.60	19.22	18.34					
H + HO → [HHO] <sup>‡</sup>	10.70	11.73	10.83					
[HHO] <sup>‡</sup> → H <sub>2</sub> + O	13.10	12.57	12.66					
H + HSH → [HHSH] <sup>‡</sup>	3.60	4.05	4.12					
[HHSH] <sup>‡</sup> → H <sub>2</sub> + SH	17.30	15.04	17.14					

Table S9: Weak interaction energies (kcal mol<sup>-1</sup>) over the 6 systems included into the WI6 dataset. All the computations are done at the def2-QZVP level of theory.

	ref.	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L
water...water 0.90R <sub>e</sub>	-4.66	-8.59	-3.95	-5.00	-3.81	-4.54	-4.95	-4.44
water...water 1.00R <sub>e</sub>	-4.95	-7.74	-4.40	-5.20	-4.24	-4.74	-4.88	-4.69
water...water 1.50R <sub>e</sub>	-2.11	-2.56	-1.93	-2.25	-2.06	-1.75	-1.96	-1.94
methane...methane 0.90R <sub>e</sub>	-0.34	-1.15	1.56	0.49	1.16	0.92	1.68	-0.15
methane...methane 1.00R <sub>e</sub>	-0.53	-0.82	0.66	-0.09	0.29	0.72	0.86	-0.50
methane...methane 1.50R <sub>e</sub>	-0.06	-0.02	0.04	-0.02	-0.01	-0.01	0.02	-0.02
	ref.	M11-L	MN12-L	MN15-L	B3LYP	PBE0	M05	M06
water...water 0.90R <sub>e</sub>	-4.66	-3.97	-3.78	-3.34	-4.45	-4.96	-4.97	-4.54
water...water 1.00R <sub>e</sub>	-4.95	-4.20	-4.37	-4.32	-4.77	-5.11	-5.31	-4.81
water...water 1.50R <sub>e</sub>	-2.11	-1.53	-1.88	-2.18	-2.03	-2.19	-2.30	-2.08
methane...methane 0.90R <sub>e</sub>	-0.34	0.16	0.07	-1.10	1.10	0.49	-0.03	-0.02
methane...methane 1.00R <sub>e</sub>	-0.53	0.20	0.18	-0.98	0.39	-0.04	-0.39	-0.26
methane...methane 1.50R <sub>e</sub>	-0.06	-0.01	-0.03	-0.01	0.03	-0.01	-0.00	-0.07
	ref.	SOGGA11-X	MN15	BMK	M06-2X	M05-2X	M06-HF	ωB97
water...water 0.90R <sub>e</sub>	-4.66	-4.54	-4.72	-4.10	-4.97	-4.99	-5.23	-5.58
water...water 1.00R <sub>e</sub>	-4.95	-4.74	-5.12	-4.46	-5.20	-5.30	-5.18	-5.74
water...water 1.50R <sub>e</sub>	-2.11	-1.75	-2.27	-1.55	-2.23	-2.28	-2.39	-2.14
methane...methane 0.90R <sub>e</sub>	-0.34	0.92	-0.69	1.12	-0.39	-0.28	0.05	-0.63
methane...methane 1.00R <sub>e</sub>	-0.53	0.72	-0.71	0.96	-0.42	-0.49	-0.27	-0.39
methane...methane 1.50R <sub>e</sub>	-0.06	-0.01	-0.00	0.01	-0.05	0.01	-0.09	0.01
	ref.	ωB97X	ωB97X-D	N12-SX	MN12-SX	M11	HF	B2-PLYP
water...water 0.90R <sub>e</sub>	-4.66	-5.55	-4.89	-5.35	-4.17	-4.78	-3.02	-4.73
water...water 1.00R <sub>e</sub>	-4.95	-5.69	-5.10	-5.43	-4.69	-5.06	-3.88	-4.99
water...water 1.50R <sub>e</sub>	-2.11	-2.25	-2.21	-2.08	-1.99	-2.19	-2.09	-2.11
methane...methane 0.90R <sub>e</sub>	-0.34	-0.56	-0.45	0.62	-0.11	-0.23	1.32	0.51
methane...methane 1.00R <sub>e</sub>	-0.53	-0.54	-0.55	0.31	-0.07	-0.31	0.36	0.03
methane...methane 1.50R <sub>e</sub>	-0.06	-0.00	-0.07	0.01	-0.05	-0.02	0.00	-0.00
	ref.	PBE-QIDH	ωB97X-2	ωB97X-noD				
water...water 0.90R <sub>e</sub>	-4.66	-5.08	-5.14	-4.39				
water...water 1.00R <sub>e</sub>	-4.95	-5.18	-5.44	-4.65				
water...water 1.50R <sub>e</sub>	-2.11	-2.18	-2.34	-2.02				
methane...methane 0.90R <sub>e</sub>	-0.34	0.15	-0.58	0.76				
methane...methane 1.00R <sub>e</sub>	-0.53	-0.20	-0.72	0.21				
methane...methane 1.50R <sub>e</sub>	-0.06	-0.03	-0.04	0.00				

Table S10: Atomization energies (kcal mol<sup>-1</sup>) over the 138 (out of 148) systems included into the G2 dataset. All the computations are done at the def2-QZVP level of theory.

	ref.	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L
H <sub>2</sub>	109.20	112.98	109.49	104.60	105.63	104.61	105.77	104.31
LiH	57.80	60.65	57.86	53.35	54.84	50.93	45.99	59.24
BeH	49.80	60.25	56.92	55.47	51.32	45.01	53.52	59.11
<sup>2</sup> CH	83.80	92.21	85.49	84.53	83.16	79.10	80.12	82.63
<sup>3</sup> CH <sub>2</sub>	190.00	212.59	190.00	194.37	188.47	189.23	190.39	192.46
<sup>1</sup> CH <sub>2</sub>	180.70	198.57	179.88	178.69	178.25	172.75	174.93	179.01
CH <sub>3</sub> •	306.60	339.13	307.15	309.93	305.11	303.24	304.76	307.05
CH <sub>4</sub>	419.20	462.32	417.08	420.00	416.42	415.24	415.93	418.12
<sup>3</sup> NH	83.50	95.14	89.35	88.30	83.36	80.37	77.39	82.22
NH <sub>2</sub> •	181.50	207.55	189.36	188.36	181.35	178.44	173.05	180.17
NH <sub>3</sub>	297.50	337.03	301.67	301.78	294.62	294.83	287.46	290.60
OH•	106.40	123.90	109.54	109.69	105.32	109.55	103.50	103.90
H <sub>2</sub> O	232.20	266.12	232.44	233.91	227.86	237.71	227.99	223.38
HF	140.80	161.89	140.86	141.76	138.26	146.44	142.46	134.51
Li <sub>2</sub>	24.40	23.55	20.46	19.99	21.87	34.74	10.31	24.43
LiF	137.50	155.30	139.43	138.07	134.23	135.52	133.08	136.07
C <sub>2</sub> H <sub>2</sub>	405.30	459.55	405.10	414.68	403.33	404.96	400.23	405.50
H <sub>2</sub> C=CH <sub>2</sub>	562.60	632.23	561.00	571.50	561.46	562.07	559.72	562.28
H <sub>3</sub> C-CH <sub>3</sub>	710.80	793.89	704.65	716.68	707.77	708.49	706.84	709.99
CN•	180.90	218.03	189.33	195.49	179.09	179.84	168.64	183.40
HCN	312.60	359.72	319.93	325.78	311.06	311.07	299.24	311.24
CO	259.30	298.10	261.70	268.64	257.51	263.94	252.11	256.83
HCO•	278.70	332.41	287.12	295.04	280.39	289.84	278.74	280.21
H <sub>2</sub> C=O	373.60	433.19	377.88	385.76	373.05	380.52	371.48	372.79
CH <sub>3</sub> -OH	511.90	586.04	510.83	519.81	508.38	515.72	508.19	505.78
N <sub>2</sub>	228.60	264.92	238.78	242.02	225.32	219.58	202.18	222.27
H <sub>2</sub> N-NH <sub>2</sub>	437.80	515.23	447.36	452.83	435.99	435.74	421.82	427.83
NO•	152.80	198.41	165.99	171.70	155.45	160.14	142.89	151.04
O <sub>2</sub>	120.50	173.06	135.31	142.87	124.97	139.41	122.30	122.85
HO-OH	268.70	334.47	275.81	281.91	264.02	282.34	264.58	257.99
F <sub>2</sub>	38.50	77.44	48.81	52.67	36.99	52.03	45.56	36.33
CO <sub>2</sub>	389.10	472.24	399.96	416.14	393.46	414.40	390.36	397.00
<sup>1</sup> SiH <sub>2</sub>	151.30	166.03	151.98	147.87	151.12	151.27	150.62	154.90
<sup>3</sup> SiH <sub>2</sub>	131.20	147.03	130.61	131.73	130.37	134.65	132.33	135.78
SiH <sub>3</sub> •	225.10	246.76	224.60	222.56	224.22	225.19	225.78	231.45
SiH <sub>4</sub>	321.40	347.29	318.08	313.65	318.38	317.27	319.68	328.00
PH <sub>2</sub> •	152.90	173.60	157.53	154.47	154.82	156.40	156.39	153.61
PH <sub>3</sub>	241.80	269.49	242.44	239.05	240.48	243.43	244.09	240.62
H <sub>2</sub> S	182.40	206.29	180.75	182.04	181.51	186.72	187.31	181.62
HCl	106.30	120.34	104.47	106.42	105.73	109.70	109.77	106.54
S <sub>2</sub>	101.60	134.95	107.70	115.25	109.15	122.65	119.97	110.27
Cl <sub>2</sub>	58.00	82.97	58.17	65.67	60.01	70.32	69.58	61.81
NaCl	98.00	103.45	91.36	94.03	98.84	102.22	90.27	109.24
SiO	192.30	223.37	195.41	196.32	187.66	199.46	189.16	187.41
CS	171.30	201.56	172.08	179.37	171.55	177.61	175.44	172.97
SO	125.10	166.63	135.01	140.96	128.20	143.55	133.29	127.15
ClO•	64.40	103.36	74.71	80.98	67.82	81.08	72.29	67.14
ClF	61.50	94.70	67.27	72.25	62.44	74.38	71.53	60.58
CH <sub>3</sub> Cl	393.90	447.03	389.72	399.88	393.71	396.64	397.95	395.62
H <sub>3</sub> C-SH	473.00	536.31	467.99	478.25	472.09	477.69	477.90	472.59
HOCl	164.40	210.64	168.74	175.34	163.56	177.78	168.42	160.85
SO <sub>2</sub>	258.40	333.70	266.54	280.06	254.53	286.58	263.28	255.91
BF <sub>3</sub>	469.90	547.86	468.67	481.43	467.54	480.55	483.16	464.55
BCl <sub>3</sub>	322.70	381.67	311.54	335.24	326.21	340.06	343.34	335.99
AlF <sub>3</sub>	426.50	482.41	421.70	427.54	420.08	429.87	437.93	417.41
AlCl <sub>3</sub>	306.10	343.60	289.54	306.55	307.01	318.93	320.07	320.04
CF <sub>4</sub>	476.30	598.18	476.84	503.37	478.71	503.68	496.36	472.20
CCl <sub>4</sub>	312.80	400.59	298.04	333.11	313.88	336.47	334.88	320.37
O=C=S	333.30	408.34	343.29	359.44	340.88	360.51	346.67	346.25
CS <sub>2</sub>	277.70	343.37	284.87	301.31	287.21	305.80	301.53	294.39
COF <sub>2</sub>	426.70	523.28	427.05	448.19	423.53	446.54	431.46	421.27
SiF <sub>4</sub>	572.80	655.11	561.29	572.74	562.35	575.29	583.91	558.42
SiCl <sub>4</sub>	383.30	443.12	357.97	386.25	382.37	402.54	404.75	399.51
N <sub>2</sub> O	270.50	359.03	295.73	309.39	275.35	289.31	258.19	277.95
CINO	191.20	264.81	213.26	224.24	194.82	213.81	192.87	199.03
NF <sub>3</sub>	205.20	311.76	228.73	245.24	210.93	234.40	217.98	205.48



PF <sub>3</sub>	363.90	442.62	367.24	376.02	361.15	381.98	378.82	353.08
O <sub>3</sub>	147.10	239.05	169.80	183.71	140.36	179.36	145.47	143.04
F <sub>2</sub> O	93.30	170.08	114.15	123.37	93.84	119.90	104.46	91.44
ClF <sub>3</sub>	125.60	229.19	150.34	166.04	131.25	167.47	159.12	128.79
F <sub>2</sub> C=CF <sub>2</sub>	583.90	743.97	596.93	630.75	595.62	624.63	614.71	590.57
Cl <sub>2</sub> C=CCl <sub>2</sub>	466.80	589.13	456.03	500.87	474.57	497.58	494.82	483.83
CF <sub>3</sub> CN	639.70	788.31	648.49	680.58	642.48	663.34	645.25	639.09
CH≡C-CH <sub>3</sub>	704.20	801.33	701.60	720.79	703.77	706.84	700.55	707.21
CH <sub>2</sub> =C=CH <sub>2</sub>	702.40	804.69	704.63	723.84	705.71	710.12	703.90	708.02
C <sub>3</sub> H <sub>4</sub>	682.10	784.50	677.04	701.54	684.47	687.04	681.02	689.15
CH <sub>2</sub> =CHCH <sub>3</sub>	859.20	970.32	853.41	873.56	857.66	860.06	855.73	859.56
C <sub>3</sub> H <sub>6</sub>	851.90	968.30	842.43	868.17	852.90	854.66	850.36	856.75
C <sub>3</sub> H <sub>8</sub>	1004.60	1127.93	993.32	1014.86	1000.24	1002.86	998.97	1003.32
C <sub>4</sub> H <sub>6</sub>	1011.20	1150.48	1006.51	1034.53	1011.38	1015.81	1009.01	1013.47
C <sub>4</sub> H <sub>6</sub>	1002.80	1141.65	996.73	1025.54	1002.90	1006.98	999.51	1007.47
C <sub>4</sub> H <sub>6</sub>	989.50	1137.86	984.54	1018.44	995.47	1000.64	992.52	999.77
C <sub>4</sub> H <sub>10</sub>	1298.50	1461.93	1281.89	1312.97	1292.66	1296.56	1291.02	1296.67
C <sub>4</sub> H <sub>10</sub>	1300.30	1463.65	1282.26	1313.73	1293.11	1297.37	1291.56	1297.60
C <sub>5</sub> H <sub>8</sub>	1282.40	1474.06	1266.51	1315.40	1287.61	1293.96	1283.55	1294.24
C <sub>6</sub> H <sub>6</sub>	1366.00	1573.22	1357.14	1409.54	1373.29	1382.06	1370.32	1375.41
H <sub>2</sub> CF <sub>2</sub>	436.20	516.73	438.02	450.85	436.58	447.15	445.77	432.20
HCF <sub>3</sub>	457.70	558.88	459.30	478.73	458.99	477.15	472.76	453.02
H <sub>2</sub> CCl <sub>2</sub>	369.60	433.53	362.44	380.42	370.55	379.79	380.17	373.24
HCCl <sub>3</sub>	343.30	418.89	332.60	358.92	344.60	360.33	359.87	348.79
H <sub>3</sub> C-NH <sub>2</sub>	581.20	660.70	582.19	590.76	578.20	577.93	570.68	575.10
CH <sub>3</sub> -CN	615.10	704.78	619.85	635.19	615.00	615.25	603.10	616.46
CH <sub>3</sub> -NO <sub>2</sub>	600.60	742.58	618.21	641.75	603.58	625.39	597.06	600.63
CH <sub>3</sub> -O-N=O	598.30	735.21	615.02	636.53	598.21	617.60	590.75	597.60
CH <sub>3</sub> -SiH <sub>3</sub>	626.10	690.37	616.99	622.03	621.13	622.28	622.80	630.30
HCOOH	500.70	597.17	506.50	522.37	500.53	519.54	500.39	497.22
HCOOCH <sub>3</sub>	784.20	921.18	787.57	811.20	783.61	800.18	783.38	783.20
CH <sub>3</sub> CONH <sub>2</sub>	867.10	1010.50	870.74	895.27	867.03	879.07	860.17	863.94
CH <sub>2</sub> -NH-CH <sub>2</sub>	719.00	831.23	718.10	739.97	720.58	721.02	711.11	721.49
NCCN	502.30	598.04	519.82	537.66	503.51	507.05	482.74	506.92
(CH <sub>3</sub> ) <sub>2</sub> CH	868.80	989.19	865.65	883.21	864.72	866.01	857.06	862.98
CH <sub>3</sub> -CH <sub>2</sub> -NH <sub>2</sub>	875.70	996.89	872.87	890.94	872.52	874.43	864.82	870.12
H <sub>2</sub> C=C=O	531.90	626.90	540.41	558.07	537.05	550.18	535.43	539.76
CH <sub>2</sub> -O-CH <sub>2</sub>	649.90	756.40	648.35	669.86	651.07	659.14	648.85	652.52
CH <sub>3</sub> CHO	676.20	778.17	676.91	694.34	675.63	686.04	674.26	676.13
O=CH-CH=O	633.40	751.73	640.79	662.94	634.49	653.37	632.28	633.80
CH <sub>3</sub> CH <sub>2</sub> OH	808.80	923.52	802.85	821.21	804.00	813.81	803.67	802.36
CH <sub>3</sub> -O-CH <sub>3</sub>	796.80	911.52	792.73	809.78	792.44	799.76	792.16	792.20
CH <sub>2</sub> -S-CH <sub>2</sub>	623.00	719.59	616.25	639.93	626.83	634.39	632.42	630.94
(CH <sub>3</sub> ) <sub>2</sub> SO	854.10	992.22	847.62	874.44	850.90	871.71	858.59	851.50
CH <sub>3</sub> -CH <sub>2</sub> -SH	767.60	870.84	757.07	776.88	764.97	772.46	770.53	766.19
CH <sub>3</sub> -S-CH <sub>3</sub>	766.00	869.50	756.93	776.63	764.48	772.40	770.47	765.81
H <sub>2</sub> C=CHF	571.30	663.47	573.87	589.87	573.45	580.93	577.28	572.35
CH <sub>3</sub> -CH <sub>2</sub> -Cl	690.10	783.45	680.77	700.39	688.44	693.75	692.56	691.31
H <sub>2</sub> C=CHCl	538.60	624.54	538.79	557.49	543.72	549.78	547.43	546.03
H <sub>2</sub> C=CHCN	763.30	878.86	767.76	790.68	763.17	765.89	750.88	764.76
CH <sub>3</sub> -CO-CH <sub>3</sub>	977.20	1120.35	972.76	999.92	975.46	986.95	973.92	977.19
CH <sub>3</sub> COOH	802.20	939.28	802.65	828.04	800.82	820.38	800.44	798.83
CH <sub>3</sub> COF	705.40	828.76	707.59	731.24	706.40	723.06	710.29	705.80
CH <sub>3</sub> COCl	666.90	782.97	666.77	692.47	669.06	685.54	673.91	672.84
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> Cl	983.80	1117.39	969.36	998.51	980.89	987.52	984.64	984.67
(CH <sub>3</sub> ) <sub>2</sub> CH-OH	1106.40	1261.78	1094.42	1122.59	1099.32	1110.60	1098.82	1099.03
CH <sub>3</sub> -CH <sub>2</sub> -O-CH <sub>3</sub>	1093.30	1248.85	1084.63	1111.07	1088.00	1097.41	1087.51	1088.84
(CH <sub>3</sub> ) <sub>3</sub> N	1158.60	1320.77	1150.42	1177.48	1152.64	1156.12	1144.85	1152.92
C <sub>4</sub> H <sub>4</sub> O	993.00	1164.94	989.91	1031.41	997.57	1014.63	996.98	997.52
C <sub>4</sub> H <sub>4</sub> S	962.10	1121.38	952.88	996.83	968.42	984.67	974.41	970.13
C <sub>4</sub> H <sub>4</sub> NH	1070.40	1249.85	1068.98	1111.03	1076.54	1086.83	1069.20	1074.17
C <sub>5</sub> H <sub>5</sub> N	1236.40	1440.09	1236.84	1285.24	1245.07	1252.90	1235.08	1244.50
SH•	86.90	99.55	87.75	87.98	87.38	90.08	89.97	86.91
C <sub>2</sub> H <sub>3</sub> •	444.00	507.08	446.61	457.50	445.94	447.47	444.72	448.85
CH <sub>3</sub> CO•	580.90	676.54	586.31	603.52	583.16	594.73	581.87	583.61
H <sub>2</sub> COH•	408.90	476.92	412.11	421.35	408.00	416.99	408.22	404.90
CH <sub>3</sub> O•	400.50	463.72	404.46	412.45	400.86	405.32	399.74	400.88
CH <sub>3</sub> CH <sub>2</sub> O•	697.10	799.88	693.11	710.44	693.11	702.42	691.95	693.81
CH <sub>3</sub> S•	380.60	435.59	379.87	389.27	382.64	386.61	385.73	382.46
C <sub>2</sub> H <sub>5</sub> •	602.20	677.03	599.82	611.85	601.47	602.00	600.55	604.31
(CH <sub>3</sub> ) <sub>2</sub> CH•	898.80	1015.70	892.59	914.18	898.02	901.24	896.82	902.02

NO <sub>2</sub> •	227.50	321.93	254.55	269.35	234.90	258.16	227.48	234.53
	ref.	M11-L	MN12-L	MN15-L	B3LYP	PBE0	M05	M06
H <sub>2</sub>	109.20	110.63	109.61	109.91	110.32	104.41	109.32	108.01
LiH	57.80	54.91	63.50	61.94	58.28	52.63	56.68	58.19
BeH	49.80	56.20	52.23	56.70	57.89	55.80	48.91	56.32
<sup>2</sup> CH	83.80	86.23	83.44	85.47	85.40	82.86	84.68	84.36
<sup>3</sup> CH <sub>2</sub>	190.00	186.29	185.76	192.01	192.18	193.65	191.99	192.28
<sup>1</sup> CH <sub>2</sub>	180.70	183.16	183.33	180.78	180.79	176.22	182.56	182.62
CH <sub>3</sub> •	306.60	303.27	306.02	306.24	310.12	308.43	309.90	307.68
CH <sub>4</sub>	419.20	415.57	419.24	416.40	421.13	417.77	421.27	419.63
<sup>3</sup> NH	83.50	85.49	82.12	84.56	87.92	85.08	84.28	82.41
NH <sub>2</sub> •	181.50	186.08	186.58	182.89	187.82	182.93	183.04	181.10
NH <sub>3</sub>	297.50	298.33	301.00	295.03	300.94	294.89	296.53	294.77
OH•	106.40	107.18	106.98	105.03	108.02	105.47	105.86	106.12
H <sub>2</sub> O	232.20	228.83	229.45	226.99	230.61	226.65	229.61	229.99
HF	140.80	135.73	139.22	137.65	138.94	136.49	140.09	140.28
Li <sub>2</sub>	24.40	13.43	76.52	25.00	20.67	19.23	22.09	24.50
LiF	137.50	117.34	135.64	132.26	136.05	131.02	134.44	137.25
C <sub>2</sub> H <sub>2</sub>	405.30	394.72	401.24	400.84	402.92	403.96	403.10	404.89
H <sub>2</sub> C=CH <sub>2</sub>	562.60	554.08	561.17	559.15	563.46	563.80	562.43	562.29
H <sub>3</sub> C-CH <sub>3</sub>	710.80	703.40	710.07	706.25	711.83	712.10	713.94	711.81
CN•	180.90	179.58	177.35	177.28	178.63	178.09	178.48	178.35
HCN	312.60	306.72	309.66	310.99	312.25	309.87	309.40	309.60
CO	259.30	252.99	255.13	259.87	254.51	254.52	256.76	258.02
HCO•	278.70	274.41	273.89	278.32	280.08	280.03	279.74	279.82
H <sub>2</sub> C=O	373.60	366.92	369.96	371.86	373.26	371.91	374.11	374.84
CH <sub>3</sub> -OH	511.90	504.45	509.59	506.87	511.49	509.64	511.97	512.10
N <sub>2</sub>	228.60	223.43	223.66	227.49	226.88	222.45	220.77	219.78
H <sub>2</sub> N-NH <sub>2</sub>	437.80	438.42	444.17	435.16	443.96	437.89	436.28	434.45
NO•	152.80	149.07	147.65	151.88	155.07	153.32	150.32	149.70
O <sub>2</sub>	120.50	109.86	107.79	118.67	122.00	121.75	119.37	117.97
HO-OH	268.70	260.95	265.05	262.98	266.58	262.35	260.26	264.05
F <sub>2</sub>	38.50	27.94	40.13	37.48	36.60	34.07	28.07	33.02
CO <sub>2</sub>	389.10	386.74	384.47	393.90	386.92	390.41	395.73	396.68
<sup>1</sup> SiH <sub>2</sub>	151.30	153.53	154.80	155.04	153.81	147.35	153.60	157.83
<sup>3</sup> SiH <sub>2</sub>	131.20	134.16	138.86	140.47	133.28	132.43	132.03	133.62
SiH <sub>3</sub> •	225.10	231.12	233.92	235.86	228.81	223.82	227.01	230.96
SiH <sub>4</sub>	321.40	325.90	329.55	330.44	324.11	315.66	322.29	328.75
PH <sub>2</sub> •	152.90	154.11	154.32	156.84	158.70	153.15	154.67	157.02
PH <sub>3</sub>	241.80	241.53	241.90	244.09	244.85	237.45	240.44	244.62
H <sub>2</sub> S	182.40	187.91	186.03	184.96	182.16	179.97	181.81	182.18
HCl	106.30	110.55	108.37	108.80	105.10	104.98	107.50	106.30
S <sub>2</sub>	101.60	115.18	105.92	107.17	103.32	106.62	106.13	105.36
Cl <sub>2</sub>	58.00	60.98	59.11	62.22	55.60	59.55	60.55	60.92
NaCl	98.00	97.57	104.05	101.66	92.41	93.32	99.96	102.47
SiO	192.30	178.39	184.00	186.55	187.35	182.22	186.45	190.37
CS	171.30	176.60	172.64	175.05	166.06	167.82	169.73	169.54
SO	125.10	125.07	120.32	126.15	125.98	125.81	123.27	123.75
ClO•	64.40	64.11	62.24	66.01	65.85	66.56	63.84	64.50
ClF	61.50	55.19	61.50	63.12	60.58	60.57	58.26	61.34
CH <sub>3</sub> Cl	393.90	392.15	394.91	394.91	392.82	395.48	398.01	395.69
H <sub>3</sub> C-SH	473.00	472.57	475.61	473.65	472.06	473.31	474.23	473.50
HOCl	164.40	161.75	163.21	164.32	162.81	162.43	161.29	163.79
SO <sub>2</sub>	258.40	252.02	247.74	257.49	249.49	250.13	252.08	254.22
BF <sub>3</sub>	469.90	458.82	477.02	470.84	464.49	466.15	470.07	474.11
BCl <sub>3</sub>	322.70	330.82	339.52	337.45	313.64	329.13	328.74	328.04
AlF <sub>3</sub>	426.50	404.17	425.43	422.09	417.03	413.32	424.77	421.30
AlCl <sub>3</sub>	306.10	316.36	325.95	322.62	294.61	305.62	313.60	311.38
CF <sub>4</sub>	476.30	467.92	481.26	486.65	468.35	478.33	480.43	483.29
CCl <sub>4</sub>	312.80	319.53	314.19	325.38	296.06	318.56	316.61	316.43
O=C=S	333.30	339.52	337.53	342.58	332.57	337.68	340.67	341.09
CS <sub>2</sub>	277.70	293.85	288.85	290.34	276.71	283.74	285.15	284.72
COF <sub>2</sub>	426.70	412.21	419.35	426.30	415.28	421.61	424.49	426.52
SiF <sub>4</sub>	572.80	551.20	573.20	572.02	557.46	555.64	565.28	567.08
SiCl <sub>4</sub>	383.30	388.29	403.77	404.85	363.99	382.93	390.66	390.17
N <sub>2</sub> O	270.50	271.73	265.65	277.16	272.67	271.72	274.55	270.80
ClNO	191.20	195.55	189.04	198.78	192.30	191.28	192.12	191.12
NF <sub>3</sub>	205.20	200.31	210.94	217.08	207.49	208.72	204.02	205.06
PF <sub>3</sub>	363.90	343.11	358.35	364.55	358.74	355.72	358.52	365.52
O <sub>3</sub>	147.10	127.60	128.38	141.95	137.68	135.00	132.60	133.48
F <sub>2</sub> O	93.30	80.41	94.20	95.73	92.91	90.27	81.54	86.87

ClF <sub>3</sub>	125.60	114.76	124.72	130.01	128.36	129.50	123.82	127.75
F <sub>2</sub> C=CF <sub>2</sub>	583.90	570.63	593.38	597.75	583.37	595.96	592.43	598.60
Cl <sub>2</sub> C=CCl <sub>2</sub>	466.80	473.27	472.88	484.41	452.51	480.44	474.85	474.35
CF <sub>3</sub> CN	639.70	626.42	640.37	647.10	632.47	642.68	639.70	642.84
CH≡C-CH <sub>3</sub>	704.20	691.80	701.75	699.90	702.44	707.44	704.84	706.00
CH <sub>2</sub> =C=CH <sub>2</sub>	702.40	693.98	704.55	702.48	704.58	709.31	703.74	705.11
C <sub>3</sub> H <sub>4</sub>	682.10	670.75	679.62	681.34	678.85	688.71	689.37	686.98
CH <sub>2</sub> =CHCH <sub>3</sub>	859.20	847.52	857.58	854.74	858.94	863.26	860.02	859.62
C <sub>3</sub> H <sub>6</sub>	851.90	840.06	851.23	850.14	849.95	859.56	860.27	856.59
C <sub>3</sub> H <sub>8</sub>	1004.60	993.11	1002.63	998.36	1003.74	1007.90	1008.03	1005.82
C <sub>4</sub> H <sub>6</sub>	1011.20	995.62	1009.32	1007.47	1009.98	1018.05	1009.52	1010.97
C <sub>4</sub> H <sub>6</sub>	1002.80	987.44	1000.77	997.54	1000.61	1009.60	1005.31	1005.84
C <sub>4</sub> H <sub>6</sub>	989.50	977.39	991.49	991.37	989.61	1003.16	999.18	996.84
C <sub>4</sub> H <sub>10</sub>	1298.50	1282.72	1295.19	1290.49	1295.57	1303.64	1302.04	1299.86
C <sub>4</sub> H <sub>10</sub>	1300.30	1284.04	1296.49	1292.23	1296.08	1304.44	1302.72	1301.32
C <sub>5</sub> H <sub>8</sub>	1282.40	1263.49	1281.63	1283.02	1276.98	1299.64	1297.66	1291.61
C <sub>6</sub> H <sub>6</sub>	1366.00	1346.32	1367.93	1367.28	1361.82	1385.70	1363.25	1367.33
H <sub>2</sub> CF <sub>2</sub>	436.20	424.53	436.34	436.99	434.79	436.34	438.84	438.77
HCF <sub>3</sub>	457.70	446.38	459.61	462.76	453.13	458.61	460.87	461.83
H <sub>2</sub> CCl <sub>2</sub>	369.60	369.92	370.41	373.95	364.05	373.02	374.51	371.69
HCCl <sub>3</sub>	343.30	346.50	344.01	351.40	332.45	348.04	348.15	345.84
H <sub>3</sub> C-NH <sub>2</sub>	581.20	577.41	583.90	577.35	584.31	581.27	581.61	579.69
CH <sub>3</sub> -CN	615.10	607.12	613.56	613.59	615.31	616.81	614.72	614.09
CH <sub>3</sub> -NO <sub>2</sub>	600.60	591.05	593.16	602.05	601.76	604.13	601.41	599.69
CH <sub>3</sub> -O-N=O	598.30	588.56	592.59	600.89	597.97	598.64	597.06	596.98
CH <sub>3</sub> -SiH <sub>3</sub>	626.10	623.31	634.00	631.54	626.10	621.55	626.11	630.95
HCOOH	500.70	493.42	496.67	500.00	498.36	499.95	501.51	502.96
HCOOCH <sub>3</sub>	784.20	771.39	780.08	783.62	782.14	785.91	786.65	788.53
CH <sub>3</sub> CONH <sub>2</sub>	867.10	858.81	868.26	865.47	867.78	871.63	868.68	868.51
CH <sub>2</sub> -NH-CH <sub>2</sub>	719.00	712.34	721.73	720.50	719.75	725.66	726.82	722.58
NCCN	502.30	493.48	500.15	504.25	500.69	502.15	495.65	497.94
(CH <sub>3</sub> ) <sub>2</sub> CH	868.80	860.61	870.59	864.16	870.72	871.02	870.01	868.44
CH <sub>3</sub> -CH <sub>2</sub> -NH <sub>2</sub>	875.70	868.93	878.22	871.39	878.12	878.94	877.52	875.36
H <sub>2</sub> C=C=O	531.90	527.83	532.80	535.43	533.46	537.43	537.29	538.30
CH <sub>2</sub> -O-CH <sub>2</sub>	649.90	638.66	647.07	650.87	647.75	654.03	656.26	654.04
CH <sub>3</sub> CHO	676.20	666.38	672.37	673.70	675.29	677.78	678.27	678.06
O=CH-CH=O	633.40	619.78	626.01	632.12	630.03	634.17	632.70	635.25
CH <sub>3</sub> CH <sub>2</sub> OH	808.80	797.39	805.32	802.09	806.71	808.60	809.26	809.09
CH <sub>3</sub> -O-CH <sub>3</sub>	796.80	784.72	794.18	791.99	796.04	796.65	798.37	798.76
CH <sub>2</sub> -S-CH <sub>2</sub>	623.00	619.29	625.64	626.43	619.90	630.19	632.72	628.92
(CH <sub>3</sub> ) <sub>2</sub> SO	854.10	846.58	851.12	853.80	848.55	855.16	854.14	853.30
CH <sub>3</sub> -CH <sub>2</sub> -SH	767.60	762.60	768.44	766.03	764.33	769.50	768.63	767.84
CH <sub>3</sub> -S-CH <sub>3</sub>	766.00	760.03	767.75	765.36	763.75	768.78	768.81	767.23
H <sub>2</sub> C=CHF	571.30	560.43	572.43	571.73	572.15	575.22	573.17	574.18
CH <sub>3</sub> -CH <sub>2</sub> -Cl	690.10	684.25	689.73	689.20	687.03	693.51	694.36	691.86
H <sub>2</sub> C=CHCl	538.60	537.14	542.63	543.79	539.78	546.75	544.38	543.51
H <sub>2</sub> C=CHCN	763.30	749.31	759.52	760.46	760.90	765.89	758.66	759.76
CH <sub>3</sub> -CO-CH <sub>3</sub>	977.20	963.40	972.63	973.35	974.53	981.05	979.58	979.42
CH <sub>3</sub> COOH	802.20	791.12	797.57	799.85	798.13	803.63	803.36	804.73
CH <sub>3</sub> COF	705.40	692.91	702.23	705.95	702.22	708.10	708.65	709.17
CH <sub>3</sub> COCl	666.90	662.52	665.49	670.51	662.88	671.86	672.30	671.62
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> Cl	983.80	973.77	982.25	981.28	978.88	989.28	988.36	985.87
(CH <sub>3</sub> ) <sub>2</sub> CH-OH	1106.40	1090.69	1101.39	1098.16	1101.61	1107.56	1106.36	1106.69
CH <sub>3</sub> -CH <sub>2</sub> -O-CH <sub>3</sub>	1093.30	1077.63	1089.91	1087.16	1091.16	1095.55	1095.56	1095.75
(CH <sub>3</sub> ) <sub>3</sub> N	1158.60	1146.42	1159.82	1154.16	1158.60	1162.62	1160.08	1159.88
C <sub>4</sub> H <sub>4</sub> O	993.00	977.26	993.75	995.12	987.94	1005.57	992.64	995.62
C <sub>4</sub> H <sub>4</sub> S	962.10	953.59	966.20	967.89	954.46	976.31	961.94	962.60
C <sub>4</sub> H <sub>4</sub> NH	1070.40	1059.00	1076.62	1072.66	1069.43	1086.82	1070.49	1071.50
C <sub>5</sub> H <sub>5</sub> N	1236.40	1221.56	1241.87	1241.30	1235.73	1255.77	1233.88	1237.43
SH•	86.90	90.44	89.60	88.62	88.23	86.78	87.11	87.37
C <sub>2</sub> H <sub>3</sub> •	444.00	440.50	445.34	444.11	447.44	449.72	447.05	447.03
CH <sub>3</sub> CO•	580.90	573.46	576.59	579.72	582.18	585.75	584.10	582.99
H <sub>2</sub> COH•	408.90	402.61	406.21	405.65	410.73	410.52	410.35	409.62
CH <sub>3</sub> O•	400.50	396.38	400.28	398.62	403.56	402.79	402.89	402.18
CH <sub>3</sub> CH <sub>2</sub> O•	697.10	685.87	692.70	690.29	695.42	698.39	696.71	695.70
CH <sub>3</sub> S•	380.60	379.88	383.25	381.43	382.49	384.50	384.00	382.81
C <sub>2</sub> H <sub>5</sub> •	602.20	596.60	602.11	600.46	605.44	607.32	607.69	604.69
(CH <sub>3</sub> ) <sub>2</sub> CH•	898.80	890.79	898.90	895.97	901.08	906.78	905.95	902.50
NO <sub>2</sub> •	227.50	225.05	219.34	231.96	231.44	231.78	230.61	227.69
	ref.	SOGGA11-X	MN15	BMK	M06-2X	M05-2X	M06-HF	ωB97
H <sub>2</sub>	109.20	105.88	107.95	107.59	107.85	107.21	110.53	105.82

LiH	57.80	53.00	60.57	56.00	56.41	58.39	51.08	57.00
BeH	49.80	52.62	52.15	56.32	53.08	48.32	47.92	52.00
<sup>2</sup> CH	83.80	83.77	81.89	83.36	83.01	82.48	84.73	83.48
<sup>3</sup> CH <sub>2</sub>	190.00	187.64	187.69	189.91	192.18	188.58	192.19	188.31
<sup>1</sup> CH <sub>2</sub>	180.70	179.33	177.77	178.70	178.63	178.51	180.94	178.94
CH <sub>3</sub> •	306.60	305.63	305.39	306.98	305.93	306.73	308.70	306.06
CH <sub>4</sub>	419.20	417.73	416.58	419.66	417.64	418.52	422.37	417.70
<sup>3</sup> NH	83.50	84.34	81.81	85.41	83.02	82.99	85.15	84.14
NH <sub>2</sub> •	181.50	182.96	182.15	184.48	180.49	181.29	181.22	182.56
NH <sub>3</sub>	297.50	295.80	296.85	298.96	295.25	296.26	299.94	296.04
OH•	106.40	105.20	106.76	106.74	106.09	105.85	104.39	105.37
H <sub>2</sub> O	232.20	226.36	230.62	230.04	230.08	230.23	231.42	227.61
HF	140.80	135.44	140.37	138.08	138.87	140.06	141.37	138.01
Li <sub>2</sub>	24.40	17.52	22.65	16.42	23.62	27.17	16.97	20.08
LiF	137.50	129.97	139.31	136.45	136.31	140.54	133.05	138.07
C <sub>2</sub> H <sub>2</sub>	405.30	400.46	402.70	401.96	403.35	402.24	404.99	399.44
H <sub>2</sub> C=CH <sub>2</sub>	562.60	561.34	559.98	562.37	561.05	562.26	566.57	559.87
H <sub>3</sub> C-CH <sub>3</sub>	710.80	710.40	707.20	712.21	709.50	711.02	716.40	710.78
CN•	180.90	173.98	175.61	177.43	176.67	172.35	171.09	174.02
HCN	312.60	308.87	310.53	312.98	309.89	308.44	310.55	308.93
CO	259.30	254.50	258.08	260.56	257.88	255.51	256.05	256.42
HCO•	278.70	276.26	277.92	281.52	277.52	276.23	273.38	278.10
H <sub>2</sub> C=O	373.60	370.07	372.89	374.93	372.08	370.84	371.68	371.39
CH <sub>3</sub> -OH	511.90	508.04	511.44	512.42	511.49	511.69	516.50	509.49
N <sub>2</sub>	228.60	224.87	224.40	226.14	223.26	221.66	223.51	226.42
H <sub>2</sub> N-NH <sub>2</sub>	437.80	438.02	440.43	442.30	436.40	437.02	444.45	439.42
NO•	152.80	152.35	153.53	154.00	151.46	149.76	149.23	156.19
O <sub>2</sub>	120.50	117.24	118.41	119.39	118.44	116.44	108.05	123.86
HO-OH	268.70	259.60	268.60	264.81	265.49	262.84	264.34	263.43
F <sub>2</sub>	38.50	29.21	38.29	31.64	32.25	28.95	29.35	37.36
CO <sub>2</sub>	389.10	385.05	390.76	393.21	388.48	385.48	372.83	388.08
<sup>1</sup> SiH <sub>2</sub>	151.30	151.25	152.64	153.14	153.32	150.93	150.54	152.53
<sup>3</sup> SiH <sub>2</sub>	131.20	129.12	134.61	131.03	134.58	127.45	135.05	131.23
SiH <sub>3</sub> •	225.10	224.44	229.57	226.82	227.47	221.87	225.67	227.89
SiH <sub>4</sub>	321.40	320.36	324.67	323.24	320.76	316.59	316.36	324.56
PH <sub>2</sub> •	152.90	154.68	154.66	155.86	156.62	155.84	159.35	155.37
PH <sub>3</sub>	241.80	241.13	241.61	243.24	242.57	241.71	245.67	241.41
H <sub>2</sub> S	182.40	181.74	183.66	181.14	181.83	182.91	185.10	180.89
HCl	106.30	105.40	106.62	105.84	105.70	106.03	106.52	105.09
S <sub>2</sub>	101.60	104.85	103.49	103.70	104.79	108.49	104.34	100.20
Cl <sub>2</sub>	58.00	57.81	59.96	61.49	59.89	59.36	61.42	55.93
NaCl	98.00	95.39	98.46	98.38	98.30	101.92	90.96	101.28
SiO	192.30	181.53	192.49	189.18	189.82	191.20	188.63	186.33
CS	171.30	168.16	171.12	166.96	168.78	169.07	167.94	164.28
SO	125.10	122.15	124.93	126.07	124.22	125.66	120.77	123.81
ClO•	64.40	63.21	65.78	64.59	63.86	63.18	60.66	63.62
ClF	61.50	57.48	64.55	60.60	61.71	61.46	65.38	61.20
CH <sub>3</sub> Cl	393.90	394.39	393.67	396.49	394.45	395.22	399.52	394.04
H <sub>3</sub> C-SH	473.00	473.29	473.23	473.73	473.07	474.97	480.26	472.69
HOCl	164.40	160.07	166.21	164.13	164.80	163.56	166.38	161.23
SO <sub>2</sub>	258.40	243.79	254.04	253.44	248.61	247.99	236.56	248.42
BF <sub>3</sub>	469.90	460.41	480.07	473.62	474.05	479.04	475.41	468.06
BCl <sub>3</sub>	322.70	325.31	331.67	331.49	326.95	326.45	322.35	324.43
AlF <sub>3</sub>	426.50	412.47	432.22	420.97	425.20	433.13	435.89	430.67
AlCl <sub>3</sub>	306.10	306.44	315.54	312.82	310.90	310.97	306.21	310.51
CF <sub>4</sub>	476.30	469.63	488.50	477.99	480.39	482.37	479.91	481.05
CCl <sub>4</sub>	312.80	311.82	317.50	314.19	315.29	315.26	318.10	312.58
O=C=S	333.30	332.99	337.68	338.53	335.18	333.97	324.31	331.27
CS <sub>2</sub>	277.70	279.70	282.99	280.69	280.22	281.48	272.95	271.11
COF <sub>2</sub>	426.70	413.92	427.18	422.30	421.07	420.37	413.59	421.93
SiF <sub>4</sub>	572.80	553.40	581.49	567.11	574.97	585.05	587.29	571.36
SiCl <sub>4</sub>	383.30	382.21	392.91	392.59	387.61	386.47	382.83	385.32
N <sub>2</sub> O	270.50	265.86	269.54	267.12	263.17	259.67	246.33	268.66
CINO	191.20	185.50	189.13	189.14	184.78	182.11	172.17	185.77
NF <sub>3</sub>	205.20	200.59	214.39	204.47	204.11	203.32	201.19	214.15
PF <sub>3</sub>	363.90	352.23	370.82	364.45	366.58	373.25	376.29	364.19
O <sub>3</sub>	147.10	122.70	135.90	129.09	124.27	118.69	101.18	133.73
F <sub>2</sub> O	93.30	82.18	95.87	86.56	87.02	83.39	82.24	93.87
ClF <sub>3</sub>	125.60	114.93	130.10	121.74	123.03	127.24	125.42	128.68
F <sub>2</sub> C=CF <sub>2</sub>	583.90	581.61	605.20	591.07	592.95	593.88	590.17	593.78
Cl <sub>2</sub> C=CCl <sub>2</sub>	466.80	469.78	476.27	469.77	473.16	472.50	472.21	469.54

CF <sub>3</sub> CN	639.70	632.54	647.79	641.15	640.32	639.83	635.68	642.04
CH≡C-CH <sub>3</sub>	704.20	701.73	701.84	703.06	703.62	702.95	706.41	700.73
CH <sub>2</sub> =C=CH <sub>2</sub>	702.40	702.97	702.57	703.91	703.34	703.69	706.52	700.30
C <sub>3</sub> H <sub>4</sub>	682.10	682.59	682.06	680.85	683.51	681.92	684.15	683.26
CH <sub>2</sub> =CHCH <sub>3</sub>	859.20	858.72	855.75	859.74	857.91	859.70	864.85	857.86
C <sub>3</sub> H <sub>6</sub>	851.90	854.45	851.62	853.82	854.11	854.41	859.26	856.40
C <sub>3</sub> H <sub>8</sub>	1004.60	1004.39	999.78	1006.31	1003.28	1005.53	1012.57	1005.68
C <sub>4</sub> H <sub>6</sub>	1011.20	1010.54	1007.47	1010.71	1009.36	1011.52	1015.70	1007.16
C <sub>4</sub> H <sub>6</sub>	1002.80	1001.74	999.74	1002.84	1002.68	1002.41	1006.71	1000.78
C <sub>4</sub> H <sub>6</sub>	989.50	994.68	992.21	993.43	994.01	993.99	997.25	995.04
C <sub>4</sub> H <sub>10</sub>	1298.50	1298.34	1292.40	1300.41	1297.08	1300.04	1308.74	1300.57
C <sub>4</sub> H <sub>10</sub>	1300.30	1299.06	1293.86	1301.41	1298.44	1301.50	1310.42	1301.79
C <sub>5</sub> H <sub>8</sub>	1282.40	1288.88	1284.92	1285.81	1288.27	1287.69	1292.40	1292.86
C <sub>6</sub> H <sub>6</sub>	1366.00	1370.90	1365.70	1368.94	1367.48	1371.57	1370.82	1364.41
H <sub>2</sub> CF <sub>2</sub>	436.20	432.22	441.25	437.85	437.48	439.99	443.74	438.16
HCF <sub>3</sub>	457.70	452.16	466.06	459.35	460.09	462.55	463.60	460.94
H <sub>2</sub> CCl <sub>2</sub>	369.60	370.32	370.75	372.43	370.96	371.53	375.46	369.94
HCCl <sub>3</sub>	343.30	343.41	345.91	345.52	345.13	345.41	348.69	343.39
H <sub>3</sub> C-NH <sub>2</sub>	581.20	580.59	580.34	583.99	579.70	580.85	588.05	581.19
CH <sub>3</sub> -CN	615.10	613.68	613.03	617.61	613.48	612.65	615.24	613.67
CH <sub>3</sub> -NO <sub>2</sub>	600.60	595.84	601.41	600.02	596.22	594.88	590.36	602.72
CH <sub>3</sub> -O-N=O	598.30	592.18	600.20	597.94	594.44	591.47	589.66	599.34
CH <sub>3</sub> -SiH <sub>3</sub>	626.10	624.06	627.17	628.61	624.63	621.99	624.92	628.83
HCOOH	500.70	495.28	502.50	503.12	500.54	499.02	497.18	498.47
HCOOCH <sub>3</sub>	784.20	779.88	787.36	789.11	785.93	784.77	786.84	783.98
CH <sub>3</sub> CONH <sub>2</sub>	867.10	865.70	868.58	873.08	866.64	867.39	869.00	868.95
CH <sub>2</sub> -NH-CH <sub>2</sub>	719.00	722.09	721.54	723.92	721.22	720.42	725.74	723.80
NCCN	502.30	496.45	499.58	501.37	496.08	491.66	487.51	494.66
(CH <sub>3</sub> ) <sub>2</sub> CH	868.80	868.56	867.71	872.40	867.98	869.31	879.99	869.98
CH <sub>3</sub> -CH <sub>2</sub> -NH <sub>2</sub>	875.70	876.38	874.74	879.94	875.24	877.14	885.79	877.87
H <sub>2</sub> C=C=O	531.90	531.11	534.59	536.53	533.55	531.97	527.82	531.72
CH <sub>2</sub> -O-CH <sub>2</sub>	649.90	649.44	652.49	652.55	652.26	651.15	653.12	651.97
CH <sub>3</sub> CHO	676.20	673.71	674.70	678.59	674.90	674.55	675.26	675.61
O=CH-CH=O	633.40	628.08	633.51	636.25	631.49	628.50	625.16	631.49
CH <sub>3</sub> CH <sub>2</sub> OH	808.80	805.15	806.98	809.61	808.20	809.13	814.91	807.47
CH <sub>3</sub> -O-CH <sub>3</sub>	796.80	793.52	796.91	798.96	797.52	797.77	806.30	795.67
CH <sub>2</sub> -S-CH <sub>2</sub>	623.00	626.84	625.37	627.27	627.15	627.83	631.31	626.30
(CH <sub>3</sub> ) <sub>2</sub> SO	854.10	849.91	851.88	853.61	851.50	854.92	857.56	852.48
CH <sub>3</sub> -CH <sub>2</sub> -SH	767.60	767.62	766.26	768.29	767.24	769.98	777.05	767.85
CH <sub>3</sub> -S-CH <sub>3</sub>	766.00	766.77	765.33	768.16	766.75	769.47	777.78	766.86
H <sub>2</sub> C=CHF	571.30	569.82	574.55	573.31	572.51	574.04	576.97	571.93
CH <sub>3</sub> -CH <sub>2</sub> -Cl	690.10	690.54	688.36	692.80	690.28	691.84	697.45	690.94
H <sub>2</sub> C=CHCl	538.60	542.39	542.26	543.44	542.64	543.40	546.65	540.96
H <sub>2</sub> C=CHCN	763.30	759.81	759.22	762.81	759.17	758.51	759.87	757.70
CH <sub>3</sub> -CO-CH <sub>3</sub>	977.20	974.99	974.77	980.23	976.03	976.54	977.78	978.01
CH <sub>3</sub> COOH	802.20	797.10	802.88	805.10	802.04	801.33	799.75	801.21
CH <sub>3</sub> COF	705.40	701.13	707.43	708.18	705.14	705.65	703.09	707.09
CH <sub>3</sub> COCl	666.90	665.35	667.52	671.23	667.22	666.56	663.81	667.02
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> Cl	983.80	984.50	980.97	986.96	984.11	986.41	993.78	985.83
(CH <sub>3</sub> ) <sub>2</sub> CH-OH	1106.40	1102.19	1103.25	1107.04	1105.54	1107.29	1114.37	1105.92
CH <sub>3</sub> -CH <sub>2</sub> -O-CH <sub>3</sub>	1093.30	1090.60	1092.42	1096.13	1094.19	1095.16	1104.60	1093.61
(CH <sub>3</sub> ) <sub>3</sub> N	1158.60	1158.26	1157.88	1162.89	1158.85	1160.49	1174.90	1161.08
C <sub>4</sub> H <sub>4</sub> O	993.00	992.72	998.01	997.95	995.36	995.66	997.21	991.65
C <sub>4</sub> H <sub>4</sub> S	962.10	965.14	964.84	963.16	963.49	967.05	967.61	960.18
C <sub>4</sub> H <sub>4</sub> NH	1070.40	1074.38	1075.55	1078.41	1073.10	1075.17	1080.53	1072.06
C <sub>5</sub> H <sub>5</sub> N	1236.40	1242.45	1239.65	1243.24	1238.54	1241.28	1242.64	1236.79
SH•	86.90	87.39	88.27	86.92	87.41	88.29	89.38	86.99
C <sub>2</sub> H <sub>3</sub> •	444.00	444.11	443.74	444.89	444.77	444.69	445.90	443.30
CH <sub>3</sub> CO•	580.90	579.87	579.91	585.21	580.19	579.92	577.97	582.15
H <sub>2</sub> COH•	408.90	406.00	410.06	410.20	409.08	409.38	410.87	408.18
CH <sub>3</sub> O•	400.50	400.64	401.09	403.31	400.47	400.61	400.86	401.02
CH <sub>3</sub> CH <sub>2</sub> O•	697.10	696.95	693.55	697.25	693.97	694.86	696.58	695.68
CH <sub>3</sub> S•	380.60	383.15	382.01	383.74	382.53	384.59	387.82	382.93
C <sub>2</sub> H <sub>5</sub> •	602.20	602.72	600.43	603.75	601.83	603.33	605.27	603.51
(CH <sub>3</sub> ) <sub>2</sub> CH•	898.80	900.27	896.34	901.13	898.68	900.80	903.17	901.67
NO <sub>2</sub> •	227.50	223.54	227.62	226.01	221.43	218.77	203.37	230.15
	ref.	ωB97X	ωB97XD	N12-SX	MN12-SX	M11	HF	B2-PLYP
H <sub>2</sub>	109.20	106.49	107.60	103.71	110.21	109.34	83.85	108.76
LiH	57.80	57.74	56.49	50.35	61.87	59.07	34.05	56.74
BeH	49.80	54.30	55.37	51.52	57.23	55.32	50.41	55.91
<sup>2</sup> CH	83.80	83.12	83.05	80.56	83.49	83.22	56.81	83.73

$^3\text{CH}_2$	190.00	189.97	190.75	190.35	188.53	188.38	155.09	190.61
$^1\text{CH}_2$	180.70	178.71	178.71	174.95	180.60	180.21	126.76	178.91
$\text{CH}_3^\bullet$	306.60	306.85	307.27	304.99	303.53	307.74	243.00	307.92
$\text{CH}_4$	419.20	418.61	419.19	415.50	415.95	420.94	328.23	419.09
$^3\text{NH}$	83.50	83.94	83.98	81.13	82.45	83.81	51.16	85.03
$\text{NH}_2^\bullet$	181.50	182.69	182.93	178.34	182.17	186.83	117.45	184.26
$\text{NH}_3$	297.50	296.57	297.13	291.99	297.17	304.42	200.59	298.19
$\text{OH}^\bullet$	106.40	106.02	106.53	106.25	107.14	107.84	68.04	106.73
$\text{H}_2\text{O}$	232.20	228.70	229.82	229.22	230.98	234.77	155.06	230.49
$\text{HF}$	140.80	137.96	138.51	139.13	139.54	142.91	96.14	139.50
$\text{Li}_2$	24.40	21.35	20.12	16.25	39.49	23.14	3.98	20.80
$\text{LiF}$	137.50	136.45	133.40	134.99	139.39	138.82	89.81	136.99
$\text{C}_2\text{H}_2$	405.30	400.48	400.74	399.37	396.76	402.31	292.57	404.41
$\text{H}_2\text{C}=\text{CH}_2$	562.60	561.22	561.78	559.45	556.05	562.10	428.35	562.11
$\text{H}_3\text{C}-\text{CH}_3$	710.80	711.53	711.87	707.92	704.76	712.73	551.40	710.03
$\text{CN}^\bullet$	180.90	174.04	174.13	170.93	172.03	176.50	90.75	179.43
$\text{HCN}$	312.60	308.59	308.30	302.92	306.03	313.09	196.23	313.96
$\text{CO}$	259.30	255.72	255.53	252.71	254.54	257.82	171.97	257.93
$\text{HCO}^\bullet$	278.70	278.29	278.75	278.04	274.25	278.92	181.20	280.45
$\text{H}_2\text{C}=\text{O}$	373.60	371.92	372.45	371.53	369.57	373.59	256.24	373.45
$\text{CH}_3-\text{OH}$	511.90	510.55	511.18	510.40	508.88	514.86	368.83	510.53
$\text{N}_2$	228.60	224.20	222.58	212.05	220.27	229.92	109.32	229.03
$\text{H}_2\text{N}-\text{NH}_2$	437.80	439.24	439.22	432.17	438.28	450.55	267.26	439.25
$\text{NO}^\bullet$	152.80	154.40	153.28	148.33	147.37	156.32	54.11	154.78
$\text{O}_2$	120.50	122.32	122.12	119.39	112.26	117.34	27.50	122.31
$\text{HO}-\text{OH}$	268.70	264.36	265.34	266.43	267.88	269.85	132.28	265.57
$\text{F}_2$	38.50	35.64	35.06	37.94	37.56	35.46	-38.16	35.84
$\text{CO}_2$	389.10	388.14	388.91	390.39	384.26	389.20	243.34	390.71
$^1\text{SiH}_2$	151.30	153.27	153.22	150.12	152.61	153.99	110.65	152.14
$^3\text{SiH}_2$	131.20	132.33	132.75	133.37	129.96	133.86	106.66	132.04
$\text{SiH}_3^\bullet$	225.10	228.42	228.19	226.53	227.24	229.09	180.62	227.13
$\text{SiH}_4$	321.40	324.66	324.08	320.29	324.98	324.83	256.78	322.61
$\text{PH}_2^\bullet$	152.90	156.98	157.44	154.22	148.09	155.77	108.98	155.30
$\text{PH}_3$	241.80	243.58	244.40	240.48	236.05	242.64	172.83	241.47
$\text{H}_2\text{S}$	182.40	182.42	183.37	182.89	184.05	183.89	129.65	181.23
$\text{HCl}$	106.30	105.68	106.27	106.51	107.89	107.52	76.98	105.38
$\text{S}_2$	101.60	102.92	104.94	111.61	107.67	104.01	50.78	103.54
$\text{Cl}_2$	58.00	57.38	58.81	63.63	60.92	60.12	18.77	56.35
$\text{NaCl}$	98.00	101.44	99.01	98.49	104.38	101.47	69.81	94.76
$\text{SiO}$	192.30	186.86	186.49	187.73	184.39	187.06	108.46	191.64
$\text{CS}$	171.30	165.60	166.97	167.97	169.40	165.72	96.75	169.53
$\text{SO}$	125.10	124.86	125.89	128.24	124.42	125.14	52.17	126.75
$\text{ClO}^\bullet$	64.40	64.56	65.45	69.04	65.33	65.17	5.82	63.68
$\text{ClF}$	61.50	60.98	60.99	64.93	62.49	63.68	6.99	60.49
$\text{CH}_3\text{Cl}$	393.90	394.66	394.82	395.53	392.38	396.28	296.69	392.92
$\text{H}_3\text{C}-\text{SH}$	473.00	474.11	474.59	474.68	471.32	475.27	350.97	471.31
$\text{HOCl}$	164.40	162.47	163.49	166.52	165.82	166.95	77.27	162.93
$\text{SO}_2$	258.40	250.02	251.64	256.20	249.51	250.64	99.51	255.74
$\text{BF}_3$	469.90	466.82	464.85	476.56	473.11	471.24	361.62	469.18
$\text{BCl}_3$	322.70	324.40	323.52	336.07	331.56	318.32	244.38	320.38
$\text{AlF}_3$	426.50	424.97	419.64	433.34	427.04	439.93	320.99	425.02
$\text{AlCl}_3$	306.10	309.59	307.70	319.59	317.43	311.33	244.27	303.63
$\text{CF}_4$	476.30	477.90	474.59	485.42	477.22	480.71	312.83	473.12
$\text{CCl}_4$	312.80	311.75	309.72	323.67	313.29	310.44	179.36	305.44
$\text{O}=\text{C}=\text{S}$	333.30	332.78	334.72	340.02	333.77	333.44	204.57	336.35
$\text{CS}_2$	277.70	274.50	278.06	288.38	282.31	274.71	163.91	280.83
$\text{COF}_2$	426.70	420.35	419.11	425.34	417.26	421.94	263.08	418.49
$\text{SiF}_4$	572.80	566.85	561.26	577.28	569.31	581.81	429.25	567.60
$\text{SiCl}_4$	383.30	385.06	383.28	399.36	390.25	382.06	284.56	376.39
$\text{N}_2\text{O}$	270.50	267.02	267.22	262.06	260.81	272.81	76.84	275.54
$\text{ClNO}$	191.20	186.25	188.22	186.89	186.37	188.61	39.71	192.49
$\text{NF}_3$	205.20	209.32	206.17	207.64	206.10	213.08	35.21	205.13
$\text{PF}_3$	363.90	363.26	360.29	368.10	354.04	367.13	234.30	361.74
$\text{O}_3$	147.10	132.73	134.43	134.99	127.86	131.14	-66.33	145.66
$\text{F}_2\text{O}$	93.30	91.53	90.55	94.32	92.53	92.51	-43.57	90.83
$\text{ClF}_3$	125.60	126.89	125.88	138.07	125.01	132.94	-23.30	127.43
$\text{F}_2\text{C}=\text{CF}_2$	583.90	591.11	588.50	602.48	586.99	592.78	373.85	585.84
$\text{Cl}_2\text{C}=\text{CCl}_2$	466.80	468.67	466.65	484.02	468.43	466.52	289.49	462.47
$\text{CF}_3\text{CN}$	639.70	638.50	634.89	640.81	632.84	640.77	396.62	639.00
$\text{CH}\equiv\text{C}-\text{CH}_3$	704.20	701.73	701.66	701.04	694.38	702.52	523.47	703.66
$\text{CH}_2=\text{C}=\text{CH}_2$	702.40	701.97	702.70	702.97	696.23	702.38	522.62	702.97

C <sub>3</sub> H <sub>4</sub>	682.10	682.20	680.55	681.89	673.38	683.80	497.20	679.25
CH <sub>2</sub> =CHCH <sub>3</sub>	859.20	859.02	859.27	856.90	849.92	858.85	655.24	857.93
C <sub>3</sub> H <sub>6</sub>	851.90	855.28	853.65	853.39	843.94	855.84	645.64	849.81
C <sub>3</sub> H <sub>8</sub>	1004.60	1006.16	1006.34	1001.69	995.23	1006.28	775.44	1002.62
C <sub>4</sub> H <sub>6</sub>	1011.20	1009.01	1009.65	1009.72	998.82	1007.39	761.92	1009.62
C <sub>4</sub> H <sub>6</sub>	1002.80	1001.70	1001.33	1001.37	990.73	1001.44	753.05	1001.74
C <sub>4</sub> H <sub>6</sub>	989.50	994.38	993.00	994.83	981.61	993.56	739.75	989.59
C <sub>4</sub> H <sub>10</sub>	1298.50	1300.77	1300.87	1295.43	1285.67	1299.88	999.41	1295.20
C <sub>4</sub> H <sub>10</sub>	1300.30	1301.85	1301.91	1296.11	1286.85	1301.15	999.67	1296.20
C <sub>5</sub> H <sub>8</sub>	1282.40	1289.72	1286.44	1289.50	1270.21	1288.40	959.37	1278.84
C <sub>6</sub> H <sub>6</sub>	1366.00	1366.49	1367.08	1373.88	1351.27	1361.72	1025.17	1366.21
H <sub>2</sub> CF <sub>2</sub>	436.20	436.84	435.50	439.88	433.97	440.11	309.31	435.51
HCF <sub>3</sub>	457.70	458.64	456.27	464.02	456.51	461.63	312.10	455.84
H <sub>2</sub> CCl <sub>2</sub>	369.60	370.20	369.81	375.00	368.63	370.85	262.37	366.67
HCCl <sub>3</sub>	343.30	343.18	342.04	351.67	342.81	342.72	223.74	338.15
H <sub>3</sub> C-NH <sub>2</sub>	581.20	581.64	581.92	576.52	578.27	588.03	416.54	581.28
CH <sub>3</sub> -CN	615.10	613.34	612.71	608.14	606.82	616.80	431.23	616.51
CH <sub>3</sub> -NO <sub>2</sub>	600.60	601.58	600.99	599.33	590.20	605.50	337.84	602.12
CH <sub>3</sub> -O-N=O	598.30	597.77	596.68	593.25	589.43	601.19	338.85	597.98
CH <sub>3</sub> -SiH <sub>3</sub>	626.10	629.00	628.23	624.88	625.14	629.33	489.78	625.13
HCOOH	500.70	499.30	499.78	501.85	497.00	502.48	329.69	499.89
HCOOCH <sub>3</sub>	784.20	784.58	784.35	786.10	777.92	786.94	545.97	783.66
CH <sub>3</sub> CONH <sub>2</sub>	867.10	869.13	868.78	867.42	860.98	874.35	606.42	867.06
CH <sub>2</sub> -NH-CH <sub>2</sub>	719.00	722.33	720.99	717.88	714.46	727.14	507.57	718.32
NCCN	502.30	493.66	493.20	488.84	490.53	497.23	284.62	505.56
(CH <sub>3</sub> ) <sub>2</sub> CH	868.80	870.25	870.24	864.22	863.06	875.23	634.99	867.96
CH <sub>3</sub> -CH <sub>2</sub> -NH <sub>2</sub>	875.70	878.08	878.14	872.11	870.39	883.25	642.26	875.70
H <sub>2</sub> C=C=O	531.90	532.53	533.29	534.67	528.24	534.08	369.36	534.00
CH <sub>2</sub> -O-CH <sub>2</sub>	649.90	651.31	650.47	651.58	644.50	653.48	459.75	648.12
CH <sub>3</sub> CHO	676.20	676.07	676.09	675.49	669.11	676.58	489.75	675.42
O=CH-CH=O	633.40	631.62	631.45	633.63	624.85	630.99	418.83	632.57
CH <sub>3</sub> CH <sub>2</sub> OH	808.80	808.30	808.44	807.37	802.33	811.36	596.13	806.31
CH <sub>3</sub> -O-CH <sub>3</sub>	796.80	796.61	796.69	795.37	791.11	799.25	585.81	794.92
CH <sub>2</sub> -S-CH <sub>2</sub>	623.00	626.21	625.52	629.78	619.95	628.05	453.10	621.52
(CH <sub>3</sub> ) <sub>2</sub> SO	854.10	853.62	853.82	856.97	846.65	854.51	600.88	850.30
CH <sub>3</sub> -CH <sub>2</sub> -SH	767.60	769.04	769.12	768.85	762.06	769.12	575.23	764.39
CH <sub>3</sub> -S-CH <sub>3</sub>	766.00	768.04	768.13	768.45	761.12	768.87	573.68	763.63
H <sub>2</sub> C=CHF	571.30	572.17	571.86	573.87	567.03	573.56	418.16	571.72
CH <sub>3</sub> -CH <sub>2</sub> -Cl	690.10	691.37	691.15	691.55	684.92	691.85	522.88	687.81
H <sub>2</sub> C=CHCl	538.60	541.87	541.98	544.51	537.70	541.96	398.54	540.70
H <sub>2</sub> C=CHCN	763.30	758.00	757.75	755.24	750.10	759.62	532.07	762.80
CH <sub>3</sub> -CO-CH <sub>3</sub>	977.20	978.21	977.79	976.83	966.63	977.80	721.00	975.17
CH <sub>3</sub> COOH	802.20	801.81	801.60	803.79	795.12	804.16	562.20	799.96
CH <sub>3</sub> COF	705.40	706.20	705.10	708.22	698.16	707.15	498.60	704.05
CH <sub>3</sub> COCl	666.90	667.39	667.45	671.22	661.45	667.21	469.25	665.48
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> Cl	983.80	985.98	985.66	985.31	975.32	985.48	746.88	980.44
(CH <sub>3</sub> ) <sub>2</sub> CH-OH	1106.40	1106.37	1106.18	1104.22	1096.03	1108.42	822.82	1102.24
CH <sub>3</sub> -CH <sub>2</sub> -O-CH <sub>3</sub>	1093.30	1094.31	1094.02	1092.28	1084.51	1095.76	813.05	1090.69
(CH <sub>3</sub> ) <sub>3</sub> N	1158.60	1161.02	1160.67	1153.54	1150.16	1164.93	854.48	1156.87
C <sub>4</sub> H <sub>4</sub> O	993.00	992.91	993.01	1000.04	984.02	992.24	709.61	991.63
C <sub>4</sub> H <sub>4</sub> S	962.10	961.75	961.97	972.22	953.49	958.61	696.02	960.18
C <sub>4</sub> H <sub>4</sub> NH	1070.40	1072.97	1073.02	1076.57	1062.77	1075.95	765.99	1071.44
C <sub>5</sub> H <sub>5</sub> N	1236.40	1238.10	1238.27	1242.51	1225.43	1236.86	891.82	1238.72
SH•	86.90	87.92	88.40	87.94	87.67	88.35	61.06	87.07
C <sub>2</sub> H <sub>3</sub> •	444.00	444.74	445.15	444.74	439.90	444.98	337.61	445.13
CH <sub>3</sub> CO•	580.90	582.31	582.21	582.21	573.46	582.41	415.11	582.20
H <sub>2</sub> COH•	408.90	409.18	409.66	410.29	406.10	412.27	289.42	409.03
CH <sub>3</sub> O•	400.50	401.86	401.95	401.95	398.73	401.84	291.55	400.10
CH <sub>3</sub> CH <sub>2</sub> O•	697.10	696.29	698.33	695.64	688.81	695.22	516.01	692.44
CH <sub>3</sub> S•	380.60	383.87	383.84	384.28	379.35	384.28	284.88	381.08
C <sub>2</sub> H <sub>5</sub> •	602.20	604.27	604.28	602.21	597.01	604.23	468.71	602.87
(CH <sub>3</sub> ) <sub>2</sub> CH•	898.80	902.33	902.11	899.86	891.19	901.44	695.04	898.63
NO <sub>2</sub> •	227.50	228.63	228.80	226.72	218.16	229.36	49.98	232.38
	ref.	PBE-QIDH	ωB97X-2					
H <sub>2</sub>	109.20	105.10	107.79					
LiH	57.80	52.80	55.83					
BeH	49.80	55.31	55.00					
<sup>2</sup> CH	83.80	81.59	81.93					
<sup>3</sup> CH <sub>2</sub>	190.00	192.62	189.81					
<sup>1</sup> CH <sub>2</sub>	180.70	175.74	176.95					
CH <sub>3</sub> •	306.60	307.69	305.67					

CH <sub>4</sub>	419.20	418.15	416.94
<sup>3</sup> NH	83.50	81.85	82.32
NH <sub>2</sub> •	181.50	179.36	180.65
NH <sub>3</sub>	297.50	292.96	294.79
OH•	106.40	104.13	105.96
H <sub>2</sub> O	232.20	227.01	229.99
HF	140.80	137.25	139.46
Li <sub>2</sub>	24.40	19.06	21.26
LiF	137.50	132.16	136.50
C <sub>2</sub> H <sub>2</sub>	405.30	403.48	401.38
H <sub>2</sub> C=CH <sub>2</sub>	562.60	562.63	558.56
H <sub>3</sub> C-CH <sub>3</sub>	710.80	712.62	707.50
CN•	180.90	172.75	173.59
HCN	312.60	307.93	310.60
CO	259.30	254.57	257.80
HCO•	278.70	276.87	278.23
H <sub>2</sub> C=O	373.60	370.18	371.52
CH <sub>3</sub> -OH	511.90	509.19	509.00
N <sub>2</sub>	228.60	219.39	226.49
H <sub>2</sub> N-NH <sub>2</sub>	437.80	432.02	433.75
NO•	152.80	147.77	152.57
O <sub>2</sub>	120.50	115.55	122.46
HO-OH	268.70	258.20	265.65
F <sub>2</sub>	38.50	28.24	36.82
CO <sub>2</sub>	389.10	387.47	389.06
<sup>1</sup> SiH <sub>2</sub>	151.30	148.27	151.35
<sup>3</sup> SiH <sub>2</sub>	131.20	132.91	133.65
SiH <sub>3</sub> •	225.10	225.52	227.73
SiH <sub>4</sub>	321.40	319.30	323.16
PH <sub>2</sub> •	152.90	151.47	153.32
PH <sub>3</sub>	241.80	236.87	239.93
H <sub>2</sub> S	182.40	180.21	181.59
HCl	106.30	105.64	105.88
S <sub>2</sub>	101.60	103.42	103.18
Cl <sub>2</sub>	58.00	57.91	57.70
NaCl	98.00	96.31	97.74
SiO	192.30	184.32	192.03
CS	171.30	167.56	168.77
SO	125.10	122.16	126.30
ClO•	64.40	59.77	62.13
ClF	61.50	57.43	61.34
CH <sub>3</sub> Cl	393.90	395.81	392.77
H <sub>3</sub> C-SH	473.00	473.49	471.33
HOCl	164.40	159.87	163.70
SO <sub>2</sub>	258.40	248.49	257.39
BF <sub>3</sub>	469.90	469.33	469.08
BCl <sub>3</sub>	322.70	332.37	325.39
AlF <sub>3</sub>	426.50	421.77	428.16
AlCl <sub>3</sub>	306.10	314.27	311.29
CF <sub>4</sub>	476.30	476.90	474.07
CCl <sub>4</sub>	312.80	320.28	313.33
O=C=S	333.30	334.94	335.01
CS <sub>2</sub>	277.70	281.60	279.03
COF <sub>2</sub>	426.70	418.06	417.91
SiF <sub>4</sub>	572.80	565.91	570.70
SiCl <sub>4</sub>	383.30	392.77	387.11
N <sub>2</sub> O	270.50	263.20	270.79
ClNO	191.20	181.48	189.40
NF <sub>3</sub>	205.20	195.94	204.27
PF <sub>3</sub>	363.90	356.15	362.43
O <sub>3</sub>	147.10	128.02	146.34
F <sub>2</sub> O	93.30	79.02	91.83
ClF <sub>3</sub>	125.60	118.28	128.36
F <sub>2</sub> C=CF <sub>2</sub>	583.90	588.74	584.23
Cl <sub>2</sub> C=CCl <sub>2</sub>	466.80	480.12	468.53
CF <sub>3</sub> CN	639.70	638.37	637.21
CH≡C-CH <sub>3</sub>	704.20	706.51	699.87
CH <sub>2</sub> =C=CH <sub>2</sub>	702.40	705.05	697.43
C <sub>3</sub> H <sub>4</sub>	682.10	686.04	676.33
CH <sub>2</sub> =CHCH <sub>3</sub>	859.20	862.22	854.07
C <sub>3</sub> H <sub>6</sub>	851.90	858.92	847.91



C <sub>3</sub> H <sub>8</sub>	1004.60	1008.96	1000.12
C <sub>4</sub> H <sub>6</sub>	1011.20	1015.25	1003.87
C <sub>4</sub> H <sub>6</sub>	1002.80	1008.39	997.28
C <sub>4</sub> H <sub>6</sub>	989.50	999.97	985.75
C <sub>4</sub> H <sub>10</sub>	1298.50	1305.32	1292.76
C <sub>4</sub> H <sub>10</sub>	1300.30	1306.57	1294.20
C <sub>5</sub> H <sub>8</sub>	1282.40	1297.88	1277.10
C <sub>6</sub> H <sub>6</sub>	1366.00	1383.07	1360.63
H <sub>2</sub> CF <sub>2</sub>	436.20	435.22	434.67
HCF <sub>3</sub>	457.70	457.25	455.85
H <sub>2</sub> CCl <sub>2</sub>	369.60	373.38	368.74
CCl <sub>3</sub>	343.30	348.82	342.86
H <sub>3</sub> C-NH <sub>2</sub>	581.20	579.02	577.22
CH <sub>3</sub> -CN	615.10	614.24	612.22
CH <sub>3</sub> -NO <sub>2</sub>	600.60	595.09	598.69
CH <sub>3</sub> -O-N=O	598.30	589.52	595.34
CH <sub>3</sub> -SiH <sub>3</sub>	626.10	625.52	625.53
HCOOH	500.70	497.29	498.27
HCOOCH <sub>3</sub>	784.20	783.34	781.62
CH <sub>3</sub> CONH <sub>2</sub>	867.10	867.14	862.24
CH <sub>2</sub> -NH-CH <sub>2</sub>	719.00	721.94	714.84
NCCN	502.30	496.21	498.72
(CH <sub>3</sub> ) <sub>2</sub> CH	868.80	868.93	863.62
CH <sub>3</sub> -CH <sub>2</sub> -NH <sub>2</sub>	875.70	877.11	871.58
H <sub>2</sub> C=C=O	531.90	533.10	530.29
CH <sub>2</sub> -O-CH <sub>2</sub>	649.90	651.72	647.04
CH <sub>3</sub> CHO	676.20	675.75	672.84
O=CH-CH=O	633.40	630.04	630.24
CH <sub>3</sub> CH <sub>2</sub> OH	808.80	808.58	804.62
CH <sub>3</sub> -O-CH <sub>3</sub>	796.80	796.05	792.82
CH <sub>2</sub> -S-CH <sub>2</sub>	623.00	629.69	622.06
(CH <sub>3</sub> ) <sub>2</sub> SO	854.10	854.48	850.72
CH <sub>3</sub> -CH <sub>2</sub> -SH	767.60	770.35	764.48
CH <sub>3</sub> -S-CH <sub>3</sub>	766.00	769.27	763.67
H <sub>2</sub> C=CHF	571.30	572.51	568.62
CH <sub>3</sub> -CH <sub>2</sub> -Cl	690.10	694.38	687.59
H <sub>2</sub> C=CHCl	538.60	545.31	539.13
H <sub>2</sub> C=CHCN	763.30	761.57	756.74
CH <sub>3</sub> -CO-CH <sub>3</sub>	977.20	979.41	972.50
CH <sub>3</sub> COOH	802.20	801.28	798.09
CH <sub>3</sub> COF	705.40	705.39	702.31
CH <sub>3</sub> COCl	666.90	669.50	664.72
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> Cl	983.80	990.80	980.30
(CH <sub>3</sub> ) <sub>2</sub> CH-OH	1106.40	1108.39	1100.86
CH <sub>3</sub> -CH <sub>2</sub> -O-CH <sub>3</sub>	1093.30	1095.47	1088.48
(CH <sub>3</sub> ) <sub>3</sub> N	1158.60	1161.42	1152.86
C <sub>4</sub> H <sub>4</sub> O	993.00	1001.97	988.40
C <sub>4</sub> H <sub>4</sub> S	962.10	975.01	959.09
C <sub>4</sub> H <sub>4</sub> NH	1070.40	1082.02	1065.71
C <sub>5</sub> H <sub>5</sub> N	1236.40	1250.02	1231.56
SH•	86.90	86.13	86.83
C <sub>2</sub> H <sub>3</sub> •	444.00	446.14	440.70
CH <sub>3</sub> CO•	580.90	582.07	579.26
H <sub>2</sub> COH•	408.90	407.97	406.93
CH <sub>3</sub> O•	400.50	398.81	397.20
CH <sub>3</sub> CH <sub>2</sub> O•	697.10	694.82	689.38
CH <sub>3</sub> S•	380.60	383.15	380.23
C <sub>2</sub> H <sub>5</sub> •	602.20	605.92	599.84
(CH <sub>3</sub> ) <sub>2</sub> CH•	898.80	905.22	895.17
NO <sub>2</sub> •	227.50	221.03	229.07

Table S11: Barrier height energies (kcal mol<sup>-1</sup>) over the 24 reactions included into the DBH24 dataset. All the computations are done at the def2-QZVP level of theory.

	ref.	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L
H + N <sub>2</sub> O → [HON <sub>2</sub> ] <sup>‡</sup>	-17.13	-2.82	-8.76	-10.19	-18.46	-13.33	-11.24	-19.37
[HON <sub>2</sub> ] <sup>‡</sup> → OH + N <sub>2</sub>	-82.47	-32.15	-61.61	-52.52	-72.52	-52.75	-58.30	-67.08
H + ClH → [HClH] <sup>‡</sup>	-18.00	-2.26	-9.96	-9.80	-18.27	-11.87	-12.69	-17.80
[HClH] <sup>‡</sup> → HCl + H	-18.00	-2.26	-9.96	-9.80	-18.27	-11.87	-12.69	-17.80
CH <sub>3</sub> + FCl → [ClFCH <sub>3</sub> ] <sup>‡</sup>	-6.75	10.46	6.04	5.41	-1.26	1.49	4.78	3.62
[ClFCH <sub>3</sub> ] <sup>‡</sup> → FCH <sub>3</sub> + Cl	-60.00	-37.59	-41.65	-41.48	-53.74	-44.44	-43.39	-47.52
Cl <sup>-</sup> ...CH <sub>3</sub> Cl → [ClCH <sub>3</sub> Cl] <sup>-‡</sup>	-13.41	-6.37	-5.31	-6.71	-10.83	-7.64	-8.21	-10.23
[ClCH <sub>3</sub> Cl] <sup>-‡</sup> → ClCH <sub>3</sub> ...Cl <sup>-</sup>	-13.41	-6.37	-5.31	-6.71	-10.83	-7.64	-8.21	-10.23
F <sup>-</sup> ...CH <sub>3</sub> Cl → [FCH <sub>3</sub> Cl] <sup>-‡</sup>	-3.44	1.70	2.42	1.44	-0.89	0.41	0.61	-0.45
[FCH <sub>3</sub> Cl] <sup>-‡</sup> → FCH <sub>3</sub> ...Cl <sup>-</sup>	-29.42	-21.84	-21.31	-21.75	-28.83	-22.13	-22.76	-28.07
HO <sup>-</sup> ...CH <sub>3</sub> F → [HOCH <sub>3</sub> F] <sup>-‡</sup>	2.44	17.48	13.11	13.77	6.10	14.73	12.64	7.04
[HOCH <sub>3</sub> F] <sup>-‡</sup> → HOCH <sub>3</sub> ...F <sup>-</sup>	-17.66	-4.02	-7.17	-7.34	-15.62	-11.73	-9.90	-13.43
H + N <sub>2</sub> → [HN <sub>2</sub> ] <sup>‡</sup>	-14.36	2.25	-5.27	-5.23	-12.32	-6.62	-6.67	-10.99
[HN <sub>2</sub> ] <sup>‡</sup> → HN <sub>2</sub>	-10.61	-9.32	-8.40	-8.99	-12.82	-11.51	-12.08	-10.69
H + C <sub>2</sub> H <sub>4</sub> → [HCH <sub>2</sub> CH <sub>2</sub> ] <sup>‡</sup>	-1.72	5.44	0.68	0.12	-4.29	-1.61	-1.30	-3.43
[HCH <sub>2</sub> CH <sub>2</sub> ] <sup>‡</sup> → CH <sub>3</sub> CH <sub>2</sub>	-41.75	-39.34	-38.20	-40.27	-44.27	-41.51	-42.08	-45.39
HCN → [HCN] <sup>‡</sup>	-48.07	-44.93	-46.88	-45.65	-46.82	-46.29	-46.28	-48.21
[HCN] <sup>‡</sup> → HNC	-32.82	-30.82	-31.88	-30.68	-33.05	-33.74	-33.58	-33.27
HO + CH <sub>4</sub> → [HOCH <sub>4</sub> ] <sup>‡</sup>	-6.70	16.76	2.37	5.24	-2.45	3.52	2.09	-3.91
[HOCH <sub>4</sub> ] <sup>‡</sup> → CH <sub>3</sub> + H <sub>2</sub> O	-19.60	-2.22	-10.54	-8.89	-13.81	-12.77	-11.45	-12.42
H + OH → [HHO] <sup>‡</sup>	-10.70	1.97	-1.42	-3.60	-8.12	-5.66	-3.37	-6.92
[HHO] <sup>‡</sup> → O + H <sub>2</sub>	-13.10	12.67	-1.51	1.34	-8.38	-0.75	-5.52	-7.28
H + H <sub>2</sub> S → [HH <sub>2</sub> S] <sup>‡</sup>	-3.60	6.74	2.12	1.12	-4.48	0.01	-1.12	-3.70
[HH <sub>2</sub> S] <sup>‡</sup> → HS + H <sub>2</sub>	-17.30	0.41	-14.40	-9.46	-15.96	-7.97	-9.49	-13.29
	ref.	M11-L	MN12-L	MN15-L	B3LYP	PBE0	M05	M06
H + N <sub>2</sub> O → [HON <sub>2</sub> ] <sup>‡</sup>	-17.13	-16.46	-16.66	-17.98	-11.59	-14.14	-18.89	-18.59
[HON <sub>2</sub> ] <sup>‡</sup> → OH + N <sub>2</sub>	-82.47	-73.57	-80.19	-72.53	-72.92	-69.05	-69.99	-72.43
H + ClH → [HClH] <sup>‡</sup>	-18.00	-15.05	-16.08	-17.65	-12.57	-13.53	-18.36	-17.44
[HClH] <sup>‡</sup> → HCl + H	-18.00	-15.05	-16.08	-17.65	-12.57	-13.53	-18.36	-17.44
CH <sub>3</sub> + FCl → [ClFCH <sub>3</sub> ] <sup>‡</sup>	-6.75	-0.93	-0.97	-1.39	0.56	-1.98	-0.92	-0.88
[ClFCH <sub>3</sub> ] <sup>‡</sup> → FCH <sub>3</sub> + Cl	-60.00	-54.25	-54.27	-51.10	-50.81	-53.29	-55.93	-54.64
Cl <sup>-</sup> ...CH <sub>3</sub> Cl → [ClCH <sub>3</sub> Cl] <sup>-‡</sup>	-13.41	-12.46	-12.14	-12.90	-8.86	-10.92	-14.08	-11.16
[ClCH <sub>3</sub> Cl] <sup>-‡</sup> → ClCH <sub>3</sub> ...Cl <sup>-</sup>	-13.41	-12.46	-12.14	-12.90	-8.86	-10.92	-14.08	-11.16
F <sup>-</sup> ...CH <sub>3</sub> Cl → [FCH <sub>3</sub> Cl] <sup>-‡</sup>	-3.44	0.62	-0.70	-1.41	0.33	-1.04	-2.91	-1.42
[FCH <sub>3</sub> Cl] <sup>-‡</sup> → FCH <sub>3</sub> ...Cl <sup>-</sup>	-29.42	-36.74	-33.94	-33.16	-26.83	-28.58	-30.22	-29.17
HO <sup>-</sup> ...CH <sub>3</sub> F → [HOCH <sub>3</sub> F] <sup>-‡</sup>	2.44	1.51	3.19	4.67	8.63	7.50	4.35	4.89
[HOCH <sub>3</sub> F] <sup>-‡</sup> → HOCH <sub>3</sub> ...F <sup>-</sup>	-17.66	-15.05	-17.57	-14.99	-12.64	-14.66	-17.38	-16.61
H + N <sub>2</sub> → [HN <sub>2</sub> ] <sup>‡</sup>	-14.36	-9.75	-10.74	-12.05	-7.56	-8.60	-11.78	-11.68
[HN <sub>2</sub> ] <sup>‡</sup> → HN <sub>2</sub>	-10.61	-10.74	-11.43	-9.81	-10.79	-11.57	-12.58	-11.39
H + C <sub>2</sub> H <sub>4</sub> → [HCH <sub>2</sub> CH <sub>2</sub> ] <sup>‡</sup>	-1.72	-2.56	-2.25	-2.40	0.15	-0.70	-2.91	-2.82
[HCH <sub>2</sub> CH <sub>2</sub> ] <sup>‡</sup> → CH <sub>3</sub> CH <sub>2</sub>	-41.75	-44.95	-43.11	-43.75	-41.81	-44.19	-48.17	-45.14
HCN → [HCN] <sup>‡</sup>	-48.07	-43.51	-44.34	-43.84	-47.49	-46.39	-45.87	-47.21
[HCN] <sup>‡</sup> → HNC	-32.82	-32.39	-35.25	-32.20	-33.54	-32.71	-32.88	-34.19
HO + CH <sub>4</sub> → [HOCH <sub>4</sub> ] <sup>‡</sup>	-6.70	-9.15	-9.34	-7.58	-2.33	-2.07	-5.44	-5.40
[HOCH <sub>4</sub> ] <sup>‡</sup> → CH <sub>3</sub> + H <sub>2</sub> O	-19.60	-18.72	-18.75	-19.44	-13.97	-14.01	-17.95	-17.42
H + OH → [HHO] <sup>‡</sup>	-10.70	-9.13	-10.10	-7.86	-4.01	-7.04	-8.27	-8.61
[HHO] <sup>‡</sup> → O + H <sub>2</sub>	-13.10	-12.47	-12.68	-12.77	-6.32	-5.95	-11.66	-10.45
H + H <sub>2</sub> S → [HH <sub>2</sub> S] <sup>‡</sup>	-3.60	-3.49	-3.23	-3.92	0.48	-1.18	-4.60	-3.95
[HH <sub>2</sub> S] <sup>‡</sup> → HS + H <sub>2</sub>	-17.30	-16.62	-16.42	-17.52	-15.92	-12.41	-19.21	-17.16
	ref.	SOGGA11-X	MN15	BMK	M06-2X	M05-2X	M06-HF	ωB97
H + N <sub>2</sub> O → [HON <sub>2</sub> ] <sup>‡</sup>	-17.13	-17.74	-15.90	-17.17	-17.41	-19.07	-16.60	-21.01
[HON <sub>2</sub> ] <sup>‡</sup> → OH + N <sub>2</sub>	-82.47	-80.19	-75.96	-82.00	-81.62	-84.97	-94.81	-82.35
H + ClH → [HClH] <sup>‡</sup>	-18.00	-17.73	-18.50	-17.04	-18.25	-19.94	-20.00	-23.11
[HClH] <sup>‡</sup> → HCl + H	-18.00	-17.73	-18.50	-17.04	-18.25	-19.94	-20.00	-23.11
CH <sub>3</sub> + FCl → [ClFCH <sub>3</sub> ] <sup>‡</sup>	-6.75	-4.24	-4.47	-3.48	-5.72	-4.80	-11.42	-5.74
[ClFCH <sub>3</sub> ] <sup>‡</sup> → FCH <sub>3</sub> + Cl	-60.00	-59.46	-56.81	-58.29	-58.92	-59.24	-64.38	-59.71
Cl <sup>-</sup> ...CH <sub>3</sub> Cl → [ClCH <sub>3</sub> Cl] <sup>-‡</sup>	-13.41	-13.52	-12.55	-13.43	-13.51	-11.61	-11.94	-17.47
[ClCH <sub>3</sub> Cl] <sup>-‡</sup> → ClCH <sub>3</sub> ...Cl <sup>-</sup>	-13.41	-13.52	-12.55	-13.43	-13.51	-11.61	-11.94	-17.47
F <sup>-</sup> ...CH <sub>3</sub> Cl → [FCH <sub>3</sub> Cl] <sup>-‡</sup>	-3.44	-2.64	-1.80	-2.88	-3.28	-1.93	-2.55	-4.83
[FCH <sub>3</sub> Cl] <sup>-‡</sup> → FCH <sub>3</sub> ...Cl <sup>-</sup>	-29.42	-31.29	-32.17	-31.61	-32.85	-30.86	-31.67	-31.30
HO <sup>-</sup> ...CH <sub>3</sub> F → [HOCH <sub>3</sub> F] <sup>-‡</sup>	2.44	3.85	5.65	3.26	5.12	6.76	8.20	6.00
[HOCH <sub>3</sub> F] <sup>-‡</sup> → HOCH <sub>3</sub> ...F <sup>-</sup>	-17.66	-17.82	-14.74	-18.55	-16.30	-14.54	-13.23	-16.23
H + N <sub>2</sub> → [HN <sub>2</sub> ] <sup>‡</sup>	-14.36	-12.57	-12.19	-13.27	-13.78	-14.72	-16.91	-15.69
[HN <sub>2</sub> ] <sup>‡</sup> → HN <sub>2</sub>	-10.61	-12.31	-12.18	-12.76	-10.98	-12.83	-13.10	-15.05

H + C <sub>2</sub> H <sub>4</sub> → [HCH <sub>2</sub> CH <sub>2</sub> ] <sup>‡</sup>	-1.72	-1.89	-2.33	-2.96	-2.79	-3.71	-3.26	-4.95
[HCH <sub>2</sub> CH <sub>2</sub> ] <sup>‡</sup> → CH <sub>3</sub> CH <sub>2</sub>	-41.75	-43.24	-42.78	-44.32	-43.50	-44.74	-41.89	-48.58
HCN → [HCN] <sup>‡</sup>	-48.07	-46.01	-45.43	-46.20	-46.05	-46.62	-46.06	-45.98
[HCN] <sup>‡</sup> → HNC	-32.82	-32.91	-33.88	-34.74	-33.21	-33.43	-34.82	-33.02
HO + CH <sub>4</sub> → [HOCH <sub>4</sub> ] <sup>‡</sup>	-6.70	-6.00	-5.84	-5.86	-5.36	-4.87	-5.81	-4.95
[HOCH <sub>4</sub> ] <sup>‡</sup> → CH <sub>3</sub> + H <sub>2</sub> O	-19.60	-15.20	-18.58	-16.61	-17.73	-17.56	-19.29	-15.64
H + OH → [HHO] <sup>‡</sup>	-10.70	-9.41	-9.85	-10.19	-9.87	-10.27	-10.05	-10.57
[HHO] <sup>‡</sup> → O + H <sub>2</sub>	-13.10	-10.01	-11.03	-10.98	-11.58	-11.55	-16.13	-11.00
H + H <sub>2</sub> S → [HH <sub>2</sub> S] <sup>‡</sup>	-3.60	-3.43	-4.30	-3.49	-4.41	-5.45	-5.79	-6.93
[HH <sub>2</sub> S] <sup>‡</sup> → HS + H <sub>2</sub>	-17.30	-14.93	-16.83	-16.85	-17.81	-18.01	-20.56	-18.86
	ref.	ωB97X	ωB97XD	N12-SX	MN12-SX	M11	HF	B2-PLYP
H + N <sub>2</sub> O → [HON <sub>2</sub> ] <sup>‡</sup>	-17.13	-19.57	-17.92	-17.22	-17.55	-17.55	-27.89	-16.79
[HON <sub>2</sub> ] <sup>‡</sup> → OH + N <sub>2</sub>	-82.47	-81.01	-78.35	-72.14	-82.41	-80.86	-124.03	-76.96
H + ClH → [HClH] <sup>‡</sup>	-18.00	-20.80	-18.34	-17.46	-18.03	-17.20	-31.46	-15.83
[HClH] <sup>‡</sup> → HCl + H	-18.00	-20.80	-18.34	-17.46	-18.03	-17.20	-31.46	-15.83
CH <sub>3</sub> + FCl → [ClFCH <sub>3</sub> ] <sup>‡</sup>	-6.75	-5.10	-4.13	-0.81	-3.20	-7.40	-16.65	-3.66
[ClFCH <sub>3</sub> ] <sup>‡</sup> → FCH <sub>3</sub> + Cl	-60.00	-58.35	-56.67	-52.28	-55.43	-59.91	-78.72	-56.36
Cl <sup>-</sup> ··· CH <sub>3</sub> Cl → [ClCH <sub>3</sub> Cl] <sup>-‡</sup>	-13.41	-15.75	-13.95	-11.34	-13.19	-15.47	-16.42	-10.59
[ClCH <sub>3</sub> Cl] <sup>-‡</sup> → ClCH <sub>3</sub> ··· Cl <sup>-</sup>	-13.41	-15.75	-13.95	-11.34	-13.19	-15.47	-16.42	-10.59
F <sup>-</sup> ··· CH <sub>3</sub> Cl → [FCH <sub>3</sub> Cl] <sup>-‡</sup>	-3.44	-3.62	-2.44	-1.51	-1.95	-4.17	-3.76	-0.72
[FCH <sub>3</sub> Cl] <sup>-‡</sup> → FCH <sub>3</sub> ··· Cl <sup>-</sup>	-29.42	-31.45	-31.03	-27.78	-33.64	-29.98	-41.57	-27.81
HO <sup>-</sup> ··· CH <sub>3</sub> F → [HOCH <sub>3</sub> F] <sup>-‡</sup>	2.44	5.77	5.23	8.18	3.57	5.17	-5.39	8.29
[HOCH <sub>3</sub> F] <sup>-‡</sup> → HOCH <sub>3</sub> ··· F <sup>-</sup>	-17.66	-16.15	-16.78	-15.18	-17.56	-17.66	-27.45	-12.90
H + N <sub>2</sub> → [HN <sub>2</sub> ] <sup>‡</sup>	-14.36	-14.19	-12.56	-11.29	-12.43	-12.27	-22.94	-12.38
[HN <sub>2</sub> ] <sup>‡</sup> → HN <sub>2</sub>	-10.61	-14.27	-13.34	-14.68	-12.02	-11.67	-13.59	-10.54
H + C <sub>2</sub> H <sub>4</sub> → [HCH <sub>2</sub> CH <sub>2</sub> ] <sup>‡</sup>	-1.72	-4.10	-3.07	-4.00	-1.37	-1.73	-4.05	-1.84
[HCH <sub>2</sub> CH <sub>2</sub> ] <sup>‡</sup> → CH <sub>3</sub> CH <sub>2</sub>	-41.75	-47.12	-45.53	-46.69	-42.27	-43.84	-44.26	-42.59
HCN → [HCN] <sup>‡</sup>	-48.07	-46.40	-46.54	-47.32	-44.92	-45.34	-47.47	-48.75
[HCN] <sup>‡</sup> → HNC	-32.82	-33.35	-33.49	-34.95	-34.11	-33.64	-37.68	-33.39
HO + CH <sub>4</sub> → [HOCH <sub>4</sub> ] <sup>‡</sup>	-6.70	-4.42	-3.72	-1.50	-7.77	-4.88	-26.65	-4.39
[HOCH <sub>4</sub> ] <sup>‡</sup> → CH <sub>3</sub> + H <sub>2</sub> O	-19.60	-15.45	-15.23	-14.13	-19.31	-18.74	-28.81	-17.03
H + OH → [HHO] <sup>‡</sup>	-10.70	-9.73	-8.78	-9.77	-10.00	-8.74	-17.36	-8.03
[HHO] <sup>‡</sup> → O + H <sub>2</sub>	-13.10	-10.15	-9.80	-7.13	-13.07	-10.24	-32.84	-10.01
H + H <sub>2</sub> S → [HH <sub>2</sub> S] <sup>‡</sup>	-3.60	-5.60	-4.17	-4.53	-4.24	-2.62	-11.91	-2.04
[HH <sub>2</sub> S] <sup>‡</sup> → HS + H <sub>2</sub>	-17.30	-17.59	-16.80	-13.27	-18.08	-16.43	-27.17	-16.62
	ref.	PBE-QIDH	ωB97X-2					
H + N <sub>2</sub> O → [HON <sub>2</sub> ] <sup>‡</sup>	-17.13	-20.89	-20.42					
[HON <sub>2</sub> ] <sup>‡</sup> → OH + N <sub>2</sub>	-82.47	-80.28	-82.18					
H + ClH → [HClH] <sup>‡</sup>	-18.00	-18.14	-19.01					
[HClH] <sup>‡</sup> → HCl + H	-18.00	-18.14	-19.01					
CH <sub>3</sub> + FCl → [ClFCH <sub>3</sub> ] <sup>‡</sup>	-6.75	-9.14	-7.71					
[ClFCH <sub>3</sub> ] <sup>‡</sup> → FCH <sub>3</sub> + Cl	-60.00	-63.65	-60.21					
Cl <sup>-</sup> ··· CH <sub>3</sub> Cl → [ClCH <sub>3</sub> Cl] <sup>-‡</sup>	-13.41	-13.68	-12.61					
[ClCH <sub>3</sub> Cl] <sup>-‡</sup> → ClCH <sub>3</sub> ··· Cl <sup>-</sup>	-13.41	-13.68	-12.61					
F <sup>-</sup> ··· CH <sub>3</sub> Cl → [FCH <sub>3</sub> Cl] <sup>-‡</sup>	-3.44	-2.79	-1.91					
[FCH <sub>3</sub> Cl] <sup>-‡</sup> → FCH <sub>3</sub> ··· Cl <sup>-</sup>	-29.42	-31.44	-28.64					
HO <sup>-</sup> ··· CH <sub>3</sub> F → [HOCH <sub>3</sub> F] <sup>-‡</sup>	2.44	5.17	8.47					
[HOCH <sub>3</sub> F] <sup>-‡</sup> → HOCH <sub>3</sub> ··· F <sup>-</sup>	-17.66	-17.15	-12.70					
H + N <sub>2</sub> → [HN <sub>2</sub> ] <sup>‡</sup>	-14.36	-14.81	-16.09					
[HN <sub>2</sub> ] <sup>‡</sup> → HN <sub>2</sub>	-10.61	-12.20	-10.98					
H + C <sub>2</sub> H <sub>4</sub> → [HCH <sub>2</sub> CH <sub>2</sub> ] <sup>‡</sup>	-1.72	-2.91	-3.39					
[HCH <sub>2</sub> CH <sub>2</sub> ] <sup>‡</sup> → CH <sub>3</sub> CH <sub>2</sub>	-41.75	-46.14	-44.69					
HCN → [HCN] <sup>‡</sup>	-48.07	-48.44	-48.48					
[HCN] <sup>‡</sup> → HNC	-32.82	-33.72	-32.75					
HO + CH <sub>4</sub> → [HOCH <sub>4</sub> ] <sup>‡</sup>	-6.70	-6.66	-5.60					
[HOCH <sub>4</sub> ] <sup>‡</sup> → CH <sub>3</sub> + H <sub>2</sub> O	-19.60	-19.22	-18.34					
H + OH → [HHO] <sup>‡</sup>	-10.70	-11.73	-10.83					
[HHO] <sup>‡</sup> → O + H <sub>2</sub>	-13.10	-12.57	-12.66					
H + H <sub>2</sub> S → [HH <sub>2</sub> S] <sup>‡</sup>	-3.60	-4.05	-4.12					
[HH <sub>2</sub> S] <sup>‡</sup> → HS + H <sub>2</sub>	-17.30	-15.04	-17.14					

Table S12: Weak interaction energies (kcal mol<sup>-1</sup>) over the 27 (out of 31) systems included into the NCB31 dataset. All the computations are done at the def2-QZVP level of theory.

	ref.	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L
(NH <sub>3</sub> ) <sub>2</sub>	3.15	5.29	2.30	3.23	2.29	2.40	2.35	2.77
(HF) <sub>2</sub>	4.57	7.39	4.38	4.96	3.90	4.04	4.81	4.41
(H <sub>2</sub> O) <sub>2</sub>	4.97	8.07	4.50	5.32	4.23	4.02	4.92	4.72
NH <sub>3</sub> ...H <sub>2</sub> O	6.41	10.19	5.92	7.02	5.68	5.03	6.34	6.18
(HCONH <sub>2</sub> ) <sub>2</sub>	14.94	21.27	12.10	14.27	11.97	9.75	13.39	14.29
(HCOOH) <sub>2</sub>	16.15	25.13	13.84	16.34	13.94	10.37	16.45	16.37
C <sub>2</sub> H <sub>4</sub> ...F <sub>2</sub>	1.06	4.37	2.44	2.89	0.74	4.45	2.46	1.38
NH <sub>3</sub> ...F <sub>2</sub>	1.81	7.21	4.70	5.12	1.73	5.85	4.52	3.02
C <sub>2</sub> H <sub>2</sub> ...ClF	3.81	10.18	4.29	6.08	3.25	3.07	4.70	5.30
HCN...ClF	4.86	9.70	4.63	5.78	3.51	3.29	4.69	5.13
NH <sub>3</sub> ...Cl <sub>2</sub>	4.88	11.66	6.37	7.80	4.62	5.08	6.35	6.63
H <sub>2</sub> O...ClF	5.36	11.32	6.07	7.30	4.62	4.50	6.25	6.50
NH <sub>3</sub> ...ClF	10.62	23.36	14.41	16.84	11.64	13.77	15.57	13.54
(H <sub>2</sub> S) <sub>2</sub>	1.66	3.37	0.67	1.74	0.90	1.70	0.69	1.30
(HCl) <sub>2</sub>	2.01	3.88	1.08	2.04	1.12	1.55	1.15	1.68
HCl...H <sub>2</sub> S	3.35	6.55	2.71	4.06	2.73	3.07	2.97	3.42
CH <sub>3</sub> Cl...HCl	3.55	6.44	1.88	3.36	1.90	2.32	2.13	3.29
HCN...CH <sub>3</sub> SH	3.59	5.83	2.16	3.50	2.47	4.08	2.31	3.40
CH <sub>3</sub> SH...HCl	4.16	9.22	3.58	5.54	3.63	4.55	4.13	5.04
HeNe	0.04	0.15	-0.09	0.10	0.01	0.10	-0.05	0.02
HeAr	0.06	0.17	-0.14	0.09	0.00	0.04	-0.12	0.03
Ne <sub>2</sub>	0.08	0.25	-0.11	0.13	-0.01	0.97	-0.06	0.07
NeAr	0.13	0.32	-0.18	0.14	-0.04	0.93	-0.16	0.06
CH <sub>4</sub> ...Ne	0.22	0.40	-0.21	0.17	-0.04	1.67	-0.21	0.23
(CH <sub>4</sub> ) <sub>2</sub>	0.51	0.94	-0.82	0.02	-0.44	3.07	-1.03	0.43
(C <sub>2</sub> H <sub>2</sub> ) <sub>2</sub>	1.34	2.09	0.09	0.98	0.48	2.25	-0.05	0.91
(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub>	1.42	2.49	-1.06	0.34	-0.55	2.14	-1.21	1.13
	ref.	M11-L	MN12-L	MN15-L	B3LYP	PBE0	M05	M06
(NH <sub>3</sub> ) <sub>2</sub>	3.15	2.45	2.38	2.57	2.56	3.04	3.18	2.91
(HF) <sub>2</sub>	4.57	3.47	4.04	4.25	4.64	4.79	5.06	4.33
(H <sub>2</sub> O) <sub>2</sub>	4.97	4.15	4.35	4.25	4.83	5.17	5.33	4.85
NH <sub>3</sub> ...H <sub>2</sub> O	6.41	5.31	5.40	5.17	6.19	6.73	6.61	6.34
(HCONH <sub>2</sub> ) <sub>2</sub>	14.94	12.91	12.78	12.08	13.06	14.22	13.40	14.02
(HCOOH) <sub>2</sub>	16.15	14.60	15.24	13.69	15.14	16.53	15.38	16.13
C <sub>2</sub> H <sub>4</sub> ...F <sub>2</sub>	1.06	0.65	0.95	1.91	1.27	1.23	1.67	0.65
NH <sub>3</sub> ...F <sub>2</sub>	1.81	1.48	1.89	2.65	2.64	2.32	2.64	1.63
C <sub>2</sub> H <sub>2</sub> ...ClF	3.81	4.66	4.41	4.82	3.70	4.58	3.98	4.69
HCN...ClF	4.86	3.90	3.95	4.19	4.43	4.79	4.65	5.12
NH <sub>3</sub> ...Cl <sub>2</sub>	4.88	6.07	5.21	5.16	5.33	5.80	5.07	5.65
H <sub>2</sub> O...ClF	5.36	5.64	5.63	5.67	5.58	5.93	5.66	5.94
NH <sub>3</sub> ...ClF	10.62	10.62	11.01	10.39	12.57	13.52	10.80	11.91
(H <sub>2</sub> S) <sub>2</sub>	1.66	1.15	0.94	1.31	0.85	1.48	1.59	1.36
(HCl) <sub>2</sub>	2.01	1.44	1.25	1.60	1.25	1.78	1.95	1.64
HCl...H <sub>2</sub> S	3.35	2.85	2.55	2.67	2.78	3.57	3.53	3.28
CH <sub>3</sub> Cl...HCl	3.55	2.72	2.66	3.21	2.17	2.99	3.18	3.27
HCN...CH <sub>3</sub> SH	3.59	2.87	2.80	3.32	2.55	3.36	3.37	3.44
CH <sub>3</sub> SH...HCl	4.16	4.00	3.88	4.27	3.70	4.89	4.68	4.81
HeNe	0.04	-0.30	-0.09	0.03	-0.04	0.06	0.08	0.08
HeAr	0.06	-0.34	-0.13	0.04	-0.07	0.05	0.09	0.11
Ne <sub>2</sub>	0.08	-0.53	-0.21	0.04	-0.05	0.08	0.14	0.06
NeAr	0.13	-0.57	-0.26	0.10	-0.09	0.07	0.17	0.05
CH <sub>4</sub> ...Ne	0.22	-0.58	-0.21	0.25	-0.10	0.10	0.23	0.13
(CH <sub>4</sub> ) <sub>2</sub>	0.51	-0.12	-0.13	1.11	-0.50	-0.03	0.38	0.20
(C <sub>2</sub> H <sub>2</sub> ) <sub>2</sub>	1.34	0.97	0.86	1.67	0.41	0.95	1.20	0.97
(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub>	1.42	0.94	0.94	2.79	-0.50	0.34	1.02	1.17
	ref.	SOGGA11-X	MN15	BMK	M06-2X	M05-2X	M06-HF	ωB97
(NH <sub>3</sub> ) <sub>2</sub>	3.15	2.60	3.07	2.28	3.06	3.06	2.75	3.65
(HF) <sub>2</sub>	4.57	4.42	4.86	4.27	4.94	5.08	4.70	5.32
(H <sub>2</sub> O) <sub>2</sub>	4.97	4.77	5.18	4.50	5.26	5.34	5.30	5.82
NH <sub>3</sub> ...H <sub>2</sub> O	6.41	6.15	6.42	5.83	6.57	6.59	6.78	7.27
(HCONH <sub>2</sub> ) <sub>2</sub>	14.94	13.89	14.07	13.25	14.54	14.81	15.07	15.62
(HCOOH) <sub>2</sub>	16.15	15.87	16.58	15.58	16.78	17.05	18.31	17.66
C <sub>2</sub> H <sub>4</sub> ...F <sub>2</sub>	1.06	0.14	1.05	-0.25	0.90	0.96	0.64	1.00
NH <sub>3</sub> ...F <sub>2</sub>	1.81	1.04	1.48	0.78	1.41	1.39	0.47	1.85
C <sub>2</sub> H <sub>2</sub> ...ClF	3.81	3.57	4.43	3.39	4.54	4.71	4.38	4.48
HCN...ClF	4.86	4.16	4.65	4.04	4.86	4.86	4.28	5.40

NH <sub>3</sub> ...Cl <sub>2</sub>	4.88	4.57	4.71	4.28	4.98	4.99	4.45	4.86
H <sub>2</sub> O...ClF	5.36	5.21	5.56	4.97	5.87	5.94	5.67	6.27
NH <sub>3</sub> ...ClF	10.62	10.55	10.14	10.73	10.35	11.38	10.78	10.44
(H <sub>2</sub> S) <sub>2</sub>	1.66	1.00	1.66	0.60	1.40	1.42	1.06	1.98
(HCl) <sub>2</sub>	2.01	1.35	1.93	0.99	1.73	1.74	1.23	2.29
HCl...H <sub>2</sub> S	3.35	2.90	3.29	2.49	3.16	3.14	2.78	3.83
CH <sub>3</sub> Cl...HCl	3.55	2.47	3.56	2.24	3.38	3.31	2.96	3.94
HCN...CH <sub>3</sub> SH	3.59	2.73	3.55	2.43	3.57	3.63	3.67	4.01
CH <sub>3</sub> SH...HCl	4.16	3.91	4.86	3.67	4.75	4.74	4.54	5.27
HeNe	0.04	-0.08	0.04	-0.33	0.14	0.04	0.13	-0.04
HeAr	0.06	-0.15	0.06	-0.41	0.13	0.04	0.13	-0.03
Ne <sub>2</sub>	0.08	-0.18	0.06	-0.54	0.17	0.10	0.17	-0.04
NeAr	0.13	-0.31	0.11	-0.67	0.17	0.13	0.15	-0.01
CH <sub>4</sub> ...Ne	0.22	-0.35	0.23	-0.73	0.26	0.22	0.24	0.04
(CH <sub>4</sub> ) <sub>2</sub>	0.51	-0.74	0.78	-0.98	0.44	0.49	0.23	0.50
(C <sub>2</sub> H <sub>2</sub> ) <sub>2</sub>	1.34	0.48	1.47	0.22	1.26	1.34	1.10	1.51
(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub>	1.42	-0.19	2.07	-0.28	1.44	1.36	1.00	1.79
	ref.	$\omega$ B97X	$\omega$ B97XD	N12-SX	MN12-SX	M11	HF	B2-PLYP
(NH <sub>3</sub> ) <sub>2</sub>	3.15	3.63	3.25	3.01	2.68	2.82	1.57	2.85
(HF) <sub>2</sub>	4.57	5.21	4.46	5.19	4.30	4.62	3.72	4.74
(H <sub>2</sub> O) <sub>2</sub>	4.97	5.76	5.15	5.49	4.70	5.14	3.70	5.04
NH <sub>3</sub> ...H <sub>2</sub> O	6.41	7.22	6.76	6.87	5.72	6.29	4.37	6.38
(HCONH <sub>2</sub> ) <sub>2</sub>	14.94	15.42	14.89	14.74	13.29	14.48	10.02	13.93
(HCOOH) <sub>2</sub>	16.15	17.48	16.85	17.46	15.29	16.79	12.07	15.72
C <sub>2</sub> H <sub>4</sub> ...F <sub>2</sub>	1.06	0.94	0.64	1.23	0.82	0.52	-1.17	1.11
NH <sub>3</sub> ...F <sub>2</sub>	1.81	1.76	1.27	2.38	1.50	0.94	-1.14	2.11
C <sub>2</sub> H <sub>2</sub> ...ClF	3.81	4.41	3.70	4.25	3.93	3.55	-0.61	3.84
HCN...ClF	4.86	5.29	4.21	4.81	4.03	4.18	1.77	4.86
NH <sub>3</sub> ...Cl <sub>2</sub>	4.88	5.15	4.88	5.52	4.76	4.03	0.67	5.16
H <sub>2</sub> O...ClF	5.36	6.22	5.31	5.91	5.41	5.31	2.41	5.60
NH <sub>3</sub> ...ClF	10.62	11.02	11.10	13.32	10.04	9.46	2.39	12.18
(H <sub>2</sub> S) <sub>2</sub>	1.66	1.98	1.57	1.27	1.07	1.09	-0.13	1.19
(HCl) <sub>2</sub>	2.01	2.27	1.75	1.66	1.39	1.38	0.17	1.58
HCl...H <sub>2</sub> S	3.35	3.81	3.36	3.34	2.55	2.72	0.75	3.04
CH <sub>3</sub> Cl...HCl	3.55	3.82	3.24	2.89	2.66	3.01	0.43	2.80
HCN...CH <sub>3</sub> SH	3.59	3.96	3.73	3.18	2.97	3.41	1.59	3.06
CH <sub>3</sub> SH...HCl	4.16	5.19	4.87	4.62	3.77	4.26	0.80	4.25
HeNe	0.04	0.02	0.01	-0.07	-0.08	0.00	-0.03	-0.01
HeAr	0.06	0.05	0.01	-0.11	-0.10	-0.01	-0.05	-0.03
Ne <sub>2</sub>	0.08	0.02	-0.01	-0.07	-0.15	-0.02	-0.06	0.00
NeAr	0.13	0.07	0.00	-0.11	-0.17	-0.01	-0.11	-0.01
CH <sub>4</sub> ...Ne	0.22	0.14	0.15	-0.13	-0.11	0.10	-0.11	0.00
(CH <sub>4</sub> ) <sub>2</sub>	0.51	0.60	0.57	-0.34	0.11	0.33	-0.53	-0.10
(C <sub>2</sub> H <sub>2</sub> ) <sub>2</sub>	1.34	1.56	1.38	0.71	1.11	1.11	0.28	0.83
(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub>	1.42	1.67	1.68	0.19	0.97	1.39	-0.87	0.35
	ref.	PBE-QIDH	$\omega$ B97X-2					
(NH <sub>3</sub> ) <sub>2</sub>	3.15	3.09	3.48					
(HF) <sub>2</sub>	4.57	4.72	5.03					
(H <sub>2</sub> O) <sub>2</sub>	4.97	5.20	5.51					
NH <sub>3</sub> ...H <sub>2</sub> O	6.41	6.67	6.91					
(HCONH <sub>2</sub> ) <sub>2</sub>	14.94	14.80	15.06					
(HCOOH) <sub>2</sub>	16.15	16.96	16.55					
C <sub>2</sub> H <sub>4</sub> ...F <sub>2</sub>	1.06	0.82	1.54					
NH <sub>3</sub> ...F <sub>2</sub>	1.81	1.39	2.21					
C <sub>2</sub> H <sub>2</sub> ...ClF	3.81	4.15	4.68					
HCN...ClF	4.86	4.90	5.54					
NH <sub>3</sub> ...Cl <sub>2</sub>	4.88	4.98	5.43					
H <sub>2</sub> O...ClF	5.36	5.50	6.09					
NH <sub>3</sub> ...ClF	10.62	11.88	11.95					
(H <sub>2</sub> S) <sub>2</sub>	1.66	1.55	1.93					
(HCl) <sub>2</sub>	2.01	1.85	2.25					
HCl...H <sub>2</sub> S	3.35	3.47	3.71					
CH <sub>3</sub> Cl...HCl	3.55	3.27	3.88					
HCN...CH <sub>3</sub> SH	3.59	3.58	4.02					
CH <sub>3</sub> SH...HCl	4.16	4.94	5.29					
HeNe	0.04	0.02	0.07					
HeAr	0.06	0.02	0.09					
Ne <sub>2</sub>	0.08	0.03	0.13					
NeAr	0.13	0.04	0.19					
CH <sub>4</sub> ...Ne	0.22	0.07	0.27					
(CH <sub>4</sub> ) <sub>2</sub>	0.51	0.16	0.74					

$(\text{C}_2\text{H}_2)_2$	1.34	1.17	1.66
$(\text{C}_2\text{H}_4)_2$	1.42	0.88	1.82

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Table S13: Density value (a.u.) at the considered critical points for the SiH<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.123448	0.124597	0.124937	0.123559	0.124257	0.124126	0.124429	0.122249	0.120773
(3,-1)	0.123448	0.124597	0.124937	0.123559	0.124257	0.124123	0.124431	0.122249	0.120769
(3,-1)	0.123449	0.124598	0.124938	0.123559	0.124258	0.124124	0.124428	0.122248	0.120767
(3,-1)	0.123449	0.124598	0.124938	0.123559	0.124258	0.124124	0.124428	0.122248	0.120767
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.123448	0.121558	0.116233	0.125301	0.123957	0.126455	0.124913	0.124383	0.122360
(3,-1)	0.123448	0.121558	0.116232	0.125301	0.123956	0.126456	0.124912	0.124382	0.122359
(3,-1)	0.123449	0.121557	0.116233	0.125302	0.123957	0.126455	0.124911	0.124383	0.122360
(3,-1)	0.123449	0.121557	0.116233	0.125302	0.123957	0.126455	0.124911	0.124383	0.122360
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97X-D	N12-SX
(3,-1)	0.123448	0.123300	0.123886	0.126945	0.129481	0.126156	0.125430	0.124618	0.124144
(3,-1)	0.123448	0.123303	0.123885	0.126944	0.129477	0.126158	0.125431	0.124620	0.124144
(3,-1)	0.123449	0.123307	0.123884	0.126947	0.129489	0.126157	0.125429	0.124616	0.124144
(3,-1)	0.123449	0.123307	0.123884	0.126947	0.129489	0.126157	0.125429	0.124616	0.124144
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.123448	0.123283	0.121554	0.124361	0.124805	0.123956	0.126157		
(3,-1)	0.123448	0.123282	0.121551	0.124360	0.124805	0.123956	0.126156		
(3,-1)	0.123449	0.123281	0.121553	0.124361	0.124806	0.123957	0.126156		
(3,-1)	0.123449	0.123281	0.121553	0.124361	0.124806	0.123957	0.126156		

Table S14: Density value (a.u.) at the considered critical points for the S<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.201548	0.196936	0.198962	0.197555	0.200172	0.201376	0.196176	0.191812	0.202840
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.201548	0.203148	0.205976	0.200682	0.199682	0.188644	0.191553	0.203748	0.202710
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97X-D	N12-SX
(3,-1)	0.201548	0.190996	0.200661	0.204643	0.213042	0.199402	0.200434	0.200627	0.198802
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.201548	0.203159	0.196822	0.207376	0.200496	0.200546	0.199402		



Table S15: Density value (a.u.) at the considered critical points for the SiO system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.194177	0.200029	0.196793	0.197285	0.197304	0.198798	0.197487	0.195098	0.191436
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.194177	0.196137	0.192826	0.197419	0.197804	0.199510	0.200324	0.198077	0.197926
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97X-D	N12-SX
(3,-1)	0.194177	0.196708	0.193623	0.194795	0.194099	0.200481	0.199615	0.199178	0.197897
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.194177	0.196118	0.197414	0.197487	0.195318	0.195733	0.200481		

Table S16: Density value (a.u.) at the considered critical points for the C<sub>3</sub>H<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.419079	0.419632	0.422452	0.417912	0.418620	0.417512	0.423724	0.407903	x.xxxxxx
(3,-1)	0.272569	0.263516	0.268412	0.265594	0.269881	0.271156	0.265486	0.271099	0.269628
(3,-1)	0.299148	0.290248	0.297344	0.294231	0.298520	0.299320	0.298114	0.291356	0.287971
(3,-1)	0.287539	0.277362	0.284906	0.281643	0.285945	0.286388	0.285256	0.280658	0.275826
(3,-1)	0.287540	0.277362	0.284907	0.281644	0.285946	0.286388	0.285250	0.280658	0.275827
(3,-1)	0.287540	0.277362	0.284907	0.281644	0.285946	0.286388	0.285250	0.280658	0.275827
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.419079	0.413727	0.409462	0.422854	0.418739	0.412066	0.413661	0.420538	0.416801
(3,-1)	0.272569	0.267342	0.269272	0.270590	0.268527	0.265830	0.268944	0.274426	0.267826
(3,-1)	0.299148	0.291288	0.293690	0.298973	0.296574	0.295711	0.290719	0.301116	0.297116
(3,-1)	0.287539	0.278910	0.281073	0.286444	0.283885	0.283238	0.278631	0.288443	0.283627
(3,-1)	0.287540	0.278911	0.281073	0.286444	0.283886	0.283238	0.278630	0.288444	0.283627
(3,-1)	0.287540	0.278911	0.281073	0.286444	0.283886	0.283238	0.278630	0.288444	0.283627
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97X-D	N12-SX
(3,-1)	0.419079	0.425249	0.422227	0.430918	0.439486	0.410104	0.415351	0.420386	0.419050
(3,-1)	0.272569	0.261631	0.269061	0.270553	0.266650	0.268816	0.269281	0.268653	0.267019
(3,-1)	0.299148	0.293044	0.301074	0.305814	0.314748	0.297784	0.297804	0.297323	0.296595
(3,-1)	0.287539	0.282074	0.287624	0.292719	0.301015	0.285387	0.285410	0.284899	0.283783
(3,-1)	0.287540	0.282081	0.287622	0.292721	0.301023	0.285385	0.285407	0.284893	0.283784
(3,-1)	0.287540	0.282081	0.287622	0.292721	0.301023	0.285385	0.285407	0.284893	0.283784
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.419079	0.418955	0.422636	0.422628	0.421335	0.418542	0.410104		
(3,-1)	0.272569	0.267651	0.267078	0.279857	0.271038	0.270546	0.268816		
(3,-1)	0.299148	0.291330	0.301122	0.305097	0.298987	0.298051	0.297784		
(3,-1)	0.287539	0.278363	0.286283	0.292593	0.287077	0.285997	0.285387		
(3,-1)	0.287540	0.278363	0.286288	0.292594	0.287078	0.285998	0.283848		
(3,-1)	0.287540	0.278363	0.286288	0.292594	0.287078	0.285998	0.283848		

Table S17: Density value (a.u.) at the considered critical points for the HCOCOH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.270180	0.257348	0.262380	0.259866	0.265975	0.268907	0.260391	0.268178	0.264954
(3,-1)	0.430008	0.433008	0.433832	0.431066	0.431956	0.429646	0.429562	0.418422	0.420447
(3,-1)	0.293140	0.281971	0.289318	0.286271	0.291535	0.292754	0.290598	0.284093	0.278043
(3,-1)	0.430008	0.433008	0.433832	0.431066	0.431956	0.429646	0.429562	0.418422	0.420447
(3,-1)	0.293140	0.281971	0.289318	0.286271	0.291535	0.292754	0.290598	0.284093	0.278043
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.270180	0.262975	0.265976	0.266043	0.264557	0.266625	0.266281	0.273448	0.262884
(3,-1)	0.430008	0.416333	0.414171	0.434482	0.431832	0.419263	0.424733	0.433254	0.427024
(3,-1)	0.293140	0.284503	0.287375	0.291695	0.289520	0.289268	0.282897	0.295590	0.289770
(3,-1)	0.430008	0.416333	0.414171	0.434482	0.431832	0.419263	0.424733	0.433254	0.427024
(3,-1)	0.293140	0.284503	0.287375	0.291695	0.289520	0.289268	0.282897	0.295590	0.289770
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97X-D	N12-SX
(3,-1)	0.270180	0.259748	0.266314	0.267793	0.261900	0.266367	0.266219	0.264822	0.263186
(3,-1)	0.430008	0.417785	0.426577	0.437401	0.439881	0.430621	0.431731	0.430605	0.432249
(3,-1)	0.293140	0.287521	0.293039	0.298962	0.305078	0.291415	0.291245	0.290546	0.289893
(3,-1)	0.430008	0.417785	0.426577	0.437401	0.439881	0.430621	0.431731	0.430605	0.432249
(3,-1)	0.293140	0.287521	0.293039	0.298962	0.305078	0.291415	0.291245	0.290546	0.289893
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.270180	0.262626	0.263818	0.281021	0.267487	0.268109	0.266367		
(3,-1)	0.430008	0.419768	0.433486	0.434721	0.432230	0.430433	0.430621		
(3,-1)	0.293140	0.283037	0.292897	0.300556	0.292288	0.291901	0.291415		
(3,-1)	0.430008	0.419768	0.433486	0.434721	0.432230	0.430433	0.430621		
(3,-1)	0.293140	0.283037	0.292897	0.300556	0.292288	0.291901	0.291415		

Table S18: Density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>8</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.090090	0.090731	0.087828	0.090769	0.091230	0.092550	0.091624	0.092964	0.086978
(3,-1)	0.240889	0.230982	0.236103	0.233585	0.238284	0.240183	0.232737	0.239007	0.241144
(3,-1)	0.240889	0.230982	0.236103	0.233585	0.238284	0.240183	0.232737	0.239007	0.241144
(3,-1)	0.240889	0.230982	0.236103	0.233585	0.238284	0.240183	0.232737	0.239007	0.241144
(3,-1)	0.240889	0.230982	0.236103	0.233585	0.238284	0.240183	0.232737	0.239007	0.241144
(3,-1)	0.289137	0.280017	0.286760	0.283764	0.287840	0.288142	0.287269	0.282591	0.276968
(3,-1)	0.287488	0.278430	0.285356	0.282264	0.286294	0.286454	0.285745	0.281325	0.275643
(3,-1)	0.289137	0.280017	0.286760	0.283764	0.287840	0.288142	0.287269	0.282591	0.276968
(3,-1)	0.287488	0.278430	0.285356	0.282264	0.286294	0.286454	0.285745	0.281325	0.275643
(3,-1)	0.289137	0.280017	0.286760	0.283764	0.287840	0.288142	0.287269	0.282591	0.276968
(3,-1)	0.287488	0.278430	0.285356	0.282264	0.286294	0.286454	0.285745	0.281325	0.275643
(3,-1)	0.289137	0.280017	0.286760	0.283764	0.287840	0.288142	0.287269	0.282591	0.276968
(3,-1)	0.287488	0.278430	0.285356	0.282264	0.286294	0.286454	0.285745	0.281325	0.275643
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.090090	0.089627	0.093297	0.088657	0.091445	0.096119	0.091040	0.091624	0.089139
(3,-1)	0.240889	0.238567	0.240375	0.238534	0.236811	0.232441	0.235991	0.243401	0.236102
(3,-1)	0.240889	0.238567	0.240375	0.238534	0.236811	0.232441	0.235991	0.243401	0.236102
(3,-1)	0.240889	0.238567	0.240375	0.238534	0.236811	0.232441	0.235991	0.243401	0.236102
(3,-1)	0.240889	0.238567	0.240375	0.238534	0.236811	0.232441	0.235991	0.243401	0.236102
(3,-1)	0.289137	0.280925	0.282631	0.288282	0.285936	0.285161	0.280763	0.290161	0.285431
(3,-1)	0.287488	0.279158	0.280838	0.286784	0.284339	0.283830	0.279293	0.288455	0.283600
(3,-1)	0.289137	0.280925	0.282631	0.288282	0.285936	0.285161	0.280763	0.290161	0.285431
(3,-1)	0.287488	0.279158	0.280838	0.286784	0.284339	0.283830	0.279293	0.288455	0.283600
(3,-1)	0.289137	0.280925	0.282631	0.288282	0.285936	0.285161	0.280763	0.290161	0.285431
(3,-1)	0.287488	0.279158	0.280838	0.286784	0.284339	0.283830	0.279293	0.288455	0.283600

Table S19: Density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>8</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97X-D	N12-SX
(3,+1)	0.090090	0.093059	0.092719	0.091058	0.092034	0.094153	0.092296	0.091390	0.090946
(3,-1)	0.240889	0.230438	0.235750	0.237903	0.233693	0.237516	0.237725	0.236749	0.235214
(3,-1)	0.240889	0.230438	0.235750	0.237903	0.233693	0.237516	0.237725	0.236749	0.235214
(3,-1)	0.240889	0.230438	0.235750	0.237903	0.233693	0.237516	0.237725	0.236749	0.235214
(3,-1)	0.240889	0.230438	0.235750	0.237903	0.233693	0.237516	0.237725	0.236749	0.235214
(3,-1)	0.289137	0.283812	0.289361	0.294556	0.302461	0.287034	0.287096	0.286669	0.285856
(3,-1)	0.287488	0.282261	0.287767	0.292868	0.300823	0.285410	0.285487	0.285082	0.284239
(3,-1)	0.289137	0.283812	0.289361	0.294556	0.302461	0.287034	0.287096	0.286669	0.285856
(3,-1)	0.287488	0.282261	0.287767	0.292868	0.300823	0.285410	0.285487	0.285082	0.284239
(3,-1)	0.289137	0.283812	0.289361	0.294556	0.302461	0.287034	0.287096	0.286669	0.285856
(3,-1)	0.287488	0.282261	0.287767	0.292868	0.300823	0.285410	0.285487	0.285082	0.284239
(3,-1)	0.289137	0.283812	0.289361	0.294556	0.302461	0.287034	0.287096	0.286669	0.285856
(3,-1)	0.287488	0.282261	0.287767	0.292868	0.300823	0.285410	0.285487	0.285082	0.284239
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.090090	0.090668	0.092936	0.090522	0.089441	0.091711	0.941526		
(3,-1)	0.240889	0.237434	0.233037	0.249585	0.239223	0.239085	0.237516		
(3,-1)	0.240889	0.237434	0.233037	0.249585	0.239223	0.239085	0.237516		
(3,-1)	0.240889	0.237434	0.233037	0.249585	0.239223	0.239085	0.237516		
(3,-1)	0.240889	0.237434	0.233037	0.249585	0.239223	0.239085	0.237516		
(3,-1)	0.289137	0.280033	0.287851	0.293748	0.288802	0.287858	0.287033		
(3,-1)	0.287488	0.278387	0.286037	0.292032	0.287240	0.286179	0.285409		
(3,-1)	0.289137	0.280033	0.287851	0.293748	0.288802	0.287858	0.287033		
(3,-1)	0.287488	0.278387	0.286037	0.292032	0.287240	0.286179	0.285409		
(3,-1)	0.289137	0.280033	0.287851	0.293748	0.288802	0.287858	0.287033		
(3,-1)	0.287488	0.278387	0.286037	0.292032	0.287240	0.286179	0.285409		
(3,-1)	0.289137	0.280033	0.287851	0.293748	0.288802	0.287858	0.287033		
(3,-1)	0.287488	0.278387	0.286037	0.292032	0.287240	0.286179	0.285409		

Table S20: Density value (a.u.) at the considered critical points for the  $[\text{H}_3\text{CHOH}]^\ddagger$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.142712	0.143322	0.144594	0.144714	0.144135	0.143100	0.143749	0.141772	0.144842
(3,-1)	0.191370	0.182431	0.189356	0.187151	0.190951	0.192438	0.189801	0.196565	0.195058
(3,-1)	0.289721	0.280360	0.287604	0.284480	0.288583	0.288731	0.288068	0.282702	0.277634
(3,-1)	0.289252	0.280058	0.287255	0.284142	0.288178	0.288239	0.287705	0.282350	0.277222
(3,-1)	0.289336	0.279927	0.287178	0.284057	0.288192	0.288356	0.287652	0.282362	0.277313
(3,-1)	0.372669	0.365448	0.376352	0.374432	0.377135	0.378812	0.378063	0.377973	0.367060
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.142712	0.143068	0.145315	0.143789	0.143686	0.143471	0.142216	0.143100	0.141948
(3,-1)	0.191370	0.187737	0.189988	0.190804	0.189386	0.192317	0.191984	0.192438	0.188229
(3,-1)	0.289721	0.280756	0.283632	0.288964	0.286473	0.285943	0.280897	0.288731	0.286401
(3,-1)	0.289252	0.280327	0.283225	0.288561	0.286066	0.285555	0.280520	0.288239	0.285913
(3,-1)	0.289336	0.280369	0.283220	0.288563	0.286080	0.285567	0.280551	0.288356	0.286025
(3,-1)	0.372669	0.361766	0.367052	0.376269	0.374931	0.377907	0.373739	0.378812	0.370788
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97X-D	N12-SX
(3,-1)	0.142712	0.142072	0.141995	0.143325	0.141277	0.143343	0.143349	0.143614	0.143957
(3,-1)	0.191370	0.187914	0.188122	0.188091	0.180502	0.191347	0.190732	0.189831	0.188819
(3,-1)	0.289721	0.284252	0.290393	0.295602	0.303696	0.288053	0.287916	0.287326	0.286404
(3,-1)	0.289252	0.283879	0.289921	0.295162	0.303270	0.287532	0.287416	0.286869	0.285981
(3,-1)	0.289336	0.283867	0.290021	0.295211	0.303325	0.287696	0.287552	0.286953	0.286023
(3,-1)	0.372669	0.372687	0.371533	0.374525	0.370468	0.379512	0.377998	0.376928	0.374204
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.142712	0.141489	0.143786	0.137059	0.143857	0.143334	0.143037		
(3,-1)	0.191370	0.190462	0.185534	0.202523	0.189960	0.189852	0.187723		
(3,-1)	0.289721	0.280643	0.289534	0.293470	0.289677	0.288572	0.287563		
(3,-1)	0.289252	0.280170	0.288867	0.292793	0.289262	0.288133	0.287096		
(3,-1)	0.289336	0.280293	0.289190	0.293151	0.289273	0.288186	0.287169		
(3,-1)	0.372669	0.365584	0.379929	0.377900	0.373622	0.372446	0.370054		

Table S21: Density value (a.u.) at the considered critical points for the [HHO]<sup>‡</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.187894	0.187711	0.189824	0.190401	0.188266	0.189471	0.189187	0.190660	0.191138
(3,-1)	0.158457	0.153766	0.158862	0.157412	0.161014	0.159391	0.162839	0.162275	0.163253
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.187894	0.190988	0.192363	0.189072	0.189632	0.189027	0.189337	0.189471	0.189552
(3,-1)	0.158457	0.156373	0.154325	0.159326	0.158119	0.164575	0.161199	0.159391	0.158181
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97X-D	N12-SX
(3,-1)	0.187894	0.187033	0.185104	0.184584	0.178059	0.188253	0.188096	0.188428	0.188522
(3,-1)	0.158457	0.158484	0.159505	0.160466	0.153350	0.161065	0.160538	0.160408	0.160002
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.187894	0.187089	0.185985	0.183685	0.189361	0.189409	0.188000		
(3,-1)	0.158457	0.161045	0.156596	0.162621	0.158204	0.157665	0.156478		

Table S22: Density value (a.u.) at the considered critical points for the [HSH]<sup>‡</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.222647	0.217004	0.221004	0.218845	0.221759	0.221758	0.220410	0.219247	0.217089
(3,-1)	0.177417	0.170349	0.174244	0.173142	0.175312	0.176503	0.174091	0.176625	0.180751
(3,-1)	0.085109	0.087071	0.088368	0.087891	0.088039	0.086071	0.087504	0.087750	0.088012
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.222647	0.217150	0.218522	0.222308	0.220553	0.220101	0.218574	0.221758	0.220502
(3,-1)	0.177417	0.171993	0.174587	0.175509	0.174882	0.174772	0.174499	0.176503	0.173606
(3,-1)	0.085109	0.087376	0.088360	0.087612	0.086871	0.084975	0.085724	0.086071	0.085568
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97X-D	N12-SX
(3,-1)	0.222647	0.218302	0.222987	0.226277	0.234285	0.221145	0.221368	0.221079	0.220382
(3,-1)	0.177417	0.170235	0.175037	0.176232	0.172172	0.175766	0.175475	0.174577	0.174407
(3,-1)	0.085109	0.085876	0.084032	0.084700	0.082108	0.086009	0.086522	0.087117	0.087572
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.222647	0.217590	0.220742	0.226556	0.222585	0.221922	0.220456		
(3,-1)	0.177417	0.176118	0.173406	0.182609	0.176711	0.177032	0.175987		
(3,-1)	0.085109	0.084806	0.084406	0.082148	0.086216	0.085153	0.084661		



Table S23: Density value (a.u.) at the considered critical points for the water...water  $0.90R_e$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.033564	0.036009	0.035196	0.035391	0.034385	0.033909	0.034532	0.033639	0.032190
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.033564	0.032410	0.032521	0.034529	0.034533	0.033576	0.033440	0.033909	0.034014
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.033564	0.033452	0.033269	0.033611	0.034774	0.034187	0.034125	0.034254	0.033959
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.033564	0.032688	0.033817	0.032113	0.034174	0.033877	0.033608		

Table S24: Density value (a.u.) at the considered critical points for the water...water  $1.00R_e$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.020607	0.022468	0.021862	0.021872	0.021048	0.021155	0.021267	0.021006	0.020117
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.020607	0.020227	0.020036	0.021346	0.021212	0.021126	0.021151	0.021155	0.021058
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.020607	0.020756	0.020409	0.020625	0.020742	0.021352	0.021250	0.021260	0.020878
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.020607	0.020309	0.020955	0.019579	0.021095	0.020761	0.021069		

Table S25: Density value (a.u.) at the considered critical points for the water...water  $1.50R_e$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.002063	0.002453	0.002435	0.002374	0.002120	0.002041	0.002241	0.001874	0.001994
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.002063	0.001993	0.002287	0.002282	0.002182	0.002171	0.001970	0.002041	0.002255
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.002063	0.002178	0.002047	0.002112	0.001981	0.002255	0.002213	0.002088	0.002210
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.002063	0.002012	0.001958	0.001891	0.002229	0.002071	0.002193		

Table S26: Density value (a.u.) at the considered critical points for the methane...methane  $0.90R_e$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.004655	0.005472	0.004802	0.004904	0.004647	0.004990	0.004720	0.004606	0.004644
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.004655	0.004902	0.004738	0.004760	0.004814	0.004563	0.005116	0.004990	0.005077
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97X-D	N12-SX
(3,-1)	0.004655	0.005107	0.005222	0.005080	0.005447	0.005094	0.005003	0.004923	0.004749
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.004655	0.005059	0.004995	0.004410	0.004755	0.004756	0.004746		

Table S27: Density value (a.u.) at the considered critical points for the methane...methane  $1.00R_e$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.002244	0.002722	0.002377	0.002403	0.002223	0.002494	0.002275	0.001996	0.002406
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.002244	0.002351	0.002439	0.002334	0.002325	0.002299	0.002356	0.002494	0.002524
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97X-D	N12-SX
(3,-1)	0.002244	0.002624	0.002497	0.002431	0.002630	0.002554	0.002490	0.002364	0.002369
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.002244	0.002472	0.002366	0.002107	0.002324	0.002277	0.002344		

Table S28: Density value (a.u.) at the considered critical points for the methane...methane  $1.50R_e$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.000055	0.000075	0.000071	0.000072	0.000060	0.000054	0.000070	0.000040	0.000050
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.000055	0.000050	0.000063	0.000064	0.000062	0.000067	0.000055	0.000054	0.000061
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97X-D	N12-SX
(3,-1)	0.000055	0.000050	0.000063	0.000059	0.000075	0.000055	0.000058	0.000057	0.000059
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.000055	0.000058	0.000054	0.000050	0.000062	0.000056	0.000061		

Table S29: Density value (a.u.) at the considered critical points for the H<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.274997	0.267080	0.276332	0.273651	0.276685	0.271245	0.280272	0.268693	0.274736
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.274997	0.271476	0.278348	0.276384	0.274098	0.280938	0.271407	0.276224	0.279935
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.274997	0.274911	0.281855	0.282752	0.288134	0.277091	0.276244	0.275983	0.275753
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.274997	0.268443	0.276264	0.275447	0.276383	0.274968	0.274203		

Table S30: Density value (a.u.) at the considered critical points for the LiH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.036594	0.038320	0.037108	0.037607	0.037427	0.038354	0.036894	0.036693	0.029610
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.036594	0.032950	0.035247	0.037578	0.037989	0.034704	0.036253	0.037830	0.036378
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.036594	0.038392	0.037322	0.036979	0.037216	0.037469	0.037448	0.037401	0.038079
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.036594	0.034522	0.037429	0.037282	0.037358	0.037806	0.037296		



Table S31: Density value (a.u.) at the considered critical points for the BeH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.092636	0.095594	0.094979	0.094669	0.093219	0.087114	0.096233	0.093650	0.088930
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.092636	0.088640	0.085274	0.095126	0.094636	0.097205	0.094742	0.094723	0.090330
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.092636	0.096956	0.094824	0.092797	0.086301	0.095133	0.094151	0.094514	0.095076
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.092636	0.093454	0.087078	0.093726	0.094426	0.094077	0.092862		

Table S32: Density value (a.u.) at the considered critical points for the  ${}^2\text{CH}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.281771	0.274565	0.280655	0.278361	0.281937	0.274799	0.282375	0.276729	0.270257
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.281771	0.277034	0.278482	0.281988	0.280226	0.284843	0.278871	0.281930	0.282977
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.281771	0.278158	0.285025	0.287656	0.292963	0.282375	0.281911	0.281057	0.280499
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.281771	0.273704	0.287296	0.286353	0.282706	0.282150	0.281179		

Table S33: Density value (a.u.) at the considered critical points for the  ${}^3\text{CH}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.291141	0.283427	0.289803	0.287547	0.289922	0.282368	0.290850	0.287625	0.287459
(3,-1)	0.291141	0.283427	0.289803	0.287547	0.289922	0.282368	0.290850	0.287625	0.287459
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.291141	0.289711	0.287013	0.290815	0.289038	0.290860	0.287758	0.290129	0.294464
(3,-1)	0.291141	0.289711	0.287013	0.290815	0.289038	0.290860	0.287758	0.290129	0.294464
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.291141	0.285035	0.294599	0.294343	0.303091	0.289223	0.289379	0.289105	0.288163
(3,-1)	0.291141	0.285035	0.294599	0.294343	0.303091	0.289223	0.289379	0.289105	0.288163
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.291141	0.284584	0.297330	0.295070	0.291427	0.290739	0.289527		
(3,-1)	0.291141	0.284584	0.297330	0.295070	0.291427	0.290739	0.289527		

Table S34: Density value (a.u.) at the considered critical points for the  ${}^1\text{CH}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.284462	0.276675	0.283369	0.280645	0.284519	0.277105	0.284618	0.278799	0.272307
(3,-1)	0.284462	0.276675	0.283369	0.280645	0.284519	0.277105	0.284618	0.278799	0.272307
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.284462	0.276034	0.279423	0.284669	0.282546	0.283690	0.276933	0.284715	0.281786
(3,-1)	0.284462	0.276034	0.279423	0.284669	0.282546	0.283690	0.276933	0.284715	0.281786
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.284462	0.281005	0.286306	0.292574	0.299977	0.284364	0.284121	0.283449	0.282763
(3,-1)	0.284462	0.281005	0.286306	0.292574	0.299977	0.284364	0.284121	0.283449	0.282763
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.284462	0.275505	0.286091	0.289323	0.285220	0.284392	0.283372		
(3,-1)	0.284462	0.275505	0.286091	0.289323	0.285220	0.284392	0.283372		

Table S35: Density value (a.u.) at the considered critical points for the  $\text{CH}_3^\bullet$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.293247	0.284773	0.291527	0.288640	0.292116	0.284543	0.292464	0.285366	0.283008
(3,-1)	0.293247	0.284773	0.291527	0.288640	0.292116	0.284543	0.292464	0.285366	0.283008
(3,-1)	0.293247	0.284773	0.291527	0.288640	0.292116	0.284543	0.292464	0.285366	0.283008
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.293247	0.286930	0.288586	0.292664	0.290332	0.289801	0.284288	0.292205	0.292503
(3,-1)	0.293247	0.286930	0.288586	0.292664	0.290332	0.289801	0.284288	0.292205	0.292503
(3,-1)	0.293247	0.286930	0.288586	0.292664	0.290332	0.289801	0.284288	0.292205	0.292503
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.293247	0.287798	0.295068	0.298808	0.308193	0.291474	0.291376	0.290946	0.290094
(3,-1)	0.293247	0.287798	0.295068	0.298808	0.308193	0.291474	0.291376	0.290946	0.290094
(3,-1)	0.293247	0.287798	0.295068	0.298808	0.308193	0.291474	0.291376	0.290946	0.290094
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.293247	0.286026	0.294873	0.296850	0.293354	0.292297	0.291224		
(3,-1)	0.293247	0.286026	0.294873	0.296850	0.293354	0.292297	0.291220		
(3,-1)	0.293247	0.286026	0.294873	0.296850	0.293354	0.292297	0.291220		

Table S36: Density value (a.u.) at the considered critical points for the CH<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.284125	0.274827	0.281997	0.278897	0.282876	0.274541	0.282325	0.278053	0.273111
(3,-1)	0.284125	0.274827	0.281997	0.278897	0.282876	0.274541	0.282325	0.278053	0.273111
(3,-1)	0.284125	0.274827	0.281997	0.278897	0.282876	0.274541	0.282325	0.278053	0.273111
(3,-1)	0.284125	0.274827	0.281997	0.278897	0.282876	0.274541	0.282325	0.278053	0.273111
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.284125	0.275970	0.278134	0.283315	0.280850	0.280417	0.276060	0.283058	0.280690
(3,-1)	0.284125	0.275970	0.278134	0.283315	0.280850	0.280417	0.276060	0.283058	0.280690
(3,-1)	0.284125	0.275970	0.278134	0.283315	0.280850	0.280417	0.276060	0.283058	0.280690
(3,-1)	0.284125	0.275970	0.278134	0.283315	0.280850	0.280417	0.276060	0.283058	0.280690
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.284125	0.279004	0.284585	0.289429	0.297732	0.282021	0.282022	0.281582	0.280712
(3,-1)	0.284125	0.279004	0.284585	0.289429	0.297732	0.282021	0.282022	0.281582	0.280712
(3,-1)	0.284125	0.279004	0.284585	0.289429	0.297732	0.282021	0.282022	0.281582	0.280712
(3,-1)	0.284125	0.279004	0.284585	0.289429	0.297732	0.282021	0.282022	0.281582	0.280712
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.284125	0.275551	0.282402	0.288493	0.283919	0.282847	0.281636		
(3,-1)	0.284125	0.275551	0.282402	0.288493	0.283919	0.282847	0.281636		
(3,-1)	0.284125	0.275551	0.282402	0.288493	0.283919	0.282847	0.281636		
(3,-1)	0.284125	0.275551	0.282402	0.288493	0.283919	0.282847	0.281636		

Table S37: Density value (a.u.) at the considered critical points for the  $^3\text{NH}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.337355	0.328952	0.337111	0.335376	0.338789	0.330111	0.339340	0.328156	0.321852
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.337355	0.320576	0.330433	0.338252	0.337167	0.336797	0.327377	0.340090	0.333415
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.337355	0.334032	0.340220	0.342977	0.347760	0.340155	0.339075	0.337806	0.336545
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.337355	0.329013	0.338404	0.343391	0.338252	0.338020	0.336200		

Table S38: Density value (a.u.) at the considered critical points for the  $\text{NH}_2^\bullet$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.341649	0.332871	0.341795	0.339442	0.343253	0.333927	0.343137	0.340861	0.332845
(3,-1)	0.341649	0.332871	0.341795	0.339442	0.343253	0.333927	0.343137	0.340861	0.332845
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.341649	0.327771	0.334349	0.342777	0.341086	0.344456	0.337410	0.344500	0.337309
(3,-1)	0.341649	0.327771	0.334349	0.342777	0.341086	0.344456	0.337410	0.344500	0.337309
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.341649	0.337670	0.343267	0.348468	0.353798	0.344298	0.343147	0.341749	0.340280
(3,-1)	0.341649	0.337670	0.343267	0.348468	0.353798	0.344298	0.343147	0.341749	0.340280
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.341649	0.331529	0.344394	0.347655	0.342317	0.341525	0.339907		
(3,-1)	0.341649	0.331529	0.344394	0.347655	0.342317	0.341525	0.339907		



Table S39: Density value (a.u.) at the considered critical points for the NH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.345392	0.336506	0.346077	0.343292	0.347277	0.337444	0.346669	0.346141	0.338615
(3,-1)	0.345392	0.336506	0.346077	0.343292	0.347277	0.337444	0.346669	0.346141	0.338615
(3,-1)	0.345392	0.336506	0.346077	0.343292	0.347277	0.337444	0.346669	0.346141	0.338615
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.345392	0.332425	0.337776	0.346904	0.344790	0.347462	0.341779	0.348529	0.340598
(3,-1)	0.345392	0.332425	0.337776	0.346904	0.344790	0.347462	0.341779	0.348529	0.340598
(3,-1)	0.345392	0.332425	0.337776	0.346904	0.344790	0.347462	0.341779	0.348529	0.340598
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.345392	0.340526	0.346560	0.351342	0.355626	0.348005	0.346889	0.345403	0.343853
(3,-1)	0.345392	0.340526	0.346560	0.351342	0.355626	0.348005	0.346889	0.345403	0.343853
(3,-1)	0.345392	0.340526	0.346560	0.351342	0.355626	0.348005	0.346889	0.345403	0.343853
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.345392	0.335326	0.349095	0.351640	0.345968	0.344748	0.343189		
(3,-1)	0.345392	0.335326	0.349095	0.351640	0.345968	0.344748	0.343192		
(3,-1)	0.345392	0.335326	0.349095	0.351640	0.345968	0.344748	0.343192		

Table S40: Density value (a.u.) at the considered critical points for the OH<sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.363327	0.355975	0.366105	0.364632	0.367029	0.360390	0.368003	0.368010	0.356979
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.363327	0.351607	0.357488	0.365975	0.365029	0.368441	0.364132	0.368594	0.360943
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.363327	0.363239	0.362078	0.365524	0.361681	0.369377	0.368001	0.367066	0.364331
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.363327	0.355815	0.369102	0.367246	0.364236	0.363309	0.361117		

Table S41: Density value (a.u.) at the considered critical points for the H<sub>2</sub>O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.367994	0.361057	0.371746	0.369806	0.372214	0.365720	0.373084	0.372908	0.361953
(3,-1)	0.367994	0.361057	0.371746	0.369806	0.372214	0.365720	0.373084	0.372908	0.361953
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.367994	0.358030	0.362319	0.371434	0.369994	0.371403	0.368328	0.373795	0.366414
(3,-1)	0.367994	0.358030	0.362319	0.371434	0.369994	0.371403	0.368328	0.373795	0.366414
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.367994	0.367748	0.366710	0.369430	0.366440	0.374715	0.373204	0.372080	0.369371
(3,-1)	0.367994	0.367748	0.366710	0.369430	0.366440	0.374715	0.373204	0.372080	0.369371
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.367994	0.361618	0.375450	0.372303	0.368884	0.367470	0.365350		
(3,-1)	0.367994	0.361618	0.375450	0.372303	0.368884	0.367470	0.365350		

Table S42: Density value (a.u.) at the considered critical points for the HF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.364639	0.359809	0.370697	0.369791	0.370133	0.368749	0.370143	0.372039	0.358472
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.364639	0.359159	0.362594	0.368853	0.368180	0.367404	0.368559	0.370417	0.367977
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.364639	0.366193	0.362321	0.362322	0.357087	0.372286	0.371095	0.370597	0.367954
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.364639	0.360940	0.369706	0.364318	0.365532	0.363901	0.361828		

Table S43: Density value (a.u.) at the considered critical points for the Li<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.012144	0.012649	0.012802	0.012372	0.012451	0.010659	0.011328	0.012517	0.014819
(3,-1)	0.012144	0.012649	0.012802	0.012372	0.012451	0.010659	0.011328	0.012517	0.014819
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.012144	0.076261	0.012554	0.012911	0.012416	0.011608	0.012155	0.012655	0.013151
(3,-1)	0.012144		0.012554	0.012911	0.012416	0.011608	0.012155	0.012655	0.013151
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.012144	0.013285	0.012570	0.012851	0.012238	0.013278	0.013208	0.012915	0.011964
(3,-1)	0.012144	0.013285	0.012570	0.012851	0.012238	0.013278	0.013208	0.012915	0.011964
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.012144	0.077621	0.009217	0.012154	0.012656	0.012330	0.012180		
(3,-1)	0.012144		0.009217	0.012154	0.012656	0.012330	0.012180		

Table S44: Density value (a.u.) at the considered critical points for the LiF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.077100	0.080545	0.078044	0.078596	0.078039	0.075897	0.077017	0.077975	0.076575
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.077100	0.406296	0.076094	0.078175	0.078573	0.077193	0.078300	0.077946	0.078535
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.077100	0.078586	0.078536	0.078920	0.079418	0.077833	0.077961	0.078199	0.077949
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.077100	0.410966	0.078197	0.077233	0.077590	0.077898	0.076977		

Table S45: Density value (a.u.) at the considered critical points for the C<sub>2</sub>H<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.411162	0.411938	0.414409	0.409993	0.410721	0.415574	0.415311	0.400311	0.287015
(3,-1)	0.298210	0.289529	0.296627	0.293545	0.297837	0.289486	0.297407	0.290500	0.287015
(3,-1)	0.298210	0.289529	0.296627	0.293545	0.297837	0.289486	0.297407	0.290500	0.287015
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.411162	0.349798	0.403457	0.414846	0.410838	0.404002	0.405461	0.409552	0.408678
(3,-1)	0.298210	0.283894	0.293474	0.298253	0.295885	0.295041	0.289856	0.298707	0.296611
(3,-1)	0.298210	0.283894	0.293474	0.298253	0.295885	0.295041	0.289856	0.298707	0.296611
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.411162	0.415397	0.414162	0.423028	0.430312	0.402410	0.407550	0.412322	0.410875
(3,-1)	0.298210	0.292312	0.300217	0.304955	0.313291	0.297216	0.297194	0.296676	0.295944
(3,-1)	0.298210	0.292312	0.300217	0.304955	0.313291	0.297216	0.297194	0.296676	0.295944
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.411162	0.351199	0.415049	0.414948	0.413346	0.410642	0.407537		
(3,-1)	0.298210	0.282971	0.300492	0.304467	0.298157	0.297246	0.295780		
(3,-1)	0.298210	0.282971	0.300492	0.304467	0.298157	0.297246	0.295780		

Table S46: Density value (a.u.) at the considered critical points for the H<sub>2</sub>C=CH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.355264	0.346222	0.352116	0.347693	0.351913	0.346710	0.349950	0.348476	0.355470
(3,-1)	0.292033	0.282723	0.289586	0.286502	0.290739	0.282010	0.290201	0.284396	0.279342
(3,-1)	0.292033	0.282723	0.289586	0.286502	0.290739	0.282010	0.290201	0.284396	0.279342
(3,-1)	0.292033	0.282723	0.289586	0.286502	0.290739	0.282010	0.290201	0.284396	0.279342
(3,-1)	0.292033	0.282723	0.289586	0.286502	0.290739	0.282010	0.290201	0.284396	0.279342
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.355264	0.246187	0.348769	0.354242	0.350718	0.343785	0.348211	0.353056	0.349747
(3,-1)	0.292033	0.276470	0.286100	0.291254	0.288858	0.287690	0.282857	0.291333	0.288885
(3,-1)	0.292033	0.276470	0.286100	0.291254	0.288858	0.287690	0.282857	0.291333	0.288885
(3,-1)	0.292033	0.276470	0.286100	0.291254	0.288858	0.287690	0.282857	0.291333	0.288885
(3,-1)	0.292033	0.276470	0.286100	0.291254	0.288858	0.287690	0.282857	0.291333	0.288885
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.355264	0.347386	0.353252	0.358151	0.358231	0.347496	0.350233	0.351774	0.349580
(3,-1)	0.292033	0.286709	0.292540	0.297845	0.305851	0.290077	0.290133	0.289652	0.288800
(3,-1)	0.292033	0.286709	0.292540	0.297845	0.305851	0.290077	0.290133	0.289652	0.288800
(3,-1)	0.292033	0.286709	0.292540	0.297845	0.305851	0.290077	0.290133	0.289652	0.288800
(3,-1)	0.292033	0.286709	0.292540	0.297845	0.305851	0.290077	0.290133	0.289652	0.288800
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.355264	0.245695	0.353306	0.363461	0.354632	0.353106	0.351810		
(3,-1)	0.292033	0.275765	0.291706	0.297494	0.291791	0.290880	0.289528		
(3,-1)	0.292033	0.275765	0.291706	0.297494	0.291791	0.290880	0.289528		
(3,-1)	0.292033	0.275765	0.291706	0.297494	0.291791	0.290880	0.289528		
(3,-1)	0.292033	0.275765	0.291706	0.297494	0.291791	0.290880	0.289528		



Table S47: Density value (a.u.) at the considered critical points for the H<sub>3</sub>C–CH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.249783	0.238918	0.244826	0.241955	0.246885	0.238510	0.241663	0.248628	0.248206
(3,-1)	0.284580	0.275402	0.282338	0.279291	0.283269	0.275445	0.282660	0.278517	0.273181
(3,-1)	0.284580	0.275402	0.282338	0.279291	0.283269	0.275445	0.282660	0.278517	0.273181
(3,-1)	0.284580	0.275402	0.282338	0.279291	0.283269	0.275445	0.282660	0.278517	0.273181
(3,-1)	0.284580	0.275402	0.282338	0.279291	0.283269	0.275445	0.282660	0.278517	0.273181
(3,-1)	0.284580	0.275402	0.282338	0.279291	0.283269	0.275445	0.282660	0.278517	0.273181
(3,-1)	0.284580	0.275402	0.282338	0.279291	0.283269	0.275445	0.282660	0.278517	0.273181
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.249783	0.467389	0.248547	0.247241	0.245201	0.242444	0.245190	0.248799	0.244635
(3,-1)	0.284580		0.278379	0.283722	0.281313	0.280881	0.276482	0.283482	0.280918
(3,-1)	0.284580		0.278379	0.283722	0.281313	0.280881	0.276482	0.283482	0.280918
(3,-1)	0.284580		0.278379	0.283722	0.281313	0.280881	0.276482	0.283482	0.280918
(3,-1)	0.284580		0.278379	0.283722	0.281313	0.280881	0.276482	0.283482	0.280918
(3,-1)	0.284580		0.278379	0.283722	0.281313	0.280881	0.276482	0.283482	0.280918
(3,-1)	0.284580		0.278379	0.283722	0.281313	0.280881	0.276482	0.283482	0.280918
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.249783	0.239444	0.245309	0.246902	0.243060	0.246407	0.246460	0.245418	0.243594
(3,-1)	0.284580	0.279467	0.284837	0.289762	0.297769	0.282470	0.282490	0.282037	0.281174
(3,-1)	0.284580	0.279467	0.284837	0.289762	0.297769	0.282470	0.282490	0.282037	0.281174
(3,-1)	0.284580	0.279467	0.284837	0.289762	0.297769	0.282470	0.282490	0.282037	0.281174
(3,-1)	0.284580	0.279467	0.284837	0.289762	0.297769	0.282470	0.282490	0.282037	0.281174
(3,-1)	0.284580	0.279467	0.284837	0.289762	0.297769	0.282470	0.282490	0.282037	0.281174
(3,-1)	0.284580	0.279467	0.284837	0.289762	0.297769	0.282470	0.282490	0.282037	0.281174
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.249783	0.471338	0.242434	0.258650	0.248149	0.247791	0.246744		
(3,-1)	0.284580		0.282706	0.288974	0.284311	0.283285	0.281994		
(3,-1)	0.284580		0.282706	0.288974	0.284311	0.283285	0.281992		
(3,-1)	0.284580		0.282706	0.288974	0.284311	0.283285	0.281991		
(3,-1)	0.284580		0.282706	0.288974	0.284311	0.283285	0.281994		
(3,-1)	0.284580		0.282706	0.288974	0.284311	0.283285	0.281991		
(3,-1)	0.284580		0.282706	0.288974	0.284311	0.283285	0.281991		

Table S48: Density value (a.u.) at the considered critical points for the CN<sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.477528	0.477612	0.475695	0.473092	0.474415	0.481759	0.477568	0.465906	0.467845
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.477528	0.457107	0.462164	0.478205	0.477404	0.466897	0.480161	0.469916	0.479651
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.477528	0.463290	0.487377	0.487902	0.514295	0.470645	0.477307	0.479249	0.482372
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.477528	0.464119	0.481512	0.507452	0.469659	0.473792	0.467984		

Table S49: Density value (a.u.) at the considered critical points for the HCN system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.473197	0.477676	0.478118	0.474031	0.475079	0.480003	0.477331	0.458135	0.468267
(3,-1)	0.297124	0.287998	0.295382	0.292361	0.296915	0.288604	0.296285	0.289537	0.286232
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.473197	0.467239	0.455996	0.478855	0.474998	0.465278	0.469228	0.472216	0.470938
(3,-1)	0.297124		0.293309	0.297082	0.294802	0.294701	0.288976	0.297997	0.295902
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.473197	0.461831	0.475033	0.488197	0.492592	0.469488	0.473951	0.476223	0.477616
(3,-1)	0.297124	0.290760	0.298914	0.303487	0.310330	0.296372	0.296233	0.295657	0.294914
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.473197	0.472160	0.480858	0.478083	0.476457	0.473904	0.471787		
(3,-1)	0.297124		0.299465	0.303609	0.296964	0.296178	0.294575		

Table S50: Density value (a.u.) at the considered critical points for the CO system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.484698	0.491793	0.491149	0.488390	0.489026	0.490411	0.486296	0.474759	0.472049
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.484698	0.421401	0.467268	0.491753	0.488998	0.476520	0.481701	0.485567	0.481854
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.484698	0.472402	0.481891	0.495476	0.495194	0.488020	0.488541	0.486298	0.489914
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.484698	0.425386	0.494267	0.491285	0.487771	0.485838	0.480892		

Table S51: Density value (a.u.) at the considered critical points for the HCO<sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.435352	0.440297	0.440053	0.437666	0.437933	0.440251	0.436076	0.424791	0.425569
(3,-1)	0.266097	0.257043	0.263156	0.260801	0.265225	0.258576	0.264676	0.260236	0.255647
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.435352	0.401574	0.420568	0.440488	0.438154	0.426636	0.431653	0.435203	0.433203
(3,-1)	0.266097	0.282050	0.259437	0.265092	0.263428	0.265075	0.259319	0.265716	0.263622
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.435352	0.424342	0.432808	0.443689	0.445141	0.437097	0.437983	0.436707	0.438602
(3,-1)	0.266097	0.260941	0.266078	0.271039	0.276777	0.265127	0.264819	0.264030	0.264032
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.435352	0.405208	0.440445	0.441103	0.437744	0.436108	0.431697		
(3,-1)	0.266097	0.280686	0.266023	0.272928	0.265438	0.265252	0.263623		

Table S52: Density value (a.u.) at the considered critical points for the H<sub>2</sub>C=O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.414683	0.417176	0.418219	0.415490	0.416537	0.417454	0.414150	0.403067	0.405584
(3,-1)	0.290643	0.279871	0.286818	0.283885	0.288912	0.279952	0.288064	0.281428	0.275753
(3,-1)	0.290643	0.279871	0.286818	0.283885	0.288912	0.279952	0.288064	0.281428	0.275753
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.414683	0.259027	0.399746	0.418970	0.416393	0.403920	0.409097	0.414521	0.412062
(3,-1)	0.290643	0.286826	0.284996	0.289111	0.286997	0.286646	0.280402	0.290080	0.287349
(3,-1)	0.290643	0.359448	0.284996	0.289111	0.286997	0.286646	0.280402	0.290080	0.287349
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.414683	0.403355	0.411663	0.422184	0.425107	0.415372	0.416432	0.415426	0.416598
(3,-1)	0.290643	0.285315	0.290533	0.296629	0.303151	0.288878	0.288677	0.287915	0.287272
(3,-1)	0.290643	0.285315	0.290533	0.296629	0.303151	0.288878	0.288677	0.287915	0.287272
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.414683	0.259082	0.417914	0.419926	0.416864	0.415182	0.411374		
(3,-1)	0.290643	0.285402	0.289930	0.297520	0.289937	0.289569	0.288108		
(3,-1)	0.290643	0.362973	0.289930	0.297520	0.289937	0.289569	0.288108		

Table S53: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>-OH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.262301	0.260612	0.262190	0.261332	0.261351	0.261247	0.259113	0.258144	0.259572
(3,-1)	0.295298	0.284760	0.292479	0.289143	0.293632	0.284638	0.293105	0.286976	0.281427
(3,-1)	0.369619	0.362628	0.373408	0.371302	0.373760	0.366999	0.374533	0.374367	0.363276
(3,-1)	0.289610	0.279152	0.286487	0.283313	0.287770	0.279269	0.287035	0.281774	0.276146
(3,-1)	0.289610	0.279152	0.286487	0.283313	0.287770	0.279269	0.287035	0.281774	0.276146
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.262301	0.644150	0.255873	0.262487	0.261605	0.252865	0.257136	0.261285	0.260552
(3,-1)	0.295298		0.289469	0.294111	0.291521	0.290814	0.285236	0.294169	0.291702
(3,-1)	0.369619		0.363829	0.373185	0.371592	0.372951	0.369638	0.375507	0.367813
(3,-1)	0.289610		0.283176	0.288204	0.285761	0.285437	0.280114	0.288332	0.285701
(3,-1)	0.289610		0.283176	0.288204	0.285761	0.285437	0.280114	0.288332	0.285701
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.262301	0.257464	0.257247	0.258618	0.257585	0.261836	0.262222	0.262013	0.259841
(3,-1)	0.295298	0.289977	0.295132	0.300699	0.307985	0.293011	0.292996	0.292482	0.291644
(3,-1)	0.369619	0.369435	0.368446	0.371234	0.368441	0.376417	0.374908	0.373734	0.370934
(3,-1)	0.289610	0.284287	0.289402	0.294951	0.302578	0.287228	0.287172	0.286595	0.285777
(3,-1)	0.289610	0.284287	0.289402	0.294951	0.302578	0.287228	0.287172	0.286595	0.285777
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.262301	0.648516	0.256283	0.260493	0.261770	0.260815	0.257816		
(3,-1)	0.295298		0.293963	0.300656	0.294945	0.293935	0.292847		
(3,-1)	0.369619		0.377143	0.374514	0.370529	0.369003	0.366866		
(3,-1)	0.289610		0.287690	0.294782	0.289097	0.288217	0.287041		
(3,-1)	0.289610		0.287690	0.294782	0.289097	0.288217	0.287041		

Table S54: Density value (a.u.) at the considered critical points for the N<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.657507	0.649576	0.654448	0.650007	0.654995	0.647550	0.654427	0.637643	0.655320
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.657507	0.309028	0.645513	0.657340	0.653964	0.635446	0.638080	0.656627	0.644162
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.657507	0.649139	0.658203	0.672468	0.682760	0.647952	0.652359	0.655252	0.651190
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.657507	0.306173	0.662692	0.667846	0.656712	0.655585	0.653068		



Table S55: Density value (a.u.) at the considered critical points for the H<sub>2</sub>N–NH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.306996	0.297934	0.300463	0.300297	0.305259	0.294102	0.298640	0.303509	0.309266
(3,-1)	0.348875	0.339483	0.348861	0.346133	0.350401	0.340240	0.349522	0.348912	0.341230
(3,-1)	0.353610	0.344260	0.353969	0.351145	0.355313	0.345224	0.354567	0.353795	0.345391
(3,-1)	0.348875	0.339483	0.348861	0.346133	0.350401	0.340240	0.349522	0.348912	0.341230
(3,-1)	0.353610	0.344260	0.353969	0.351145	0.355313	0.345224	0.354567	0.353795	0.345391
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.306996	0.611681	0.310138	0.303605	0.304157	0.294961	0.297314	0.308525	0.301573
(3,-1)	0.348875		0.340729	0.350029	0.348029	0.351174	0.344834	0.351999	0.343539
(3,-1)	0.353610		0.345398	0.354984	0.352886	0.356241	0.349701	0.356926	0.348316
(3,-1)	0.348875		0.340729	0.350029	0.348029	0.351174	0.344834	0.351999	0.343539
(3,-1)	0.353610		0.345398	0.354984	0.352886	0.356241	0.349701	0.356926	0.348316
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.306996	0.297841	0.301212	0.302939	0.303091	0.306701	0.305229	0.302935	0.299739
(3,-1)	0.348875	0.344119	0.349883	0.355172	0.359295	0.351369	0.350269	0.348729	0.347042
(3,-1)	0.353610	0.348979	0.354464	0.359988	0.363450	0.356233	0.355160	0.353651	0.351928
(3,-1)	0.348875	0.344119	0.349883	0.355172	0.359295	0.351369	0.350269	0.348729	0.347042
(3,-1)	0.353610	0.348979	0.354464	0.359988	0.363450	0.356233	0.355160	0.353651	0.351928
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.306996	0.612438	0.297634	0.316684	0.304498	0.306239	0.302832		
(3,-1)	0.348875		0.352126	0.355960	0.349249	0.348244	0.346588		
(3,-1)	0.353610		0.357053	0.360564	0.354112	0.352967	0.351402		
(3,-1)	0.348875		0.352126	0.355960	0.349249	0.348244	0.346588		
(3,-1)	0.353610		0.357053	0.360564	0.354112	0.352967	0.351402		

Table S56: Density value (a.u.) at the considered critical points for the NO<sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.620755	0.615734	0.618307	0.615926	0.620042	0.613109	0.615286	0.603271	0.615847
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.620755	0.495658	0.608744	0.621168	0.619484	0.599529	0.604401	0.620805	0.611810
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.620755	0.606257	0.617431	0.629192	0.638621	0.616418	0.618239	0.617742	0.616431
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.620755	0.493731	0.620677	0.631815	0.619487	0.619351	0.613960		

Table S57: Density value (a.u.) at the considered critical points for the O<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.493712	0.487385	0.487475	0.488818	0.494450	0.481756	0.485430	0.490023	0.499650
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.493712	0.274860	0.498719	0.491840	0.493960	0.483205	0.485143	0.499199	0.488608
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.493712	0.485687	0.494203	0.495406	0.505638	0.494965	0.493821	0.491528	0.485572
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.493712	0.273168	0.488894	0.508010	0.490406	0.493768	0.487190		

Table S58: Density value (a.u.) at the considered critical points for the HO–OH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.271538	0.266326	0.265222	0.267410	0.271813	0.266093	0.266009	0.273950	0.278413
(3,-1)	0.368699	0.361179	0.372111	0.370256	0.372624	0.366282	0.372950	0.373803	0.362624
(3,-1)	0.368699	0.361179	0.372111	0.370256	0.372624	0.366282	0.372950	0.373803	0.362624
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.271538	0.275648	0.278175	0.269103	0.272001	0.274211	0.272527	0.276431	0.269440
(3,-1)	0.368699		0.362397	0.371762	0.370430	0.373473	0.369410	0.374419	0.366316
(3,-1)	0.368699		0.362397	0.371762	0.370430	0.373473	0.369410	0.374419	0.366316
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.271538	0.271060	0.270066	0.267486	0.262270	0.274678	0.273580	0.272643	0.267708
(3,-1)	0.368699	0.368783	0.366648	0.370438	0.364820	0.375237	0.373732	0.372629	0.369465
(3,-1)	0.368699	0.368783	0.366648	0.370438	0.364820	0.375237	0.373732	0.372629	0.369465
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.271538	0.279748	0.267297	0.283754	0.269082	0.272901	0.268165		
(3,-1)	0.368699		0.375078	0.372633	0.369178	0.367795	0.365675		
(3,-1)	0.368699		0.375078	0.372633	0.369178	0.367795	0.365675		

Table S59: Density value (a.u.) at the considered critical points for the F<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.277927	0.276178	0.273416	0.276177	0.280949	0.278604	0.272274	0.276847	0.285600
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.277927	0.438027	0.285507	0.278050	0.281696	0.285141	0.281181	0.285721	0.279181
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.277927	0.281621	0.283620	0.283767	0.282318	0.281273	0.281452	0.281308	0.277059
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.277927	0.444162	0.281832	0.295355	0.276893	0.281718	0.276380		

Table S60: Density value (a.u.) at the considered critical points for the CO<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.454306	0.452980	0.454223	0.450985	0.454730	0.453478	0.451404	0.438736	0.443785
(3,-1)	0.454306	0.452980	0.454223	0.450985	0.454730	0.453478	0.451404	0.438736	0.443785
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.454306	0.114223	0.435812	0.457226	0.454625	0.442179	0.447252	0.453992	0.450187
(3,-1)	0.454306	0.114223	0.435812	0.457226	0.454625	0.442179	0.447252	0.453992	0.450187
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.454306	0.440238	0.453707	0.464466	0.474764	0.453871	0.455019	0.453535	0.455751
(3,-1)	0.454306	0.440238	0.453707	0.464466	0.474764	0.453871	0.455019	0.453535	0.455751
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.454306	0.116053	0.459504	0.465826	0.453556	0.452860	0.447854		
(3,-1)	0.454306	0.116053	0.459504	0.465826	0.453556	0.452860	0.447854		

Table S61: Density value (a.u.) at the considered critical points for the  $^1\text{SiH}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.116130	0.118418	0.117922	0.117184	0.117526	0.116747	0.118230	0.116368	0.115240
(3,-1)	0.116130	0.118418	0.117922	0.117184	0.117526	0.116747	0.118230	0.116368	0.115240
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.116130	0.119678	0.110664	0.118217	0.117415	0.119730	0.118410	0.117407	0.115548
(3,-1)	0.116130	0.119678	0.110664	0.118217	0.117415	0.119730	0.118410	0.117407	0.115548
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.116130	0.116406	0.116890	0.118231	0.111732	0.118846	0.118385	0.117804	0.117952
(3,-1)	0.116130	0.116406	0.116890	0.118231	0.111732	0.118846	0.118385	0.117804	0.117952
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.116130	0.121570	0.114021	0.116847	0.117582	0.117035	0.115879		
(3,-1)	0.116130	0.121570	0.114021	0.116847	0.117582	0.117035	0.115879		

Table S62: Density value (a.u.) at the considered critical points for the  ${}^3\text{SiH}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.120624	0.122240	0.121685	0.121021	0.121029	0.119743	0.121824	0.118665	0.120314
(3,-1)	0.120624	0.122240	0.121685	0.121021	0.121029	0.119743	0.121824	0.118665	0.120314
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.120624	0.120476	0.115926	0.122216	0.121510	0.121808	0.121637	0.120967	0.120588
(3,-1)	0.120624	0.120476	0.115926	0.122216	0.121510	0.121808	0.121637	0.120967	0.120588
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.120624	0.120498	0.121517	0.122992	0.124027	0.121944	0.121990	0.121833	0.121733
(3,-1)	0.120624	0.120498	0.121517	0.122992	0.124027	0.121944	0.121990	0.121833	0.121733
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.120624	0.122307	0.117505	0.122410	0.121842	0.121529	0.120475		
(3,-1)	0.120624	0.122307	0.117505	0.122410	0.121842	0.121529	0.120475		



Table S63: Density value (a.u.) at the considered critical points for the  $\text{SiH}_3^\bullet$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.121918	0.123418	0.123316	0.122211	0.122671	0.120926	0.123128	0.120625	0.120298
(3,-1)	0.121918	0.123418	0.123316	0.122211	0.122671	0.120926	0.123128	0.120625	0.120298
(3,-1)	0.121918	0.123418	0.123316	0.122211	0.122671	0.120926	0.123128	0.120625	0.120298
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.121918	0.120582	0.115941	0.123711	0.122594	0.124423	0.123599	0.122543	0.121323
(3,-1)	0.121918	0.120582	0.115941	0.123711	0.122594	0.124423	0.123599	0.122543	0.121323
(3,-1)	0.121918	0.120582	0.115941	0.123711	0.122594	0.124423	0.123599	0.122543	0.121323
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.121918	0.121657	0.122682	0.124928	0.124239	0.124041	0.123632	0.123050	0.122955
(3,-1)	0.121918	0.121657	0.122682	0.124928	0.124239	0.124041	0.123632	0.123050	0.122955
(3,-1)	0.121918	0.121657	0.122682	0.124928	0.124239	0.124041	0.123632	0.123050	0.122955
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.121918	0.122284	0.119326	0.122996	0.123254	0.122569	0.121563		
(3,-1)	0.121918	0.122284	0.119326	0.122996	0.123254	0.122569	0.121563		
(3,-1)	0.121918	0.122284	0.119326	0.122996	0.123254	0.122569	0.121563		

Table S64: Density value (a.u.) at the considered critical points for the SiH<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.122424	0.123549	0.123885	0.122518	0.123213	0.121298	0.123373	0.121195	0.119752
(3,-1)	0.122424	0.123549	0.123885	0.122518	0.123213	0.121298	0.123373	0.121195	0.119752
(3,-1)	0.122424	0.123549	0.123885	0.122518	0.123213	0.121298	0.123373	0.121195	0.119752
(3,-1)	0.122424	0.123549	0.123885	0.122518	0.123213	0.121298	0.123373	0.121195	0.119752
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.122424	0.164125	0.115285	0.124250	0.122916	0.125372	0.123843	0.123068	0.121331
(3,-1)	0.122424	0.164125	0.115285	0.124250	0.122916	0.125372	0.123843	0.123068	0.121331
(3,-1)	0.122424		0.115285	0.124250	0.122916	0.125372	0.123843	0.123068	0.121331
(3,-1)	0.122424		0.115285	0.124250	0.122916	0.125372	0.123843	0.123068	0.121331
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.122424	0.122218	0.122854	0.125904	0.128437	0.125096	0.124383	0.123580	0.123093
(3,-1)	0.122424	0.122218	0.122854	0.125904	0.128437	0.125096	0.124383	0.123580	0.123093
(3,-1)	0.122424	0.122218	0.122854	0.125904	0.128437	0.125096	0.124383	0.123580	0.123093
(3,-1)	0.122424	0.122218	0.122854	0.125904	0.128437	0.125096	0.124383	0.123580	0.123093
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.122424	0.164824	0.120736	0.123314	0.123763	0.122920	0.121883		
(3,-1)	0.122424	0.164824	0.120736	0.123314	0.123763	0.122920	0.121883		
(3,-1)	0.122424		0.120736	0.123314	0.123763	0.122920	0.121883		
(3,-1)	0.122424		0.120736	0.123314	0.123763	0.122920	0.121883		

Table S65: Density value (a.u.) at the considered critical points for the  $\text{PH}_2^\bullet$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.166147	0.167130	0.167202	0.165910	0.166703	0.166140	0.167792	0.162580	0.164925
(3,-1)	0.166147	0.167130	0.167202	0.165910	0.166703	0.166140	0.167792	0.162580	0.164925
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.166147	0.163202	0.162017	0.167756	0.166456	0.166280	0.165855	0.166049	0.167780
(3,-1)	0.166147	0.163202	0.162017	0.167756	0.166456	0.166280	0.165855	0.166049	0.167780
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.166147	0.163974	0.166550	0.169484	0.175037	0.166700	0.166953	0.166947	0.167072
(3,-1)	0.166147	0.163974	0.166550	0.169484	0.175037	0.166700	0.166953	0.166947	0.167072
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.166147	0.163881	0.165829	0.167100	0.167346	0.166571	0.165145		
(3,-1)	0.166147	0.163881	0.165829	0.167100	0.167346	0.166571	0.165144		

Table S66: Density value (a.u.) at the considered critical points for the PH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.166619	0.166991	0.167665	0.165943	0.167015	0.166794	0.167097	0.162446	0.164026
(3,-1)	0.166619	0.166991	0.167665	0.165943	0.167015	0.166794	0.167097	0.162446	0.164026
(3,-1)	0.166619	0.166991	0.167665	0.165943	0.167015	0.166794	0.167097	0.162446	0.164026
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.166619	0.216401	0.160506	0.168261	0.166615	0.165901	0.166263	0.166441	0.167254
(3,-1)	0.166619	0.216401	0.160506	0.168261	0.166615	0.165901	0.166263	0.166441	0.167254
(3,-1)	0.166619		0.160506	0.168261	0.166615	0.165901	0.166263	0.166441	0.167254
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.166619	0.162878	0.165890	0.169779	0.173866	0.166479	0.166970	0.166908	0.166945
(3,-1)	0.166619	0.162878	0.165890	0.169779	0.173866	0.166479	0.166970	0.166908	0.166945
(3,-1)	0.166619	0.162878	0.165890	0.169779	0.173866	0.166479	0.166970	0.166908	0.166945
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.166619	0.216993	0.166145	0.167978	0.167835	0.166854	0.165549		
(3,-1)	0.166619	0.216993	0.166145	0.167978	0.167835	0.166854	0.165550		
(3,-1)	0.166619		0.166145	0.167978	0.167835	0.166854	0.165550		

Table S67: Density value (a.u.) at the considered critical points for the H<sub>2</sub>S system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.222006	0.216135	0.220135	0.218003	0.220904	0.217313	0.219670	0.218446	0.216337
(3,-1)	0.222006	0.216135	0.220135	0.218003	0.220904	0.217313	0.219670	0.218446	0.216337
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.222006	0.246754	0.217652	0.221502	0.219795	0.219141	0.217832	0.221086	0.219746
(3,-1)	0.222006		0.217652	0.221502	0.219795	0.219141	0.217832	0.221086	0.219746
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.222006	0.217783	0.222265	0.225494	0.233705	0.220327	0.220583	0.220324	0.219660
(3,-1)	0.222006	0.217783	0.222265	0.225494	0.233705	0.220327	0.220583	0.220324	0.219660
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.222006	0.249512	0.220102	0.226095	0.221915	0.221330	0.219885		
(3,-1)	0.222006		0.220102	0.226095	0.221915	0.221330	0.219885		

Table S68: Density value (a.u.) at the considered critical points for the HCl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.255339	0.248168	0.254537	0.252009	0.255077	0.249188	0.252634	0.252625	0.250867
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.255339	0.193686	0.249853	0.255362	0.253273	0.252853	0.250785	0.255307	0.251691
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.255339	0.244990	0.256768	0.260311	0.270061	0.254892	0.254789	0.253811	0.253150
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.255339	0.193474	0.257428	0.259279	0.255229	0.254049	0.253534		

Table S69: Density value (a.u.) at the considered critical points for the S<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.191759	0.187225	0.189096	0.187910	0.190588	0.187432	0.186131	0.182750	0.192932
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.191759	0.161776	0.196617	0.190833	0.190035	0.179603	0.182466	0.191782	0.192988
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.191759	0.180907	0.190994	0.194583	0.202599	0.190038	0.190865	0.190730	0.189140
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.191759	0.159706	0.186899	0.197577	0.190619	0.190820	0.189497		

Table S70: Density value (a.u.) at the considered critical points for the Cl<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.159956	0.153890	0.154313	0.155160	0.158232	0.152840	0.152928	0.157682	0.158028
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.159956	0.032236	0.163576	0.156793	0.158082	0.155757	0.156053	0.160811	0.157808
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.159956	0.154079	0.157635	0.156488	0.157838	0.161542	0.159791	0.157362	0.156607
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.159956	0.032697	0.154458	0.166932	0.157560	0.159552	0.157299		



Table S71: Density value (a.u.) at the considered critical points for the NaCl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.032710	0.034788	0.033727	0.034070	0.033452	0.033003	0.032799	0.033078	0.031279
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.032710	0.183366	0.032082	0.033734	0.033984	0.032700	0.033239	0.033738	0.032995
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.032710	0.034376	0.033966	0.034118	0.034263	0.033589	0.033656	0.033694	0.033636
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.032710	0.183218	0.033285	0.032952	0.033330	0.033406	0.033525		

Table S72: Density value (a.u.) at the considered critical points for the SiO system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.181532	0.187073	0.183977	0.184408	0.184399	0.184210	0.184534	0.182509	0.178190
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.181532	0.281829	0.180163	0.184600	0.184936	0.186839	0.187813	0.185824	0.185211
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.181532	0.184057	0.180851	0.181844	0.180450	0.187578	0.186751	0.186309	0.185097
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.181532	0.286303	0.184278	0.184761	0.182491	0.182882	0.180307		

Table S73: Density value (a.u.) at the considered critical points for the CS system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.286193	0.290037	0.289767	0.287315	0.287813	0.289831	0.291458	0.276018	0.290908
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.286193	0.254770	0.278670	0.290226	0.287925	0.280111	0.281614	0.287422	0.290437
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.286193	0.285637	0.288317	0.295787	0.303696	0.284909	0.287609	0.290406	0.288477
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.286193	0.255543	0.291221	0.288470	0.288724	0.287189	0.285035		

Table S74: Density value (a.u.) at the considered critical points for the SO system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.255291	0.260013	0.257808	0.257466	0.257541	0.258013	0.257244	0.250293	0.255449
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.255291	0.264252	0.251329	0.258270	0.257856	0.252302	0.256355	0.257605	0.259963
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.255291	0.251492	0.254693	0.257026	0.260689	0.259129	0.258731	0.258211	0.257449
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.255291	0.263120	0.256653	0.257379	0.256665	0.256668	0.253402		

Table S75: Density value (a.u.) at the considered critical points for the ClO• system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.261892	0.258187	0.258096	0.258792	0.262287	0.257118	0.257264	0.259314	0.265160
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.261892	0.209117	0.265608	0.260962	0.262103	0.256950	0.258637	0.264996	0.262060
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.261892	0.256522	0.261202	0.260126	0.264345	0.263997	0.263305	0.262141	0.259413
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.261892	0.208838	0.257424	0.268370	0.260619	0.262534	0.258951		

Table S76: Density value (a.u.) at the considered critical points for the CIF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.209068	0.206555	0.205290	0.206922	0.208660	0.207566	0.204200	0.207858	0.213670
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.209068	0.191283	0.209359	0.207082	0.208965	0.208717	0.208134	0.210390	0.208010
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.209068	0.205359	0.207411	0.205819	0.202094	0.209867	0.209270	0.208440	0.206972
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.209068	0.190082	0.206636	0.210857	0.206679	0.208588	0.204661		

Table S77: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>Cl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.191053	0.184341	0.186778	0.186034	0.188788	0.183848	0.183460	0.184825	0.190632
(3,-1)	0.294000	0.283639	0.291358	0.288063	0.292636	0.283257	0.291970	0.286390	0.281078
(3,-1)	0.294000	0.283639	0.291358	0.288063	0.292636	0.283257	0.291970	0.286390	0.281078
(3,-1)	0.294000	0.283639	0.291358	0.288063	0.292636	0.283257	0.291970	0.286390	0.281078
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.191053	0.185137	0.192741	0.188402	0.188030	0.179615	0.182239	0.190132	0.188019
(3,-1)	0.294000	0.217261	0.288315	0.293021	0.290474	0.289853	0.284460	0.293237	0.290633
(3,-1)	0.294000	0.279575	0.288315	0.293021	0.290474	0.289853	0.284460	0.293237	0.290633
(3,-1)	0.294000	0.280702	0.288315	0.293021	0.290474	0.289853	0.284460	0.293237	0.290633
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.191053	0.181295	0.186084	0.188334	0.189063	0.189691	0.188987	0.187273	0.186482
(3,-1)	0.294000	0.288385	0.294252	0.299634	0.307270	0.292142	0.292053	0.291450	0.290436
(3,-1)	0.294000	0.288385	0.294252	0.299634	0.307270	0.292142	0.292053	0.291450	0.290436
(3,-1)	0.294000	0.288385	0.294252	0.299634	0.307270	0.292142	0.292053	0.291450	0.290436
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.191053	0.184338	0.182926	0.194689	0.189110	0.189478	0.187901		
(3,-1)	0.294000	0.217665	0.293139	0.299776	0.293679	0.292687	0.291515		
(3,-1)	0.294000	0.278869	0.293139	0.299776	0.293679	0.292687	0.291513		
(3,-1)	0.294000	0.280031	0.293139	0.299776	0.293679	0.292687	0.291513		

Table S78: Density value (a.u.) at the considered critical points for the H<sub>3</sub>C–SH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.185818	0.177466	0.180979	0.179485	0.183428	0.177183	0.178016	0.180292	0.186580
(3,-1)	0.222783	0.217132	0.220754	0.218757	0.221603	0.218163	0.220333	0.219068	0.217157
(3,-1)	0.287856	0.278237	0.285582	0.282405	0.286676	0.277852	0.286123	0.281283	0.276377
(3,-1)	0.289255	0.279542	0.286850	0.283704	0.287994	0.279060	0.287358	0.282404	0.277315
(3,-1)	0.289255	0.279542	0.286850	0.283704	0.287994	0.279060	0.287358	0.282404	0.277315
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.185818	0.209370	0.187998	0.183253	0.182363	0.173838	0.177593	0.185240	0.182927
(3,-1)	0.222783	0.350845	0.218248	0.222170	0.220586	0.219765	0.218543	0.221832	0.220367
(3,-1)	0.287856		0.281955	0.287059	0.284569	0.283986	0.279131	0.287015	0.284478
(3,-1)	0.289255		0.283204	0.288374	0.285918	0.285303	0.280364	0.288417	0.285792
(3,-1)	0.289255		0.283204	0.288374	0.285918	0.285303	0.280364	0.288417	0.285792
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.185818	0.175646	0.180578	0.182988	0.181907	0.184356	0.183914	0.182461	0.181131
(3,-1)	0.222783	0.218463	0.222767	0.226089	0.234032	0.221092	0.221351	0.221077	0.220427
(3,-1)	0.287856	0.282428	0.288240	0.293440	0.301407	0.286021	0.285947	0.285408	0.284499
(3,-1)	0.289255	0.283763	0.289604	0.294868	0.302846	0.287415	0.287339	0.286758	0.285798
(3,-1)	0.289255	0.283763	0.289604	0.294868	0.302846	0.287415	0.287339	0.286758	0.285798
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.185818	0.207447	0.178046	0.193301	0.183957	0.184308	0.183121		
(3,-1)	0.222783	0.354418	0.220436	0.226558	0.222606	0.222119	0.220575		
(3,-1)	0.287856		0.286802	0.292916	0.287587	0.286540	0.285268		
(3,-1)	0.289255		0.288156	0.294412	0.288955	0.287948	0.286702		
(3,-1)	0.289255		0.288156	0.294412	0.288955	0.287948	0.286702		



Table S79: Density value (a.u.) at the considered critical points for the HOCl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.206498	0.201386	0.201089	0.202311	0.205723	0.201301	0.200526	0.205286	0.208923
(3,-1)	0.361589	0.354437	0.365442	0.363436	0.365648	0.359236	0.366260	0.367003	0.355757
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.206498	0.285217	0.210130	0.204004	0.205751	0.204167	0.204548	0.208800	0.205290
(3,-1)	0.361589	0.285217	0.355821	0.364947	0.363421	0.366093	0.362534	0.367267	0.359897
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.206498	0.201669	0.204523	0.202544	0.201259	0.208212	0.207136	0.205640	0.203708
(3,-1)	0.361589	0.361705	0.359525	0.362773	0.357428	0.368385	0.366837	0.365694	0.362616
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.206498	0.286256	0.201591	0.215056	0.203892	0.206359	0.202901		
(3,-1)	0.361589	0.286256	0.367882	0.365276	0.362088	0.360483	0.358412		

Table S80: Density value (a.u.) at the considered critical points for the SO<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.288441	0.291243	0.289469	0.288461	0.290035	0.288713	0.288650	0.281256	0.286048
(3,-1)	0.288441	0.291243	0.289469	0.288461	0.290035	0.288713	0.288650	0.281256	0.286048
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.288441	0.210903	0.280475	0.290972	0.290105	0.283511	0.289007	0.290914	0.291909
(3,-1)	0.288441	0.210903	0.280475	0.290972	0.290105	0.283511	0.289007	0.290914	0.291909
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.288441	0.282014	0.286606	0.290387	0.296121	0.291708	0.291259	0.290130	0.289767
(3,-1)	0.288441	0.282014	0.286606	0.290387	0.296121	0.291708	0.291259	0.290130	0.289767
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.288441	0.211552	0.289090	0.294560	0.287844	0.287814	0.283624		
(3,-1)	0.288441	0.211552	0.289090	0.294560	0.287844	0.287814	0.283624		

Table S81: Density value (a.u.) at the considered critical points for the BF<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.214240	0.219753	0.218217	0.217731	0.215739	0.219118	0.214696	0.216961	0.204407
(3,-1)	0.214240	0.219753	0.218217	0.217731	0.215739	0.219118	0.214696	0.216961	0.204407
(3,-1)	0.214240	0.219753	0.218217	0.217731	0.215739	0.219118	0.214696	0.216961	0.204407
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.214240	0.154276	0.208540	0.217771	0.217043	0.217392	0.220775	0.215205	0.214508
(3,-1)	0.214240	0.154276	0.208540	0.217771	0.217043	0.217392	0.220775	0.215205	0.214508
(3,-1)	0.214240	0.154276	0.208540	0.217771	0.217043	0.217392	0.220775	0.215205	0.214508
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.214240	0.216975	0.213970	0.212763	0.205922	0.217111	0.217731	0.217783	0.216391
(3,-1)	0.214240	0.216975	0.213970	0.212763	0.205922	0.217111	0.217731	0.217783	0.216391
(3,-1)	0.214240	0.216975	0.213970	0.212763	0.205922	0.217111	0.217731	0.217783	0.216391
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.214240	0.157363	0.214712	0.213437	0.215899	0.214880	0.212473		
(3,-1)	0.214240	0.157363	0.214712	0.213437	0.215899	0.214880	0.212474		
(3,-1)	0.214240	0.157363	0.214712	0.213437	0.215899	0.214880	0.212474		

Table S82: Density value (a.u.) at the considered critical points for the BCl<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.163000	0.162134	0.164240	0.161598	0.161773	0.161554	0.157972	0.155491	0.156880
(3,-1)	0.163000	0.162134	0.164240	0.161598	0.161773	0.161554	0.157972	0.155491	0.156880
(3,-1)	0.163000	0.162134	0.164240	0.161598	0.161773	0.161554	0.157972	0.155491	0.156880
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.163000	0.116022	0.154808	0.164388	0.161849	0.154174	0.158834	0.160772	0.160317
(3,-1)	0.163000	0.116022	0.154808	0.164388	0.161849	0.154174	0.158834	0.160772	0.160317
(3,-1)	0.163000	0.116022	0.154808	0.164388	0.161849	0.154174	0.158834	0.160772	0.160317
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.163000	0.155436	0.159061	0.164914	0.161691	0.162490	0.162713	0.161426	0.160510
(3,-1)	0.163000	0.155436	0.159061	0.164914	0.161691	0.162490	0.162713	0.161426	0.160510
(3,-1)	0.163000	0.155436	0.159061	0.164914	0.161691	0.162490	0.162713	0.161426	0.160510
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.163000	0.117334	0.160520	0.163427	0.163492	0.161509	0.160239		
(3,-1)	0.163000	0.117334	0.160520	0.163427	0.163492	0.161509	0.160232		
(3,-1)	0.163000	0.117334	0.160520	0.163427	0.163492	0.161509	0.160232		

Table S83: Density value (a.u.) at the considered critical points for the  $\text{AlF}_3$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.115839	0.120550	0.118344	0.118846	0.117791	0.122440	0.116604	0.115404	0.113437
(3,-1)	0.115839	0.120550	0.118344	0.118846	0.117791	0.122440	0.116604	0.115404	0.113437
(3,-1)	0.115839	0.120550	0.118344	0.118846	0.117791	0.122440	0.116604	0.115404	0.113437
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.115839	0.080451	0.113669	0.118275	0.118616	0.118005	0.117958	0.117616	0.118087
(3,-1)	0.115839	0.080451	0.113669	0.118275	0.118616	0.118005	0.117958	0.117616	0.118087
(3,-1)	0.115839	0.080451	0.113669	0.118275	0.118616	0.118005	0.117958	0.117616	0.118087
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.115839	0.119001	0.117534	0.118367	0.117971	0.117834	0.118116	0.118170	0.118976
(3,-1)	0.115839	0.119001	0.117534	0.118367	0.117971	0.117834	0.118116	0.118170	0.118976
(3,-1)	0.115839	0.119001	0.117534	0.118367	0.117971	0.117834	0.118116	0.118170	0.118976
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.115839	0.081206	0.115672	0.116106	0.117082	0.117120	0.116137		
(3,-1)	0.115839	0.081206	0.115672	0.116106	0.117082	0.117120	0.116137		
(3,-1)	0.115839	0.081206	0.115672	0.116106	0.117082	0.117120	0.116137		

Table S84: Density value (a.u.) at the considered critical points for the  $\text{AlCl}_3$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.080940	0.083514	0.082728	0.082607	0.082046	0.081594	0.083060	0.081716	0.075700
(3,-1)	0.080940	0.083514	0.082728	0.082607	0.082046	0.081594	0.083060	0.081716	0.075700
(3,-1)	0.080940	0.083514	0.082728	0.082607	0.082046	0.081594	0.083060	0.081716	0.075700
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.080940	0.302402	0.079337	0.082750	0.082537	0.082980	0.083497	0.082832	0.081161
(3,-1)	0.080940	0.302402	0.079337	0.082750	0.082537	0.082980	0.083497	0.082832	0.081161
(3,-1)	0.080940	0.302402	0.079337	0.082750	0.082537	0.082980	0.083497	0.082832	0.081161
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.080940	0.083707	0.081339	0.080896	0.080043	0.084386	0.084135	0.083877	0.083270
(3,-1)	0.080940	0.083707	0.081339	0.080896	0.080043	0.084386	0.084135	0.083877	0.083270
(3,-1)	0.080940	0.083707	0.081339	0.080896	0.080043	0.084386	0.084135	0.083877	0.083270
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.080940	0.301686	0.081442	0.081487	0.081963	0.081654	0.080853		
(3,-1)	0.080940	0.301686	0.081442	0.081487	0.081963	0.081654	0.080854		
(3,-1)	0.080940	0.301686	0.081442	0.081487	0.081963	0.081654	0.080854		

Table S85: Density value (a.u.) at the considered critical points for the CF<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.307191	0.307795	0.309760	0.307747	0.306379	0.309752	0.304842	0.303045	0.301416
(3,-1)	0.307191	0.307795	0.309760	0.307747	0.306379	0.309752	0.304842	0.303045	0.301416
(3,-1)	0.307191	0.307795	0.309760	0.307747	0.306379	0.309752	0.304842	0.303045	0.301416
(3,-1)	0.307191	0.307795	0.309760	0.307747	0.306379	0.309752	0.304842	0.303045	0.301416
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.307191	0.206200	0.295820	0.309249	0.307040	0.299499	0.305210	0.305016	0.305128
(3,-1)	0.307191	0.206200	0.295820	0.309249	0.307040	0.299499	0.305210	0.305016	0.305128
(3,-1)	0.307191	0.206200	0.295820	0.309249	0.307040	0.299499	0.305210	0.305016	0.305128
(3,-1)	0.307191	0.206200	0.295820	0.309249	0.307040	0.299499	0.305210	0.305016	0.305128
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.307191	0.301115	0.301987	0.303760	0.302488	0.306172	0.307285	0.307266	0.307045
(3,-1)	0.307191	0.301115	0.301987	0.303760	0.302488	0.306172	0.307285	0.307266	0.307045
(3,-1)	0.307191	0.301115	0.301987	0.303760	0.302488	0.306172	0.307285	0.307266	0.307045
(3,-1)	0.307191	0.301115	0.301987	0.303760	0.302488	0.306172	0.307285	0.307266	0.307045
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.307191	0.204571	0.303386	0.303573	0.307750	0.305384	0.302307		
(3,-1)	0.307191	0.204571	0.303386	0.303573	0.307750	0.305384	0.302307		
(3,-1)	0.307191	0.204571	0.303386	0.303573	0.307750	0.305384	0.302307		
(3,-1)	0.307191	0.204571	0.303386	0.303573	0.307750	0.305384	0.302307		

Table S86: Density value (a.u.) at the considered critical points for the CCl<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.206355	0.196953	0.199599	0.198700	0.203116	0.195627	0.196351	0.198298	0.205492
(3,-1)	0.206355	0.196953	0.199599	0.198700	0.203116	0.195627	0.196351	0.198298	0.205492
(3,-1)	0.206355	0.196953	0.199599	0.198700	0.203116	0.195627	0.196351	0.198298	0.205492
(3,-1)	0.206355	0.196953	0.199599	0.198700	0.203116	0.195627	0.196351	0.198298	0.205492
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.206355	0.236463	0.207899	0.202497	0.202237	0.192105	0.195642	0.205344	0.202538
(3,-1)	0.206355	0.436729	0.207899	0.202497	0.202237	0.192105	0.195642	0.205344	0.202538
(3,-1)	0.206355		0.207899	0.202497	0.202237	0.192105	0.195642	0.205344	0.202538
(3,-1)	0.206355		0.207899	0.202497	0.202237	0.192105	0.195642	0.205344	0.202538
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.206355	0.194697	0.200779	0.203641	0.204552	0.205045	0.204091	0.201801	0.200596
(3,-1)	0.206355	0.194697	0.200779	0.203641	0.204552	0.205045	0.204091	0.201801	0.200596
(3,-1)	0.206355	0.194697	0.200779	0.203641	0.204552	0.205045	0.204091	0.201801	0.200596
(3,-1)	0.206355	0.194697	0.200779	0.203641	0.204552	0.205045	0.204091	0.201801	0.200596
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.206355	0.239812	0.198261	0.214077	0.203228	0.204242	0.202314		
(3,-1)	0.206355	0.442286	0.198261	0.214077	0.203228	0.204242	0.202314		
(3,-1)	0.206355		0.198261	0.214077	0.203228	0.204242	0.202314		
(3,-1)	0.206355		0.198261	0.214077	0.203228	0.204242	0.202314		



Table S87: Density value (a.u.) at the considered critical points for the O=C=S system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.238519	0.246837	0.245100	0.243756	0.242107	0.246245	0.245129	0.232285	0.244133
(3,-1)	0.453561	0.453293	0.453954	0.450984	0.454102	0.453505	0.450570	0.437911	0.440929
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.238519	0.249408	0.234436	0.243836	0.242173	0.235434	0.237040	0.240142	0.243277
(3,-1)	0.453561	0.249408	0.435009	0.456637	0.454199	0.440596	0.446302	0.453174	0.449556
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.238519	0.236533	0.240035	0.246038	0.249272	0.238160	0.240316	0.242430	0.242462
(3,-1)	0.453561	0.440282	0.451901	0.463225	0.471484	0.454371	0.455254	0.453400	0.455036
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.238519	0.252809	0.240544	0.237622	0.242029	0.240202	0.237800		
(3,-1)	0.453561	0.252809	0.459507	0.464224	0.452882	0.452154	0.447310		

Table S88: Density value (a.u.) at the considered critical points for the CS<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.251829	0.258473	0.257470	0.255565	0.254567	0.258269	0.257762	0.243789	0.255802
(3,-1)	0.251829	0.258473	0.257470	0.255565	0.254567	0.258269	0.257762	0.243789	0.255802
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.251829	0.443678	0.246644	0.256727	0.254650	0.246690	0.249063	0.253071	0.256344
(3,-1)	0.251829	0.294032	0.246644	0.256727	0.254650	0.246690	0.249063	0.253071	0.256344
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.251829	0.249138	0.253423	0.259442	0.264768	0.250868	0.253294	0.255691	0.255294
(3,-1)	0.251829	0.249138	0.253423	0.259442	0.264768	0.250868	0.253294	0.255691	0.255294
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.251829	0.449084	0.254155	0.251860	0.254903	0.252977	0.250803		
(3,-1)	0.251829	0.293566	0.254155	0.251860	0.254903	0.252977	0.250803		

Table S89: Density value (a.u.) at the considered critical points for the COF<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.459999	0.459058	0.460965	0.457295	0.460299	0.458939	0.457402	0.445073	0.450703
(3,-1)	0.298942	0.299910	0.300914	0.299393	0.298299	0.301402	0.296436	0.294879	0.292905
(3,-1)	0.298942	0.299910	0.300914	0.299393	0.298299	0.301402	0.296436	0.294879	0.292905
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.459999	0.151197	0.441462	0.463213	0.460066	0.447632	0.452918	0.459006	0.456015
(3,-1)	0.298942	0.151197	0.287998	0.300772	0.299088	0.292666	0.298199	0.297373	0.296709
(3,-1)	0.298942	0.151197	0.287998	0.300772	0.299088	0.292666	0.298199	0.297373	0.296709
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.459999	0.445737	0.457536	0.469337	0.474966	0.458820	0.460247	0.459033	0.461350
(3,-1)	0.298942	0.293226	0.293970	0.295122	0.293753	0.298454	0.299458	0.299421	0.298723
(3,-1)	0.298942	0.293226	0.293970	0.295122	0.293753	0.298454	0.299458	0.299421	0.298723
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.459999	0.151795	0.464242	0.468817	0.460906	0.459413	0.455252		
(3,-1)	0.298942	0.151795	0.295493	0.296922	0.299174	0.297407	0.293779		
(3,-1)	0.298942	0.151795	0.295493	0.296922	0.299174	0.297407	0.293779		

Table S90: Density value (a.u.) at the considered critical points for the SiF<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.150416	0.155340	0.153362	0.153390	0.152203	0.155559	0.151761	0.150741	0.146639
(3,-1)	0.150416	0.155340	0.153362	0.153390	0.152203	0.155559	0.151761	0.150741	0.146639
(3,-1)	0.150416	0.155340	0.153362	0.153390	0.152203	0.155559	0.151761	0.150741	0.146639
(3,-1)	0.150416	0.155340	0.153362	0.153390	0.152203	0.155559	0.151761	0.150741	0.146639
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.150416	0.107958	0.147142	0.153187	0.153054	0.153927	0.155282	0.152585	0.152410
(3,-1)	0.150416	0.107958	0.147142	0.153187	0.153054	0.153927	0.155282	0.152585	0.152410
(3,-1)	0.150416	0.107958	0.147142	0.153187	0.153054	0.153927	0.155282	0.152585	0.152410
(3,-1)	0.150416	0.107958	0.147142	0.153187	0.153054	0.153927	0.155282	0.152585	0.152410
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.150416	0.153996	0.151765	0.151728	0.148747	0.153488	0.153575	0.153516	0.154006
(3,-1)	0.150416	0.153996	0.151765	0.151728	0.148747	0.153488	0.153575	0.153516	0.154006
(3,-1)	0.150416	0.153996	0.151765	0.151728	0.148747	0.153488	0.153575	0.153516	0.154006
(3,-1)	0.150416	0.153996	0.151765	0.151728	0.148747	0.153488	0.153575	0.153516	0.154006
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.150416	0.109247	0.150747	0.150497	0.151813	0.151432	0.150083		
(3,-1)	0.150416	0.109247	0.150747	0.150497	0.151813	0.151432	0.150083		
(3,-1)	0.150416	0.109247	0.150747	0.150497	0.151813	0.151432	0.150083		
(3,-1)	0.150416	0.109247	0.150747	0.150497	0.151813	0.151432	0.150083		

Table S91: Density value (a.u.) at the considered critical points for the SiCl<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.110011	0.111331	0.111556	0.110370	0.110365	0.110077	0.109422	0.107044	0.108536
(3,-1)	0.110011	0.111331	0.111556	0.110370	0.110365	0.110077	0.109422	0.107044	0.108536
(3,-1)	0.110011	0.111331	0.111556	0.110370	0.110365	0.110077	0.109422	0.107044	0.108536
(3,-1)	0.110011	0.111331	0.111556	0.110370	0.110365	0.110077	0.109422	0.107044	0.108536
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.110011	0.519100	0.106418	0.111632	0.110439	0.107711	0.109914	0.110250	0.109939
(3,-1)	0.110011	0.533864	0.106418	0.111632	0.110439	0.107711	0.109914	0.110250	0.109939
(3,-1)	0.110011		0.106418	0.111632	0.110439	0.107711	0.109914	0.110250	0.109939
(3,-1)	0.110011		0.106418	0.111632	0.110439	0.107711	0.109914	0.110250	0.109939
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.110011	0.107790	0.108506	0.111416	0.110818	0.112869	0.112056	0.110943	0.110042
(3,-1)	0.110011	0.107790	0.108506	0.111416	0.110818	0.112869	0.112056	0.110943	0.110042
(3,-1)	0.110011	0.107790	0.108506	0.111416	0.110818	0.112869	0.112056	0.110943	0.110042
(3,-1)	0.110011	0.107790	0.108506	0.111416	0.110818	0.112869	0.112056	0.110943	0.110042
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.110011	0.525143	0.110020	0.110679	0.110801	0.109807	0.108549		
(3,-1)	0.110011	0.534237	0.110020	0.110679	0.110801	0.109807	0.108549		
(3,-1)	0.110011		0.110020	0.110679	0.110801	0.109807	0.108549		
(3,-1)	0.110011		0.110020	0.110679	0.110801	0.109807	0.108549		

Table S92: Density value (a.u.) at the considered critical points for the N<sub>2</sub>O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.531013	0.529265	0.530645	0.527863	0.530153	0.527906	0.529187	0.512558	0.526464
(3,-1)	0.536395	0.529517	0.531440	0.530437	0.536074	0.525135	0.528063	0.524258	0.534535
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.531013	0.114639	0.519221	0.532234	0.529797	0.512790	0.516442	0.529648	0.526041
(3,-1)	0.536395	0.603954	0.533278	0.535260	0.535133	0.516499	0.521544	0.538937	0.528793
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.531013	0.520374	0.533619	0.543781	0.563416	0.524733	0.528123	0.529864	0.528525
(3,-1)	0.536395	0.521818	0.536930	0.542031	0.557029	0.533782	0.534317	0.532874	0.529264
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.531013	0.113864	0.533860	0.535627	0.530043	0.528990	0.524631		
(3,-1)	0.536395	0.605085	0.533497	0.548425	0.533514	0.535054	0.529844		

Table S93: Density value (a.u.) at the considered critical points for the ClNO system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.114793	0.109615	0.108904	0.110145	0.112722	0.110848	0.109568	0.111807	0.113534
(3,-1)	0.612448	0.604211	0.607368	0.605001	0.611225	0.600971	0.604834	0.594144	0.606374
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.114793	0.330686	0.114874	0.111432	0.113113	0.114200	0.113414	0.115399	0.111408
(3,-1)	0.612448	0.330686	0.601862	0.611832	0.610531	0.588616	0.594040	0.614016	0.602018
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.114793	0.112996	0.112623	0.111570	0.108658	0.115151	0.114476	0.113648	0.112809
(3,-1)	0.612448	0.598976	0.610884	0.621430	0.634862	0.608223	0.610008	0.609451	0.606688
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.114793	0.328065	0.112133	0.120807	0.110899	0.113378	0.110967		
(3,-1)	0.612448	0.328065	0.612038	0.627947	0.609952	0.610873	0.605498		

Table S94: Density value (a.u.) at the considered critical points for the  $\text{NF}_3$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.328876	0.319867	0.320362	0.321454	0.326126	0.320264	0.319110	0.326842	0.333451
(3,-1)	0.328876	0.319867	0.320362	0.321454	0.326126	0.320264	0.319110	0.326842	0.333451
(3,-1)	0.328876	0.319867	0.320362	0.321454	0.326126	0.320264	0.319110	0.326842	0.333451
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.328876	0.169296	0.329818	0.324269	0.326082	0.322944	0.324467	0.330047	0.323419
(3,-1)	0.328876	0.169296	0.329818	0.324269	0.326082	0.322944	0.324467	0.330047	0.323419
(3,-1)	0.328876	0.169296	0.329818	0.324269	0.326082	0.322944	0.324467	0.330047	0.323419
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.328876	0.321638	0.324075	0.321512	0.320590	0.327367	0.326816	0.325701	0.322351
(3,-1)	0.328876	0.321638	0.324075	0.321512	0.320590	0.327367	0.326816	0.325701	0.322351
(3,-1)	0.328876	0.321638	0.324075	0.321512	0.320590	0.327367	0.326816	0.325701	0.322351
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.328876	0.169068	0.319077	0.337392	0.324629	0.327541	0.322262		
(3,-1)	0.328876	0.169068	0.319077	0.337392	0.324629	0.327541	0.322261		
(3,-1)	0.328876	0.169068	0.319077	0.337392	0.324629	0.327541	0.322261		



Table S95: Density value (a.u.) at the considered critical points for the PF<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.168995	0.174638	0.172761	0.172580	0.171015	0.175527	0.170675	0.168328	0.168515
(3,-1)	0.168995	0.174638	0.172761	0.172580	0.171015	0.175527	0.170675	0.168328	0.168515
(3,-1)	0.168995	0.174638	0.172761	0.172580	0.171015	0.175527	0.170675	0.168328	0.168515
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.168995	0.426204	0.164706	0.172145	0.171694	0.172089	0.174806	0.170451	0.171156
(3,-1)	0.168995	0.426204	0.164706	0.172145	0.171694	0.172089	0.174806	0.170451	0.171156
(3,-1)	0.168995		0.164706	0.172145	0.171694	0.172089	0.174806	0.170451	0.171156
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.168995	0.169216	0.168369	0.169612	0.163825	0.171867	0.171983	0.171885	0.171867
(3,-1)	0.168995	0.169216	0.168369	0.169612	0.163825	0.171867	0.171983	0.171885	0.171867
(3,-1)	0.168995	0.169216	0.168369	0.169612	0.163825	0.171867	0.171983	0.171885	0.171867
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.168995	0.424313	0.170304	0.167643	0.170535	0.169701	0.167749		
(3,-1)	0.168995	0.424313	0.170304	0.167643	0.170535	0.169701	0.167750		
(3,-1)	0.168995		0.170304	0.167643	0.170535	0.169701	0.167750		

Table S96: Density value (a.u.) at the considered critical points for the O<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.425838	0.419843	0.419010	0.421068	0.425806	0.415038	0.417873	0.426886	0.431958
(3,-1)	0.425838	0.419843	0.419010	0.421068	0.425806	0.415038	0.417873	0.426886	0.431958
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.425838	0.291858	0.429963	0.422805	0.425460	0.420838	0.421354	0.430191	0.419166
(3,-1)	0.425838	0.291858	0.429963	0.422805	0.425460	0.420838	0.421354	0.430191	0.419166
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.425838	0.419416	0.423084	0.421579	0.424480	0.427532	0.425967	0.424058	0.417094
(3,-1)	0.425838	0.419416	0.423084	0.421579	0.424480	0.427532	0.425967	0.424058	0.417094
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.425838	0.293022	0.418707	0.432672	0.422572	0.426252	0.419991		
(3,-1)	0.425838	0.293022	0.418707	0.432672	0.422572	0.426252	0.419991		

Table S97: Density value (a.u.) at the considered critical points for the F<sub>2</sub>O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.292718	0.286906	0.285126	0.287634	0.292777	0.288372	0.285056	0.293547	0.300938
(3,-1)	0.292718	0.286906	0.285126	0.287634	0.292777	0.288372	0.285056	0.293547	0.300938
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.292718	0.234834	0.297942	0.289889	0.293290	0.297142	0.294858	0.297906	0.290328
(3,-1)	0.292718	0.190332	0.297942	0.289889	0.293290	0.297142	0.294858	0.297906	0.290328
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.292718	0.292572	0.292638	0.290592	0.285343	0.294482	0.294054	0.293492	0.288645
(3,-1)	0.292718	0.292572	0.292638	0.290592	0.285343	0.294482	0.294054	0.293492	0.288645
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.292718	0.234278	0.289967	0.307010	0.289457	0.294083	0.288491		
(3,-1)	0.292718	0.189938	0.289967	0.307010	0.289457	0.294083	0.288491		

Table S98: Density value (a.u.) at the considered critical points for the ClF<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.235780	0.228706	0.228424	0.229502	0.232943	0.229792	0.227050	0.232135	0.238787
(3,-1)	0.191096	0.188565	0.187374	0.189061	0.190494	0.189938	0.186522	0.190266	0.195707
(3,-1)	0.191096	0.188565	0.187374	0.189061	0.190494	0.189938	0.186522	0.190266	0.195707
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.235780	0.360540	0.234346	0.231526	0.233168	0.232073	0.233010	0.235979	0.233143
(3,-1)	0.191096	0.283542	0.191406	0.188804	0.190643	0.192388	0.190706	0.191616	0.188816
(3,-1)	0.191096	0.283542	0.191406	0.188804	0.190643	0.192388	0.190706	0.191616	0.188816
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.235780	0.229137	0.232337	0.230391	0.228694	0.234512	0.234014	0.233012	0.231234
(3,-1)	0.191096	0.187790	0.188737	0.188094	0.182245	0.191069	0.190440	0.189848	0.189170
(3,-1)	0.191096	0.187790	0.188737	0.188094	0.182245	0.191069	0.190440	0.189848	0.189170
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.235780	0.360900	0.229512	0.243055	0.231303	0.233766	0.229261		
(3,-1)	0.191096	0.283659	0.188902	0.189846	0.188851	0.190610	0.187008		
(3,-1)	0.191096	0.283659	0.188902	0.189846	0.188851	0.190610	0.187008		

Table S99: Density value (a.u.) at the considered critical points for the F<sub>2</sub>C=CF<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.364954	0.354977	0.360442	0.356279	0.361319	0.355320	0.359460	0.360320	0.365621
(3,-1)	0.289375	0.290202	0.290132	0.289282	0.288060	0.290950	0.285325	0.284633	0.281407
(3,-1)	0.289375	0.290202	0.290132	0.289282	0.288060	0.290950	0.285325	0.284633	0.281407
(3,-1)	0.289375	0.290202	0.290132	0.289282	0.288060	0.290950	0.285325	0.284633	0.281407
(3,-1)	0.289375	0.290202	0.290132	0.289282	0.288060	0.290950	0.285325	0.284633	0.281407
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.364954	0.341433	0.357936	0.363443	0.360338	0.360537	0.363275	0.362965	0.359350
(3,-1)	0.289375	0.221905	0.277739	0.290218	0.289223	0.281741	0.287915	0.287675	0.287283
(3,-1)	0.289375	0.221905	0.277739	0.290218	0.289223	0.281741	0.287915	0.287675	0.287283
(3,-1)	0.289375	0.221905	0.277739	0.290218	0.289223	0.281741	0.287915	0.287675	0.287283
(3,-1)	0.289375	0.221905	0.277739	0.290218	0.289223	0.281741	0.287915	0.287675	0.287283
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.364954	0.357983	0.363673	0.366795	0.364527	0.357389	0.360011	0.361502	0.359651
(3,-1)	0.289375	0.284297	0.284997	0.285190	0.285005	0.288735	0.289672	0.289589	0.288164
(3,-1)	0.289375	0.284297	0.284997	0.285190	0.285005	0.288735	0.289672	0.289589	0.288164
(3,-1)	0.289375	0.284297	0.284997	0.285190	0.285005	0.288735	0.289672	0.289589	0.288164
(3,-1)	0.289375	0.284297	0.284997	0.285190	0.285005	0.288735	0.289672	0.289589	0.288164
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.364954	0.341727	0.362232	0.373765	0.363850	0.362959	0.360687		
(3,-1)	0.289375	0.220901	0.285511	0.286926	0.289101	0.287988	0.284265		
(3,-1)	0.289375	0.220901	0.285511	0.286926	0.289101	0.287988	0.284265		
(3,-1)	0.289375	0.220901	0.285511	0.286926	0.289101	0.287988	0.284265		
(3,-1)	0.289375	0.220901	0.285511	0.286926	0.289101	0.287988	0.284265		

Table S100: Density value (a.u.) at the considered critical points for the Cl<sub>2</sub>C=CCL<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.346181	0.336243	0.341177	0.337450	0.342449	0.336544	0.339354	0.339668	0.346672
(3,-1)	0.222819	0.213793	0.216523	0.215325	0.219478	0.212819	0.212658	0.212963	0.221018
(3,-1)	0.222819	0.213793	0.216523	0.215325	0.219478	0.212819	0.212658	0.212963	0.221018
(3,-1)	0.222819	0.213793	0.216523	0.215325	0.219478	0.212819	0.212658	0.212963	0.221018
(3,-1)	0.222819	0.213793	0.216523	0.215325	0.219478	0.212819	0.212658	0.212963	0.221018
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.346181	0.279427	0.339700	0.344175	0.341437	0.335362	0.340271	0.343951	0.340864
(3,-1)	0.222819	0.291899	0.223161	0.219249	0.218661	0.206944	0.211256	0.221512	0.219027
(3,-1)	0.222819	0.291899	0.223161	0.219249	0.218661	0.206944	0.211256	0.221512	0.219027
(3,-1)	0.222819	0.291899	0.223161	0.219249	0.218661	0.206944	0.211256	0.221512	0.219027
(3,-1)	0.222819	0.452234	0.223161	0.219249	0.218661	0.206944	0.211256	0.221512	0.219027
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.346181	0.335990	0.342811	0.347471	0.346071	0.340103	0.342125	0.342824	0.340251
(3,-1)	0.222819	0.209516	0.217552	0.220881	0.223323	0.220496	0.220190	0.218370	0.217026
(3,-1)	0.222819	0.209516	0.217552	0.220881	0.223323	0.220496	0.220190	0.218370	0.217026
(3,-1)	0.222819	0.209516	0.217552	0.220881	0.223323	0.220496	0.220190	0.218370	0.217026
(3,-1)	0.222819	0.209516	0.217552	0.220881	0.223323	0.220496	0.220190	0.218370	0.217026
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.346181	0.279267	0.343248	0.354993	0.344400	0.343750	0.341832		
(3,-1)	0.222819	0.291340	0.214970	0.230215	0.219830	0.220530	0.218729		
(3,-1)	0.222819	0.291340	0.214970	0.230215	0.219830	0.220530	0.218729		
(3,-1)	0.222819	0.291340	0.214970	0.230215	0.219830	0.220530	0.218729		
(3,-1)	0.222819	0.291340	0.214970	0.230215	0.219830	0.220530	0.218729		
(3,-1)	0.222819	0.459257	0.214970	0.230215	0.219830	0.220530	0.218729		

Table S101: Density value (a.u.) at the considered critical points for the CF<sub>3</sub>CN system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.287888	0.274475	0.280304	0.277168	0.283396	0.273808	0.278322	0.286333	0.280714
(3,-1)	0.296732	0.297267	0.298690	0.297143	0.295846	0.299217	0.293696	0.292571	0.290814
(3,-1)	0.296732	0.297267	0.298690	0.297143	0.295846	0.299217	0.293696	0.292571	0.290814
(3,-1)	0.296732	0.297267	0.298690	0.297143	0.295846	0.299217	0.293696	0.292571	0.290814
(3,-1)	0.467547	0.472134	0.472812	0.468840	0.469691	0.474576	0.472040	0.453281	0.464166
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.287888	0.402419	0.281281	0.283872	0.281830	0.285327	0.285069	0.285861	0.280129
(3,-1)	0.296732	0.268153	0.285720	0.298356	0.296645	0.289164	0.294757	0.294790	0.294653
(3,-1)	0.296732	0.288952	0.285720	0.298356	0.296645	0.289164	0.294757	0.294790	0.294653
(3,-1)	0.296732	0.276614	0.285720	0.298356	0.296645	0.289164	0.294757	0.294790	0.294653
(3,-1)	0.467547	0.276614	0.451356	0.473387	0.469630	0.460208	0.464038	0.466921	0.465533
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.287888	0.275938	0.284831	0.285868	0.282527	0.282809	0.283112	0.282253	0.280782
(3,-1)	0.296732	0.291044	0.291850	0.293042	0.292069	0.295990	0.297039	0.297006	0.296205
(3,-1)	0.296732	0.291044	0.291850	0.293042	0.292069	0.295990	0.297039	0.297006	0.296205
(3,-1)	0.296732	0.291044	0.291850	0.293042	0.292069	0.295990	0.297039	0.297006	0.296205
(3,-1)	0.467547	0.457527	0.469843	0.482461	0.487220	0.463940	0.468436	0.470938	0.472053
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.287888	0.407374	0.282336	0.298227	0.285030	0.285192	0.283385		
(3,-1)	0.296732	0.268504	0.292977	0.293264	0.296944	0.295033	0.291804		
(3,-1)	0.296732	0.289080	0.292977	0.293264	0.296944	0.295033	0.291802		
(3,-1)	0.296732	0.276104	0.292977	0.293264	0.296944	0.295033	0.291802		
(3,-1)	0.467547	0.276104	0.474612	0.472254	0.470844	0.468287	0.466025		

Table S102: Density value (a.u.) at the considered critical points for the  $\text{CH}\equiv\text{C}-\text{CH}_3$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.407289	0.407699	0.410458	0.406086	0.406866	0.411351	0.411490	0.396204	0.273597
(3,-1)	0.273480	0.264434	0.269324	0.266488	0.270775	0.264405	0.266410	0.271919	0.270476
(3,-1)	0.296792	0.287947	0.294988	0.291912	0.296195	0.287651	0.295734	0.289101	0.285746
(3,-1)	0.285144	0.275013	0.282504	0.279281	0.283574	0.275102	0.282824	0.278373	0.273597
(3,-1)	0.285144	0.275013	0.282504	0.279281	0.283574	0.275102	0.282824	0.278373	0.273597
(3,-1)	0.285144	0.275013	0.282504	0.279281	0.283574	0.275102	0.282824	0.278373	0.273597
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.407289	0.353871	0.398964	0.410910	0.406959	0.400039	0.401672	0.405855	0.405120
(3,-1)	0.273480	0.353871	0.270082	0.271508	0.269429	0.266672	0.269841	0.272045	0.268730
(3,-1)	0.296792	0.279017	0.291394	0.296625	0.294256	0.293455	0.288486	0.297009	0.294821
(3,-1)	0.285144	0.279017	0.278785	0.284045	0.281521	0.280925	0.276340	0.284029	0.281259
(3,-1)	0.285144	0.279017	0.278785	0.284045	0.281521	0.280925	0.276340	0.284029	0.281259
(3,-1)	0.285144	0.279017	0.278785	0.284045	0.281521	0.280925	0.276340	0.284029	0.281259
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.407289	0.412213	0.410328	0.418978	0.427417	0.398581	0.403684	0.408540	0.407119
(3,-1)	0.273480	0.262528	0.269989	0.271510	0.267636	0.269713	0.270198	0.269579	0.267944
(3,-1)	0.296792	0.290671	0.298743	0.303473	0.312402	0.295522	0.295515	0.295004	0.294278
(3,-1)	0.285144	0.279681	0.285218	0.290292	0.298505	0.283063	0.283057	0.282519	0.281410
(3,-1)	0.285144	0.279681	0.285218	0.290292	0.298505	0.283063	0.283057	0.282519	0.281410
(3,-1)	0.285144	0.279681	0.285218	0.290292	0.298505	0.283063	0.283057	0.282519	0.281410
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.407289	0.355968	0.410727	0.411059	0.409412	0.406760	0.403502		
(3,-1)	0.273480	0.355968	0.268034	0.280783	0.271934	0.271433	0.270017		
(3,-1)	0.296792	0.278812	0.298817	0.302776	0.296607	0.295694	0.294200		
(3,-1)	0.285144	0.278812	0.283868	0.290211	0.284674	0.283618	0.282378		
(3,-1)	0.285144	0.278812	0.283868	0.290211	0.284674	0.283618	0.282374		
(3,-1)	0.285144	0.278812	0.283868	0.290211	0.284674	0.283618	0.282374		



Table S103: Density value (a.u.) at the considered critical points for the CH<sub>2</sub>=C=CH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.359546	0.353039	0.357848	0.353698	0.356957	0.354590	0.356229	0.351180	0.360082
(3,-1)	0.359546	0.353039	0.357848	0.353698	0.356957	0.354590	0.356229	0.351180	0.360082
(3,-1)	0.288040	0.277674	0.284927	0.281729	0.286193	0.277314	0.285392	0.280227	0.275719
(3,-1)	0.288040	0.277674	0.284927	0.281729	0.286193	0.277314	0.285392	0.280227	0.275719
(3,-1)	0.288040	0.277674	0.284927	0.281729	0.286193	0.277314	0.285392	0.280227	0.275719
(3,-1)	0.288040	0.277674	0.284927	0.281729	0.286193	0.277314	0.285392	0.280227	0.275719
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.359546	0.217711	0.352241	0.359532	0.356124	0.348423	0.352707	0.357267	0.355068
(3,-1)	0.359546	0.238608	0.352241	0.359532	0.356124	0.348423	0.352707	0.357267	0.355068
(3,-1)	0.288040	0.238608	0.281112	0.286719	0.284250	0.283116	0.278793	0.286961	0.284286
(3,-1)	0.288040	0.353577	0.281112	0.286719	0.284250	0.283116	0.278793	0.286961	0.284286
(3,-1)	0.288040	0.281335	0.281112	0.286719	0.284250	0.283116	0.278793	0.286961	0.284286
(3,-1)	0.288040	0.281335	0.281112	0.286719	0.284250	0.283116	0.278793	0.286961	0.284286
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.359546	0.352454	0.358077	0.363328	0.364408	0.352120	0.355162	0.357148	0.355425
(3,-1)	0.359546	0.352454	0.358077	0.363328	0.364408	0.352120	0.355162	0.357148	0.355425
(3,-1)	0.288040	0.281995	0.288171	0.293294	0.302023	0.285890	0.285899	0.285302	0.284142
(3,-1)	0.288040	0.281995	0.288171	0.293294	0.302023	0.285890	0.285899	0.285302	0.284142
(3,-1)	0.288040	0.281995	0.288171	0.293294	0.302023	0.285890	0.285899	0.285302	0.284142
(3,-1)	0.288040	0.281995	0.288171	0.293294	0.302023	0.285890	0.285899	0.285302	0.284142
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.359546	0.216120	0.358175	0.365490	0.359403	0.357719	0.355933		
(3,-1)	0.359546	0.238353	0.358175	0.365490	0.359403	0.357719	0.355933		
(3,-1)	0.288040	0.238353	0.287421	0.293450	0.287249	0.286314	0.284942		
(3,-1)	0.288040	0.356102	0.287421	0.293450	0.287249	0.286314	0.284942		
(3,-1)	0.288040	0.280426	0.287421	0.293450	0.287249	0.286314	0.284942		
(3,-1)	0.288040	0.280426	0.287421	0.293450	0.287249	0.286314	0.284942		

Table S104: Density value (a.u.) at the considered critical points for the C<sub>3</sub>H<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.216391	0.215618	0.214219	0.215910	0.218318	0.213723	0.210365	0.217870	0.222994
(3,-1)	0.238677	0.233229	0.235189	0.234526	0.237784	0.232323	0.232578	0.233951	0.241781
(3,-1)	0.238677	0.233229	0.235189	0.234526	0.237784	0.232323	0.232578	0.233951	0.241781
(3,-1)	0.357168	0.352716	0.356375	0.352881	0.354828	0.355718	0.358349	0.346935	0.360882
(3,-1)	0.289796	0.280397	0.287050	0.284113	0.288313	0.279948	0.287580	0.282691	0.277284
(3,-1)	0.289796	0.280397	0.287050	0.284113	0.288313	0.279948	0.287580	0.282691	0.277284
(3,-1)	0.291480	0.282400	0.289070	0.286234	0.290526	0.282026	0.289974	0.283874	0.280036
(3,-1)	0.291480	0.282400	0.289070	0.286234	0.290526	0.282026	0.289974	0.283874	0.280036
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.216391	0.349672	0.220902	0.215145	0.216814	0.216460	0.220336	0.218092	0.215500
(3,-1)	0.238677	0.281283	0.240384	0.236863	0.236564	0.228844	0.232089	0.238755	0.236678
(3,-1)	0.238677	0.282930	0.240384	0.236863	0.236564	0.228844	0.232089	0.238755	0.236678
(3,-1)	0.357168	0.260698	0.352466	0.357679	0.354760	0.345231	0.345902	0.355574	0.353467
(3,-1)	0.289796	0.282670	0.283259	0.288714	0.286443	0.285482	0.280983	0.288838	0.285999
(3,-1)	0.289796	0.276689	0.283259	0.288714	0.286443	0.285482	0.280983	0.288838	0.285999
(3,-1)	0.291480	0.273953	0.285746	0.290830	0.288674	0.287437	0.282598	0.291302	0.288731
(3,-1)	0.291480	0.273953	0.285746	0.290830	0.288674	0.287437	0.282598	0.291302	0.288731
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.216391	0.190327	0.217619	0.216068	0.213237	0.215613	0.215981	0.214312	0.214087
(3,-1)	0.238677	0.229200	0.235879	0.238279	0.239299	0.236611	0.236698	0.235714	0.234666
(3,-1)	0.238677	0.229200	0.235879	0.238279	0.239299	0.236611	0.236698	0.235714	0.234666
(3,-1)	0.357168	0.357726	0.355758	0.361911	0.367797	0.350650	0.353837	0.357564	0.354265
(3,-1)	0.289796	0.284185	0.289953	0.295330	0.303577	0.287604	0.287660	0.287155	0.286286
(3,-1)	0.289796	0.284185	0.289953	0.295330	0.303577	0.287604	0.287660	0.287155	0.286286
(3,-1)	0.291480	0.285885	0.292535	0.297771	0.306251	0.289973	0.289958	0.289454	0.288664
(3,-1)	0.291480	0.285885	0.292535	0.297771	0.306251	0.289973	0.289958	0.289454	0.288664
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.216391	0.350807	0.213970	0.217487	0.215910	0.217439	0.216845		
(3,-1)	0.238677	0.280648	0.233423	0.243581	0.237344	0.237883	0.236092		
(3,-1)	0.238677	0.282177	0.233423	0.243581	0.237344	0.237883	0.236091		
(3,-1)	0.357168	0.260208	0.356416	0.362526	0.357264	0.355825	0.352484		
(3,-1)	0.289796	0.281430	0.288303	0.294784	0.289336	0.288514	0.287109		
(3,-1)	0.289796	0.276021	0.288303	0.294784	0.289336	0.288514	0.287109		
(3,-1)	0.291480	0.273530	0.292562	0.297264	0.291127	0.290411	0.288815		
(3,-1)	0.291480	0.273530	0.292562	0.297264	0.291127	0.290411	0.288815		

Table S105: Density value (a.u.) at the considered critical points for the CH<sub>2</sub>=CHCH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.354838	0.345972	0.351635	0.347316	0.351537	0.346264	0.349474	0.348420	0.355215
(3,-1)	0.289694	0.280148	0.287159	0.284061	0.288329	0.280081	0.287757	0.282275	0.277065
(3,-1)	0.291192	0.281751	0.288620	0.285538	0.289778	0.281264	0.289190	0.283646	0.278597
(3,-1)	0.265123	0.254284	0.259905	0.256896	0.261919	0.253515	0.256823	0.263619	0.262410
(3,-1)	0.290593	0.281315	0.287948	0.284965	0.289306	0.280468	0.288589	0.283330	0.277851
(3,-1)	0.284702	0.275390	0.282732	0.279579	0.283655	0.276057	0.283066	0.278730	0.273246
(3,-1)	0.282425	0.272696	0.279833	0.276723	0.280878	0.272775	0.280122	0.276176	0.271136
(3,-1)	0.282425	0.272696	0.279833	0.276723	0.280878	0.272775	0.280122	0.276176	0.271136
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.354838	0.206690	0.348440	0.353814	0.350392	0.343499	0.348207	0.352659	0.349361
(3,-1)	0.289694	0.244317	0.283259	0.288814	0.286415	0.285387	0.280669	0.288805	0.286204
(3,-1)	0.291192	0.244317	0.284954	0.290293	0.287900	0.286759	0.282144	0.290340	0.287875
(3,-1)	0.265123	0.244317	0.262781	0.262524	0.260384	0.257884	0.260761	0.263962	0.259705
(3,-1)	0.290593	0.282853	0.284513	0.289755	0.287475	0.286345	0.281694	0.289908	0.287310
(3,-1)	0.284702	0.282853	0.278689	0.284099	0.281607	0.281250	0.276522	0.283822	0.281045
(3,-1)	0.282425	0.282853	0.275868	0.281337	0.278898	0.278595	0.274280	0.281216	0.278554
(3,-1)	0.282425	0.282853	0.275868	0.281337	0.278898	0.278595	0.274280	0.281216	0.278554
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.354838	0.346746	0.352772	0.357584	0.357522	0.347237	0.349949	0.351459	0.349215
(3,-1)	0.289694	0.284269	0.290105	0.295305	0.303742	0.287497	0.287570	0.287153	0.286369
(3,-1)	0.291192	0.285744	0.291699	0.296914	0.305288	0.289051	0.289123	0.288661	0.287832
(3,-1)	0.265123	0.254485	0.261086	0.262669	0.258789	0.261340	0.261657	0.260776	0.258784
(3,-1)	0.290593	0.285293	0.290941	0.296254	0.303816	0.288805	0.288836	0.288325	0.287421
(3,-1)	0.284702	0.279664	0.285043	0.289990	0.297865	0.282687	0.282720	0.282325	0.281542
(3,-1)	0.282425	0.277026	0.282522	0.287419	0.295637	0.280330	0.280313	0.279773	0.278773
(3,-1)	0.282425	0.277026	0.282522	0.287419	0.295637	0.280330	0.280313	0.279773	0.278773
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.354838	0.203789	0.352909	0.362977	0.354156	0.352713	0.351329		
(3,-1)	0.289694	0.243783	0.288971	0.294956	0.289334	0.288414	0.286995		
(3,-1)	0.291192	0.243783	0.290723	0.296434	0.290830	0.289917	0.288542		
(3,-1)	0.265123	0.243783	0.258635	0.274351	0.263361	0.263000	0.261865		
(3,-1)	0.290593	0.282051	0.290145	0.296269	0.290216	0.289431	0.287937		
(3,-1)	0.284702	0.282051	0.283166	0.289630	0.284515	0.283417	0.282103		
(3,-1)	0.282425	0.282051	0.280567	0.287093	0.281964	0.280953	0.279667		
(3,-1)	0.282425	0.282051	0.280567	0.287093	0.281964	0.280953	0.279667		

Table S106: Density value (a.u.) at the considered critical points for the C<sub>3</sub>H<sub>6</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.203761	0.199449	0.199171	0.200499	0.204171	0.197083	0.195947	0.202334	0.208667
(3,-1)	0.244756	0.237286	0.240906	0.239284	0.243006	0.236564	0.238508	0.240547	0.247884
(3,-1)	0.244756	0.237286	0.240906	0.239284	0.243006	0.236564	0.238508	0.240547	0.247884
(3,-1)	0.244756	0.237286	0.240906	0.239284	0.243006	0.236564	0.238508	0.240547	0.247884
(3,-1)	0.291198	0.281923	0.288797	0.285702	0.289807	0.281399	0.289177	0.284132	0.279127
(3,-1)	0.291198	0.281923	0.288797	0.285702	0.289807	0.281399	0.289177	0.284132	0.279127
(3,-1)	0.291198	0.281923	0.288797	0.285702	0.289807	0.281399	0.289177	0.284132	0.279127
(3,-1)	0.291198	0.281923	0.288797	0.285702	0.289807	0.281399	0.289177	0.284132	0.279127
(3,-1)	0.291198	0.281923	0.288797	0.285702	0.289807	0.281399	0.289177	0.284132	0.279127
(3,-1)	0.291198	0.281923	0.288797	0.285702	0.289807	0.281399	0.289177	0.284132	0.279127
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.203761	0.248434	0.208402	0.201002	0.202584	0.200306	0.204003	0.205140	0.201750
(3,-1)	0.244756	0.248434	0.245698	0.242786	0.241731	0.233932	0.237401	0.244407	0.241783
(3,-1)	0.244756	0.276784	0.245698	0.242786	0.241731	0.233932	0.237401	0.244407	0.241783
(3,-1)	0.244756	0.276784	0.245698	0.242786	0.241731	0.233932	0.237401	0.244407	0.241783
(3,-1)	0.291198	0.275834	0.284736	0.290325	0.287888	0.286726	0.282328	0.290199	0.287578
(3,-1)	0.291198	0.275834	0.284736	0.290325	0.287888	0.286726	0.282328	0.290199	0.287578
(3,-1)	0.291198	0.275165	0.284736	0.290325	0.287888	0.286726	0.282328	0.290199	0.287578
(3,-1)	0.291198	0.275165	0.284736	0.290325	0.287888	0.286726	0.282328	0.290199	0.287578
(3,-1)	0.291198	0.275165	0.284736	0.290325	0.287888	0.286726	0.282328	0.290199	0.287578
(3,-1)	0.291198	0.275165	0.284736	0.290325	0.287888	0.286726	0.282328	0.290199	0.287578
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.203761	0.177581	0.203878	0.202645	0.203798	0.202976	0.203057	0.201299	0.200212
(3,-1)	0.244756	0.236203	0.240419	0.243167	0.243105	0.242207	0.242261	0.241550	0.239910
(3,-1)	0.244756	0.236203	0.240419	0.243167	0.243105	0.242207	0.242261	0.241550	0.239910
(3,-1)	0.244756	0.236203	0.240419	0.243167	0.243105	0.242207	0.242261	0.241550	0.239910
(3,-1)	0.291198	0.285458	0.291556	0.296722	0.304915	0.289083	0.289162	0.288692	0.287755
(3,-1)	0.291198	0.285458	0.291556	0.296722	0.304915	0.289083	0.289162	0.288692	0.287755
(3,-1)	0.291198	0.285458	0.291556	0.296722	0.304915	0.289083	0.289162	0.288692	0.287755
(3,-1)	0.291198	0.285458	0.291556	0.296722	0.304915	0.289083	0.289162	0.288692	0.287755
(3,-1)	0.291198	0.285458	0.291556	0.296722	0.304915	0.289083	0.289162	0.288692	0.287755
(3,-1)	0.291198	0.285458	0.291556	0.296722	0.304915	0.289083	0.289162	0.288692	0.287755
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.203761	0.247695	0.197934	0.207444	0.202269	0.204147	0.203970		
(3,-1)	0.244756	0.247695	0.238228	0.250922	0.243337	0.243444	0.241539		
(3,-1)	0.244756	0.275806	0.238228	0.250922	0.243337	0.243444	0.241539		
(3,-1)	0.244756	0.275806	0.238228	0.250922	0.243337	0.243444	0.241542		
(3,-1)	0.291198	0.275163	0.290265	0.295989	0.290879	0.289861	0.288561		
(3,-1)	0.291198	0.275163	0.290265	0.295989	0.290879	0.289861	0.288561		
(3,-1)	0.291198	0.274567	0.290265	0.295989	0.290879	0.289861	0.288563		
(3,-1)	0.291198	0.274567	0.290265	0.295989	0.290879	0.289861	0.288564		
(3,-1)	0.291198	0.274567	0.290265	0.295989	0.290879	0.289861	0.288564		
(3,-1)	0.291198	0.274567	0.290265	0.295989	0.290879	0.289861	0.288564		

Table S107: Density value (a.u.) at the considered critical points for the C<sub>3</sub>H<sub>8</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.251951	0.241152	0.246936	0.244058	0.249020	0.240501	0.243693	0.250984	0.250355
(3,-1)	0.251951	0.241152	0.246936	0.244058	0.249020	0.240501	0.243693	0.250984	0.250355
(3,-1)	0.284884	0.275775	0.282511	0.279516	0.283523	0.275840	0.282880	0.278833	0.273082
(3,-1)	0.284884	0.275775	0.282511	0.279516	0.283523	0.275840	0.282880	0.278833	0.273082
(3,-1)	0.283827	0.274632	0.281622	0.278564	0.282569	0.274777	0.281956	0.277898	0.272488
(3,-1)	0.283827	0.274632	0.281622	0.278564	0.282569	0.274777	0.281956	0.277898	0.272488
(3,-1)	0.283292	0.274097	0.281177	0.278108	0.282102	0.274657	0.281519	0.277398	0.271976
(3,-1)	0.283292	0.274097	0.281177	0.278108	0.282102	0.274657	0.281519	0.277398	0.271976
(3,-1)	0.283292	0.274097	0.281177	0.278108	0.282102	0.274657	0.281519	0.277398	0.271976
(3,-1)	0.283292	0.274097	0.281177	0.278108	0.282102	0.274657	0.281519	0.277398	0.271976
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.251951	0.283171	0.250691	0.249416	0.247373	0.244542	0.247486	0.250948	0.246734
(3,-1)	0.251951	0.346637	0.250691	0.249416	0.247373	0.244542	0.247486	0.250948	0.246734
(3,-1)	0.284884	0.283847	0.278404	0.283973	0.281619	0.281131	0.276739	0.283739	0.281013
(3,-1)	0.284884	0.346637	0.278404	0.283973	0.281619	0.281131	0.276739	0.283739	0.281013
(3,-1)	0.283827	0.283847	0.277650	0.283017	0.280603	0.280196	0.275865	0.282772	0.280176
(3,-1)	0.283827	0.281926	0.277650	0.283017	0.280603	0.280196	0.275865	0.282772	0.280176
(3,-1)	0.283292	0.282394	0.276998	0.282534	0.280109	0.279790	0.275294	0.282236	0.279547
(3,-1)	0.283292	0.282394	0.276998	0.282534	0.280109	0.279790	0.275294	0.282236	0.279547
(3,-1)	0.283292	0.281926	0.276998	0.282534	0.280109	0.279790	0.275294	0.282236	0.279547
(3,-1)	0.283292	0.281926	0.276998	0.282534	0.280109	0.279790	0.275294	0.282236	0.279547
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.251951	0.241450	0.247451	0.249044	0.244916	0.248651	0.248709	0.247623	0.245719
(3,-1)	0.251951	0.241450	0.247451	0.249044	0.244916	0.248651	0.248709	0.247623	0.245719
(3,-1)	0.284884	0.279718	0.284943	0.289943	0.297634	0.282783	0.282833	0.282396	0.281489
(3,-1)	0.284884	0.279718	0.284943	0.289943	0.297634	0.282783	0.282833	0.282396	0.281489
(3,-1)	0.283827	0.278712	0.284140	0.289031	0.297079	0.281752	0.281780	0.281353	0.280487
(3,-1)	0.283827	0.278712	0.284140	0.289031	0.297079	0.281752	0.281780	0.281353	0.280487
(3,-1)	0.283292	0.278188	0.283549	0.288432	0.296462	0.281180	0.281215	0.280818	0.279994
(3,-1)	0.283292	0.278188	0.283549	0.288432	0.296462	0.281180	0.281215	0.280818	0.279994
(3,-1)	0.283292	0.278188	0.283549	0.288432	0.296462	0.281180	0.281215	0.280818	0.279994
(3,-1)	0.283292	0.278188	0.283549	0.288432	0.296462	0.281180	0.281215	0.280818	0.279994
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.251951	0.282913	0.244770	0.260976	0.250255	0.249901	0.248815		
(3,-1)	0.251951	0.347729	0.244770	0.260976	0.250255	0.249901	0.248815		
(3,-1)	0.284884	0.283063	0.282952	0.289296	0.284528	0.283555	0.282176		
(3,-1)	0.284884	0.347729	0.282952	0.289296	0.284528	0.283555	0.282176		
(3,-1)	0.283827	0.283063	0.282094	0.288321	0.283547	0.282516	0.281206		
(3,-1)	0.283827	0.281274	0.282094	0.288321	0.283547	0.282516	0.281206		
(3,-1)	0.283292	0.281195	0.281331	0.287761	0.283050	0.281998	0.280663		
(3,-1)	0.283292	0.281195	0.281331	0.287761	0.283050	0.281998	0.280663		
(3,-1)	0.283292	0.281274	0.281331	0.287761	0.283050	0.281998	0.280663		
(3,-1)	0.283292	0.281274	0.281331	0.287761	0.283050	0.281998	0.280663		

Table S108: Density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>6</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.288854	0.277823	0.283202	0.279909	0.285083	0.276861	0.280242	0.286286	0.284862
(3,-1)	0.351712	0.342921	0.348734	0.344395	0.348607	0.343298	0.346435	0.346049	0.351924
(3,-1)	0.291968	0.282628	0.289467	0.286410	0.290679	0.282024	0.290085	0.284438	0.279432
(3,-1)	0.351712	0.342921	0.348734	0.344395	0.348607	0.343298	0.346435	0.346049	0.351924
(3,-1)	0.291968	0.282628	0.289467	0.286410	0.290679	0.282024	0.290085	0.284438	0.279432
(3,-1)	0.290212	0.280811	0.287792	0.284719	0.288990	0.280690	0.288410	0.282852	0.277674
(3,-1)	0.290319	0.280881	0.287881	0.284795	0.289174	0.280730	0.288503	0.283057	0.277437
(3,-1)	0.290319	0.280881	0.287881	0.284795	0.289174	0.280730	0.288503	0.283057	0.277437
(3,-1)	0.290212	0.280811	0.287792	0.284719	0.288990	0.280690	0.288410	0.282852	0.277674
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.288854	0.399200	0.284628	0.286087	0.283727	0.280772	0.284341	0.287196	0.283003
(3,-1)	0.351712	0.267414	0.345682	0.350852	0.347404	0.340729	0.345426	0.349710	0.346255
(3,-1)	0.291968	0.267414	0.285951	0.291168	0.288802	0.287678	0.282941	0.291288	0.288801
(3,-1)	0.351712	0.276197	0.345682	0.350852	0.347404	0.340729	0.345426	0.349710	0.346255
(3,-1)	0.291968	0.276197	0.285951	0.291168	0.288802	0.287678	0.282941	0.291288	0.288801
(3,-1)	0.290212	0.276197	0.283988	0.289451	0.287073	0.286076	0.281227	0.289487	0.286879
(3,-1)	0.290319	0.276197	0.284319	0.289630	0.287258	0.286176	0.281268	0.289710	0.286965
(3,-1)	0.290319	0.276197	0.284319	0.289630	0.287258	0.286176	0.281268	0.289710	0.286965
(3,-1)	0.290212	0.276197	0.283988	0.289451	0.287073	0.286076	0.281227	0.289487	0.286879
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.288854	0.277706	0.285295	0.287131	0.283857	0.284382	0.285096	0.284465	0.282134
(3,-1)	0.351712	0.343475	0.349729	0.354351	0.354002	0.344161	0.346819	0.348286	0.346230
(3,-1)	0.291968	0.286565	0.292607	0.297849	0.306109	0.289995	0.290052	0.289581	0.288734
(3,-1)	0.351712	0.343475	0.349729	0.354351	0.354002	0.344161	0.346819	0.348286	0.346230
(3,-1)	0.291968	0.286565	0.292607	0.297849	0.306109	0.289995	0.290052	0.289581	0.288734
(3,-1)	0.290212	0.284837	0.290757	0.295989	0.304323	0.288167	0.288227	0.287802	0.287027
(3,-1)	0.290319	0.285006	0.290605	0.295877	0.303315	0.288473	0.288531	0.288085	0.287255
(3,-1)	0.290319	0.285006	0.290605	0.295877	0.303315	0.288473	0.288531	0.288085	0.287255
(3,-1)	0.290212	0.284837	0.290757	0.295989	0.304323	0.288167	0.288227	0.287802	0.287027
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.288854	0.404210	0.283563	0.298606	0.286828	0.286418	0.285211		
(3,-1)	0.351712	0.267868	0.349780	0.359919	0.351098	0.349601	0.348209		
(3,-1)	0.291968	0.267868	0.291807	0.297453	0.291630	0.290747	0.289342		
(3,-1)	0.351712	0.275659	0.349780	0.359919	0.351098	0.349601	0.348209		
(3,-1)	0.291968	0.275659	0.291807	0.297453	0.291630	0.290747	0.289342		
(3,-1)	0.290212	0.275659	0.289791	0.295656	0.289893	0.288990	0.287550		
(3,-1)	0.290319	0.275659	0.289925	0.296199	0.289959	0.289073	0.287564		
(3,-1)	0.290319	0.275659	0.289925	0.296199	0.289959	0.289073	0.287564		
(3,-1)	0.290212	0.275659	0.289791	0.295656	0.289893	0.288990	0.287550		

Table S109: Density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>6</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.403536	0.403656	0.406610	0.402331	0.403162	0.407469	0.407858	0.392554	0.414740
(3,-1)	0.272756	0.263577	0.268543	0.265675	0.270009	0.263708	0.265601	0.270786	0.269753
(3,-1)	0.272756	0.263577	0.268543	0.265675	0.270009	0.263708	0.265601	0.270786	0.269753
(3,-1)	0.284665	0.274610	0.282015	0.278822	0.283097	0.274757	0.282340	0.277994	0.273179
(3,-1)	0.284665	0.274610	0.282015	0.278822	0.283097	0.274757	0.282340	0.277994	0.273179
(3,-1)	0.284665	0.274610	0.282015	0.278822	0.283097	0.274757	0.282340	0.277994	0.273179
(3,-1)	0.284665	0.274610	0.282015	0.278822	0.283097	0.274757	0.282340	0.277994	0.273179
(3,-1)	0.284665	0.274610	0.282015	0.278822	0.283097	0.274757	0.282340	0.277994	0.273179
(3,-1)	0.284665	0.274610	0.282015	0.278822	0.283097	0.274757	0.282340	0.277994	0.273179
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.403536	0.263416	0.396289	0.407084	0.403239	0.396521	0.398220	0.402419	0.401690
(3,-1)	0.272756	0.263416	0.269340	0.270755	0.268649	0.265377	0.268755	0.271285	0.267988
(3,-1)	0.272756	0.206638	0.269340	0.270755	0.268649	0.265377	0.268755	0.271285	0.267988
(3,-1)	0.284665	0.228990	0.278288	0.283563	0.281064	0.280499	0.275961	0.283542	0.280753
(3,-1)	0.284665	0.348414	0.278288	0.283563	0.281064	0.280499	0.275961	0.283542	0.280753
(3,-1)	0.284665	0.279998	0.278288	0.283563	0.281064	0.280499	0.275961	0.283542	0.280753
(3,-1)	0.284665	0.279998	0.278288	0.283563	0.281064	0.280499	0.275961	0.283542	0.280753
(3,-1)	0.284665	0.279998	0.278288	0.283563	0.281064	0.280499	0.275961	0.283542	0.280753
(3,-1)	0.284665	0.279998	0.278288	0.283563	0.281064	0.280499	0.275961	0.283542	0.280753
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.403536	0.409552	0.406587	0.414912	0.424437	0.394951	0.399976	0.404921	0.403465
(3,-1)	0.272756	0.261634	0.269215	0.270822	0.267439	0.268934	0.269436	0.268810	0.267179
(3,-1)	0.272756	0.261634	0.269215	0.270822	0.267439	0.268934	0.269436	0.268810	0.267179
(3,-1)	0.284665	0.279265	0.284731	0.289806	0.298006	0.282586	0.282581	0.282045	0.280943
(3,-1)	0.284665	0.279265	0.284731	0.289806	0.298006	0.282586	0.282581	0.282045	0.280943
(3,-1)	0.284665	0.279265	0.284731	0.289806	0.298006	0.282586	0.282581	0.282045	0.280943
(3,-1)	0.284665	0.279265	0.284731	0.289806	0.298006	0.282586	0.282581	0.282045	0.280943
(3,-1)	0.284665	0.279265	0.284731	0.289806	0.298006	0.282586	0.282581	0.282045	0.280943
(3,-1)	0.284665	0.279265	0.284731	0.289806	0.298006	0.282586	0.282581	0.282045	0.280943
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.403536	0.263204	0.406577	0.407396	0.405573	0.403017	0.399543		
(3,-1)	0.272756	0.263204	0.267314	0.280230	0.271166	0.270650	0.269240		
(3,-1)	0.272756	0.204124	0.267314	0.280230	0.271166	0.270650	0.269240		
(3,-1)	0.284665	0.228340	0.283250	0.289699	0.284189	0.283152	0.281887		
(3,-1)	0.284665	0.350163	0.283250	0.289699	0.284189	0.283152	0.281883		
(3,-1)	0.284665	0.279472	0.283250	0.289699	0.284189	0.283152	0.281883		
(3,-1)	0.284665	0.279472	0.283250	0.289699	0.284189	0.283152	0.281887		
(3,-1)	0.284665	0.279472	0.283250	0.289699	0.284189	0.283152	0.281883		
(3,-1)	0.284665	0.279472	0.283250	0.289699	0.284189	0.283152	0.281883		

Table S110: Density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>6</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.265073	0.257488	0.261199	0.259176	0.262918	0.257696	0.259333	0.260232	0.266998
(3,-1)	0.265073	0.257488	0.261199	0.259176	0.262918	0.257696	0.259333	0.260232	0.266998
(3,+1)	0.204064	0.200770	0.200062	0.201633	0.205038	0.198328	0.196414	0.203605	0.209688
(3,-1)	0.229195	0.221915	0.224796	0.223829	0.227733	0.220598	0.222085	0.225249	0.232491
(3,-1)	0.353864	0.346027	0.351163	0.346992	0.350744	0.346987	0.349514	0.345458	0.354354
(3,-1)	0.288606	0.278940	0.285951	0.282827	0.287062	0.278396	0.286321	0.281487	0.276775
(3,-1)	0.288606	0.278940	0.285951	0.282827	0.287062	0.278396	0.286321	0.281487	0.276775
(3,-1)	0.288606	0.278940	0.285951	0.282827	0.287062	0.278396	0.286321	0.281487	0.276775
(3,-1)	0.288606	0.278940	0.285951	0.282827	0.287062	0.278396	0.286321	0.281487	0.276775
(3,-1)	0.289999	0.280316	0.287209	0.284164	0.288482	0.279684	0.287800	0.282443	0.277399
(3,-1)	0.289999	0.280316	0.287209	0.284164	0.288482	0.279684	0.287800	0.282443	0.277399
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.265073	0.250317	0.264563	0.263307	0.261911	0.253849	0.257201	0.264483	0.261516
(3,-1)	0.265073	0.248128	0.264563	0.263307	0.261911	0.253849	0.257201	0.264483	0.261516
(3,+1)	0.204064	0.275798	0.208750	0.201688	0.203431	0.201871	0.205648	0.205680	0.202470
(3,-1)	0.229195	0.248128	0.230797	0.226788	0.226335	0.219100	0.222562	0.229117	0.226554
(3,-1)	0.353864	0.275798	0.347152	0.353193	0.349839	0.341224	0.345939	0.351661	0.348810
(3,-1)	0.288606	0.275204	0.281889	0.287563	0.285119	0.284041	0.279768	0.287569	0.284820
(3,-1)	0.288606	0.275204	0.281889	0.287563	0.285119	0.284041	0.279768	0.287569	0.284820
(3,-1)	0.288606	0.275204	0.281889	0.287563	0.285119	0.284041	0.279768	0.287569	0.284820
(3,-1)	0.288606	0.275204	0.281889	0.287563	0.285119	0.284041	0.279768	0.287569	0.284820
(3,-1)	0.289999	0.275462	0.283522	0.288939	0.286596	0.285559	0.280998	0.289131	0.286566
(3,-1)	0.289999	0.275462	0.283522	0.288939	0.286596	0.285559	0.280998	0.289131	0.286566
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.265073	0.257562	0.260551	0.263752	0.263042	0.261973	0.262431	0.262223	0.260291
(3,-1)	0.265073	0.257562	0.260551	0.263752	0.263042	0.261973	0.262431	0.262223	0.260291
(3,+1)	0.204064	0.178697	0.204413	0.203048	0.202480	0.203724	0.203551	0.201357	0.200918
(3,-1)	0.229195	0.219369	0.225306	0.227610	0.227553	0.227403	0.227113	0.225767	0.224389
(3,-1)	0.353864	0.347126	0.351640	0.356974	0.357904	0.346324	0.349193	0.350996	0.348919
(3,-1)	0.288606	0.282648	0.288791	0.293966	0.302209	0.286527	0.286571	0.286042	0.284998
(3,-1)	0.288606	0.282648	0.288791	0.293966	0.302209	0.286527	0.286571	0.286042	0.284998
(3,-1)	0.288606	0.282648	0.288791	0.293966	0.302209	0.286527	0.286571	0.286042	0.284998
(3,-1)	0.288606	0.282648	0.288791	0.293966	0.302209	0.286527	0.286571	0.286042	0.284998
(3,-1)	0.289999	0.284418	0.290503	0.295697	0.304276	0.287893	0.287918	0.287409	0.286518
(3,-1)	0.289999	0.284418	0.290503	0.295697	0.304276	0.287893	0.287918	0.287409	0.286518
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.265073	0.249319	0.259110	0.272221	0.263656	0.263590	0.261330		
(3,-1)	0.265073	0.247430	0.259110	0.272221	0.263656	0.263590	0.261330		
(3,+1)	0.204064	0.275134	0.199379	0.207183	0.202781	0.204677	0.204266		
(3,-1)	0.229195	0.247430	0.222601	0.235199	0.227507	0.228097	0.226447		
(3,-1)	0.353864	0.275134	0.352033	0.361350	0.353293	0.351808	0.350019		
(3,-1)	0.288606	0.274612	0.287689	0.293611	0.288121	0.287126	0.285798		
(3,-1)	0.288606	0.274612	0.287689	0.293611	0.288121	0.287126	0.285798		
(3,-1)	0.288606	0.274612	0.287689	0.293611	0.288121	0.287126	0.285798		
(3,-1)	0.288606	0.274612	0.287689	0.293611	0.288121	0.287126	0.285798		
(3,-1)	0.289999	0.274607	0.289539	0.295239	0.289512	0.288660	0.287272		
(3,-1)	0.289999	0.274607	0.289539	0.295239	0.289512	0.288660	0.287272		



Table S111: Density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>10</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.251064	0.242967	0.248630	0.245752	0.250745	0.242188	0.245319	0.252917	0.252146
(3,-1)	0.248981	0.240803	0.246654	0.243751	0.248734	0.240309	0.243403	0.250732	0.250028
(3,-1)	0.280983	0.274591	0.281581	0.278523	0.282525	0.274809	0.281897	0.277866	0.272480
(3,-1)	0.248981	0.240803	0.246654	0.243751	0.248734	0.240309	0.243403	0.250732	0.250028
(3,-1)	0.280983	0.274591	0.281581	0.278523	0.282525	0.274809	0.281897	0.277866	0.272480
(3,-1)	0.280532	0.274143	0.281227	0.278153	0.282141	0.274728	0.281544	0.277431	0.272025
(3,-1)	0.280532	0.274143	0.281227	0.278153	0.282141	0.274728	0.281544	0.277431	0.272025
(3,-1)	0.280532	0.274143	0.281227	0.278153	0.282141	0.274728	0.281544	0.277431	0.272025
(3,-1)	0.280794	0.274470	0.281360	0.278336	0.282354	0.275014	0.281701	0.277719	0.271896
(3,-1)	0.280794	0.274470	0.281360	0.278336	0.282354	0.275014	0.281701	0.277719	0.271896
(3,-1)	0.280794	0.274470	0.281360	0.278336	0.282354	0.275014	0.281701	0.277719	0.271896
(3,-1)	0.280794	0.274470	0.281360	0.278336	0.282354	0.275014	0.281701	0.277719	0.271896
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.251064	0.276763	0.252455	0.251172	0.249135	0.246171	0.249313	0.252676	0.248428
(3,-1)	0.248981	0.249729	0.250341	0.249139	0.247078	0.244277	0.247229	0.250641	0.246410
(3,-1)	0.280983	0.273858	0.277618	0.282975	0.280560	0.280155	0.275836	0.282726	0.280136
(3,-1)	0.248981	0.275155	0.250341	0.249139	0.247078	0.244277	0.247229	0.250641	0.246410
(3,-1)	0.280983	0.275155	0.277618	0.282975	0.280560	0.280155	0.275836	0.282726	0.280136
(3,-1)	0.280532	0.249729	0.277058	0.282580	0.280149	0.279830	0.275331	0.282275	0.279591
(3,-1)	0.280532	0.273858	0.277058	0.282580	0.280149	0.279830	0.275331	0.282275	0.279591
(3,-1)	0.280532	0.275155	0.277058	0.282580	0.280149	0.279830	0.275331	0.282275	0.279591
(3,-1)	0.280532	0.275155	0.277058	0.282580	0.280149	0.279830	0.275331	0.282275	0.279591
(3,-1)	0.280794	0.249729	0.277017	0.282789	0.280414	0.280056	0.275554	0.282491	0.279625
(3,-1)	0.280794	0.273858	0.277017	0.282789	0.280414	0.280056	0.275554	0.282491	0.279625
(3,-1)	0.280794	0.275155	0.277017	0.282789	0.280414	0.280056	0.275554	0.282491	0.279625
(3,-1)	0.280794	0.275155	0.277017	0.282789	0.280414	0.280056	0.275554	0.282491	0.279625
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.251064	0.243022	0.249143	0.250755	0.246315	0.250477	0.250534	0.249406	0.247430
(3,-1)	0.248981	0.241132	0.247158	0.248736	0.244681	0.248329	0.248398	0.247326	0.245452
(3,-1)	0.280983	0.278663	0.284100	0.288989	0.297039	0.281702	0.281730	0.281295	0.280441
(3,-1)	0.248981	0.241132	0.247158	0.248736	0.244681	0.248329	0.248398	0.247326	0.245452
(3,-1)	0.280983	0.278663	0.284100	0.288989	0.297039	0.281702	0.281730	0.281295	0.280441
(3,-1)	0.280532	0.278234	0.283587	0.288480	0.296529	0.281214	0.281246	0.280838	0.280032
(3,-1)	0.280532	0.278234	0.283587	0.288480	0.296529	0.281214	0.281246	0.280838	0.280032
(3,-1)	0.280532	0.278234	0.283587	0.288480	0.296529	0.281214	0.281246	0.280838	0.280032
(3,-1)	0.280794	0.278463	0.283640	0.288602	0.296336	0.281478	0.281539	0.281141	0.280310
(3,-1)	0.280794	0.278463	0.283640	0.288602	0.296336	0.281478	0.281539	0.281141	0.280310
(3,-1)	0.280794	0.278463	0.283640	0.288602	0.296336	0.281478	0.281539	0.281141	0.280310
(3,-1)	0.280794	0.278463	0.283640	0.288602	0.296336	0.281478	0.281539	0.281141	0.280310
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.251064	0.275539	0.246684	0.262884	0.251940	0.251596	0.250464		
(3,-1)	0.248981	0.248713	0.244541	0.260733	0.249921	0.249550	0.248447		
(3,-1)	0.280983	0.273418	0.282042	0.288281	0.283491	0.282457	0.281144		
(3,-1)	0.248981	0.274579	0.244541	0.260733	0.249921	0.249550	0.248447		
(3,-1)	0.280983	0.274579	0.282042	0.288281	0.283491	0.282457	0.281144		
(3,-1)	0.280532	0.248713	0.281370	0.287802	0.283096	0.282036	0.280704		
(3,-1)	0.280532	0.273418	0.281370	0.287802	0.283096	0.282036	0.280704		
(3,-1)	0.280532	0.274579	0.281370	0.287802	0.283096	0.282036	0.280704		
(3,-1)	0.280794	0.248713	0.281556	0.288081	0.283264	0.282258	0.280829		
(3,-1)	0.280794	0.273418	0.281556	0.288081	0.283264	0.282258	0.280829		
(3,-1)	0.280794	0.274579	0.281556	0.288081	0.283264	0.282258	0.280829		
(3,-1)	0.280794	0.274579	0.281556	0.288081	0.283264	0.282258	0.280829		

Table S112: Density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>10</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.282078	0.275778	0.282362	0.279421	0.283491	0.275649	0.282776	0.278896	0.272714
(3,-1)	0.250442	0.242346	0.247960	0.245111	0.250122	0.241145	0.244663	0.252316	0.251554
(3,-1)	0.279223	0.272819	0.280085	0.276980	0.280990	0.273879	0.280410	0.276310	0.270814
(3,-1)	0.280404	0.274039	0.281182	0.278082	0.282081	0.274762	0.281486	0.277355	0.271855
(3,-1)	0.280404	0.274039	0.281182	0.278082	0.282081	0.274762	0.281486	0.277355	0.271855
(3,-1)	0.250442	0.242346	0.247960	0.245111	0.250122	0.241145	0.244663	0.252316	0.251554
(3,-1)	0.279223	0.272819	0.280085	0.276980	0.280990	0.273879	0.280410	0.276310	0.270814
(3,-1)	0.280405	0.274039	0.281182	0.278082	0.282081	0.274762	0.281486	0.277355	0.271855
(3,-1)	0.280404	0.274039	0.281182	0.278082	0.282081	0.274762	0.281486	0.277355	0.271855
(3,-1)	0.250442	0.242346	0.247960	0.245111	0.250122	0.241145	0.244663	0.252316	0.251554
(3,-1)	0.279223	0.272819	0.280085	0.276980	0.280990	0.273879	0.280410	0.276310	0.270814
(3,-1)	0.280404	0.274039	0.281182	0.278082	0.282081	0.274762	0.281486	0.277355	0.271855
(3,-1)	0.280405	0.274039	0.281182	0.278082	0.282081	0.274762	0.281486	0.277355	0.271855
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.282078	0.255895	0.277987	0.283906	0.281617	0.281032	0.276692	0.283667	0.280767
(3,-1)	0.250442	0.255895	0.251812	0.250518	0.248509	0.245459	0.248709	0.252047	0.247852
(3,-1)	0.279223	0.206578	0.275623	0.281410	0.278956	0.278784	0.274112	0.281036	0.278171
(3,-1)	0.280404	0.234426	0.276964	0.282534	0.280082	0.279769	0.275270	0.282200	0.279477
(3,-1)	0.280404	0.255895	0.276964	0.282534	0.280082	0.279769	0.275270	0.282200	0.279477
(3,-1)	0.250442	0.255895	0.251812	0.250518	0.248509	0.245459	0.248709	0.252047	0.247852
(3,-1)	0.279223	0.206578	0.275623	0.281410	0.278956	0.278784	0.274112	0.281036	0.278171
(3,-1)	0.280405	0.234426	0.276964	0.282534	0.280082	0.279769	0.275270	0.282200	0.279477
(3,-1)	0.280404	0.281426	0.276964	0.282534	0.280082	0.279769	0.275270	0.282200	0.279477
(3,-1)	0.250442	0.281426	0.251812	0.250518	0.248509	0.245459	0.248709	0.252047	0.247852
(3,-1)	0.279223	0.281426	0.275623	0.281410	0.278956	0.278784	0.274112	0.281036	0.278171
(3,-1)	0.280404	0.281426	0.276964	0.282534	0.280082	0.279769	0.275270	0.282200	0.279477
(3,-1)	0.280405	0.281426	0.276964	0.282534	0.280082	0.279769	0.275270	0.282200	0.279477
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.282078	0.279620	0.284716	0.289812	0.297205	0.282748	0.282831	0.282433	0.281504
(3,-1)	0.250442	0.242417	0.248517	0.250154	0.245765	0.249876	0.249928	0.248800	0.246813
(3,-1)	0.279223	0.276953	0.282294	0.287143	0.295226	0.279924	0.279978	0.279620	0.278874
(3,-1)	0.280404	0.278135	0.283522	0.288406	0.296503	0.281109	0.281161	0.280776	0.279988
(3,-1)	0.280404	0.278135	0.283522	0.288406	0.296503	0.281109	0.281161	0.280776	0.279988
(3,-1)	0.250442	0.242417	0.248517	0.250154	0.245765	0.249876	0.249928	0.248800	0.246813
(3,-1)	0.279223	0.276953	0.282294	0.287143	0.295226	0.279924	0.279978	0.279620	0.278874
(3,-1)	0.280405	0.278135	0.283522	0.288406	0.296503	0.281109	0.281161	0.280776	0.279988
(3,-1)	0.280404	0.278135	0.283522	0.288406	0.296503	0.281109	0.281161	0.280776	0.279988
(3,-1)	0.250442	0.242417	0.248517	0.250154	0.245765	0.249876	0.249928	0.248800	0.246813
(3,-1)	0.279223	0.276953	0.282294	0.287143	0.295226	0.279924	0.279978	0.279620	0.278874
(3,-1)	0.280404	0.278135	0.283522	0.288406	0.296503	0.281109	0.281161	0.280776	0.279988
(3,-1)	0.280405	0.278135	0.283522	0.288406	0.296503	0.281109	0.281161	0.280776	0.279988
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.282078	0.255365	0.283002	0.289288	0.284397	0.283494	0.281971		
(3,-1)	0.250442	0.255365	0.246093	0.262200	0.251283	0.250972	0.249811		
(3,-1)	0.279223	0.203928	0.280001	0.286620	0.281840	0.280745	0.279377		
(3,-1)	0.280404	0.233713	0.281415	0.287795	0.282984	0.281900	0.280562		
(3,-1)	0.280404	0.255365	0.281415	0.287795	0.282984	0.281900	0.280562		
(3,-1)	0.250442	0.255365	0.246093	0.262200	0.251283	0.250972	0.249813		
(3,-1)	0.279223	0.203928	0.280001	0.286620	0.281840	0.280745	0.279377		
(3,-1)	0.280405	0.233713	0.281415	0.287795	0.282984	0.281900	0.280562		
(3,-1)	0.280404	0.280703	0.281415	0.287795	0.282984	0.281900	0.280564		
(3,-1)	0.250442	0.280703	0.246093	0.262200	0.251283	0.250972	0.249813		
(3,-1)	0.279223	0.280703	0.280001	0.286620	0.281840	0.280745	0.279377		
(3,-1)	0.280404	0.280703	0.281415	0.287795	0.282984	0.281900	0.280564		
(3,-1)	0.280405	0.280703	0.281415	0.287795	0.282984	0.281900	0.280562		



Table S113: Density value (a.u.) at the considered critical points for the  $C_5H_8$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.253723	0.249324	0.252891	0.251040	0.254757	0.248899	0.250740	0.252101	0.259384
(3,-1)	0.253723	0.249324	0.252891	0.251040	0.254757	0.248899	0.250740	0.252101	0.259384
(3,+1)	0.201408	0.200369	0.199762	0.201273	0.204737	0.197943	0.196427	0.203219	0.209112
(3,-1)	0.231504	0.227166	0.230348	0.229154	0.232994	0.226252	0.227765	0.230506	0.237819
(3,-1)	0.253723	0.249324	0.252891	0.251040	0.254757	0.248899	0.250740	0.252101	0.259384
(3,-1)	0.253723	0.249324	0.252891	0.251040	0.254757	0.248899	0.250740	0.252101	0.259384
(3,+1)	0.201408	0.200369	0.199762	0.201273	0.204737	0.197943	0.196427	0.203219	0.209112
(3,-1)	0.231504	0.227166	0.230348	0.229154	0.232994	0.226252	0.227765	0.230506	0.237819
(3,-1)	0.286992	0.280406	0.287309	0.284243	0.288389	0.279942	0.287722	0.282797	0.277760
(3,-1)	0.286992	0.280406	0.287309	0.284243	0.288389	0.279942	0.287722	0.282797	0.277760
(3,-1)	0.286992	0.280406	0.287309	0.284243	0.288389	0.279942	0.287722	0.282797	0.277760
(3,-1)	0.286992	0.280406	0.287309	0.284243	0.288389	0.279942	0.287722	0.282797	0.277760
(3,-1)	0.286992	0.280406	0.287309	0.284243	0.288389	0.279942	0.287722	0.282797	0.277760
(3,-1)	0.286992	0.280406	0.287309	0.284243	0.288389	0.279942	0.287722	0.282797	0.277760
(3,-1)	0.286992	0.280406	0.287309	0.284243	0.288389	0.279942	0.287722	0.282797	0.277760
(3,-1)	0.286992	0.280406	0.287309	0.284243	0.288389	0.279942	0.287722	0.282797	0.277760
(3,-1)	0.286992	0.280406	0.287309	0.284243	0.288389	0.279942	0.287722	0.282797	0.277760
(3,-1)	0.286992	0.280406	0.287309	0.284243	0.288389	0.279942	0.287722	0.282797	0.277760
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.253723	0.024340	0.256930	0.254945	0.253680	0.245171	0.248889	0.256301	0.253531
(3,-1)	0.253723	0.315932	0.256930	0.254945	0.253680	0.245171	0.248889	0.256301	0.253531
(3,+1)	0.201408	0.315932	0.208578	0.201454	0.203158	0.201326	0.205139	0.205499	0.202210
(3,-1)	0.231504	0.315932	0.236007	0.232284	0.231627	0.224109	0.227589	0.234350	0.231745
(3,-1)	0.253723	0.315932	0.256930	0.254945	0.253680	0.245171	0.248889	0.256301	0.253531
(3,-1)	0.253723	0.315932	0.256930	0.254945	0.253680	0.245171	0.248889	0.256301	0.253531
(3,+1)	0.201408	0.315932	0.208578	0.201454	0.203158	0.201326	0.205139	0.205499	0.202210
(3,-1)	0.231504	0.284068	0.236007	0.232284	0.231627	0.224109	0.227589	0.234350	0.231745
(3,-1)	0.286992	0.284068	0.283257	0.288859	0.286460	0.285409	0.281038	0.288814	0.286093
(3,-1)	0.286992	0.284068	0.283257	0.288859	0.286460	0.285409	0.281038	0.288814	0.286093
(3,-1)	0.286992	0.284068	0.283257	0.288859	0.286460	0.285409	0.281038	0.288814	0.286093
(3,-1)	0.286992	0.284068	0.283257	0.288859	0.286460	0.285409	0.281038	0.288814	0.286093
(3,-1)	0.286992	0.284068	0.283257	0.288859	0.286460	0.285409	0.281038	0.288814	0.286093
(3,-1)	0.286992	0.284068	0.283257	0.288859	0.286460	0.285409	0.281038	0.288814	0.286093
(3,-1)	0.286992	0.284068	0.283257	0.288859	0.286460	0.285409	0.281038	0.288814	0.286093
(3,-1)	0.286992	0.284068	0.283257	0.288859	0.286460	0.285409	0.281038	0.288814	0.286093
(3,-1)	0.286992	0.284068	0.283257	0.288859	0.286460	0.285409	0.281038	0.288814	0.286093
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.253723	0.248801	0.252167	0.255104	0.254722	0.254041	0.254310	0.253859	0.251869
(3,-1)	0.253723	0.248801	0.252167	0.255104	0.254722	0.254041	0.254310	0.253859	0.251869
(3,+1)	0.201408	0.178348	0.204199	0.202870	0.202725	0.203457	0.203422	0.201475	0.200762
(3,-1)	0.231504	0.225020	0.230453	0.232916	0.232984	0.232421	0.232254	0.231164	0.229741
(3,-1)	0.253723	0.248801	0.252167	0.255104	0.254722	0.254041	0.254310	0.253859	0.251869
(3,-1)	0.253723	0.248801	0.252167	0.255104	0.254722	0.254041	0.254310	0.253859	0.251869
(3,+1)	0.201408	0.178348	0.204199	0.202870	0.202725	0.203457	0.203422	0.201475	0.200762
(3,-1)	0.231504	0.225020	0.230453	0.232916	0.232984	0.232421	0.232254	0.231164	0.229741
(3,-1)	0.286992	0.284006	0.290125	0.295300	0.303518	0.287662	0.287724	0.287259	0.286351
(3,-1)	0.286992	0.284006	0.290125	0.295300	0.303518	0.287662	0.287724	0.287259	0.286351
(3,-1)	0.286992	0.284006	0.290125	0.295300	0.303518	0.287662	0.287724	0.287259	0.286351
(3,-1)	0.286992	0.284006	0.290125	0.295300	0.303518	0.287662	0.287724	0.287259	0.286351
(3,-1)	0.286992	0.284006	0.290125	0.295300	0.303518	0.287662	0.287724	0.287259	0.286351
(3,-1)	0.286992	0.284006	0.290125	0.295300	0.303518	0.287662	0.287724	0.287259	0.286351
(3,-1)	0.286992	0.284006	0.290125	0.295300	0.303518	0.287662	0.287724	0.287259	0.286351
(3,-1)	0.286992	0.284006	0.290125	0.295300	0.303518	0.287662	0.287724	0.287259	0.286351
(3,-1)	0.286992	0.284006	0.290125	0.295300	0.303518	0.287662	0.287724	0.287259	0.286351
(3,-1)	0.286992	0.284006	0.290125	0.295300	0.303518	0.287662	0.287724	0.287259	0.286351
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.253723	0.024760	0.250291	0.263614	0.255339	0.255323	0.253101		
(3,-1)	0.253723	0.316463	0.250291	0.263614	0.255339	0.255323	0.253101		
(3,+1)	0.201408	0.316463	0.198838	0.207216	0.202578	0.204473	0.204109		
(3,-1)	0.231504	0.316463	0.227891	0.240490	0.232947	0.233369	0.231607		
(3,-1)	0.253723	0.316463	0.250291	0.263614	0.255339	0.255323	0.253101		
(3,-1)	0.253723	0.316463	0.250291	0.263614	0.255339	0.255323	0.253101		
(3,+1)	0.201408	0.316463	0.198838	0.207216	0.202578	0.204473	0.204109		
(3,-1)	0.231504	0.282831	0.227891	0.240490	0.232947	0.233369	0.231607		
(3,-1)	0.286992	0.282831	0.288873	0.294598	0.289385	0.288404	0.287059		
(3,-1)	0.286992	0.282831	0.288873	0.294598	0.289385	0.288404	0.287059		
(3,-1)	0.286992	0.282831	0.288873	0.294598	0.289385	0.288404	0.287059		
(3,-1)	0.286992	0.282831	0.288873	0.294598	0.289385	0.288404	0.287059		
(3,-1)	0.286992	0.282831	0.288873	0.294598	0.289385	0.288404	0.287059		
(3,-1)	0.286992	0.282831	0.288873	0.294598	0.289385	0.288404	0.287059		
(3,-1)	0.286992	0.282831	0.288873	0.294598	0.289385	0.288404	0.287059		
(3,-1)	0.286992	0.282831	0.288873	0.294598	0.289385	0.288404	0.287059		
(3,-1)	0.286992	0.282831	0.288873	0.294598	0.289385	0.288404	0.287059		
(3,-1)	0.286992	0.282831	0.288873	0.294598	0.289385	0.288404	0.287059		

Table S114: Density value (a.u.) at the considered critical points for the C<sub>6</sub>H<sub>6</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.022791	0.025368	0.023305	0.024357	0.023625	0.026399	0.023468	0.022334	0.024078
(3,-1)	0.318279	0.311409	0.317196	0.313288	0.318035	0.311390	0.314364	0.317203	0.319348
(3,-1)	0.318278	0.311409	0.317196	0.313288	0.318035	0.311390	0.314364	0.317203	0.319348
(3,-1)	0.318279	0.311409	0.317196	0.313288	0.318035	0.311390	0.314364	0.317203	0.319348
(3,-1)	0.318279	0.311409	0.317196	0.313288	0.318035	0.311390	0.314364	0.317203	0.319348
(3,-1)	0.318279	0.311409	0.317196	0.313288	0.318035	0.311390	0.314364	0.317203	0.319348
(3,-1)	0.318278	0.311409	0.317196	0.313288	0.318035	0.311390	0.314364	0.317203	0.319348
(3,-1)	0.289181	0.282521	0.289238	0.286228	0.290535	0.281741	0.289879	0.284396	0.279030
(3,-1)	0.289181	0.282521	0.289238	0.286228	0.290535	0.281741	0.289879	0.284396	0.279030
(3,-1)	0.289181	0.282521	0.289238	0.286228	0.290535	0.281741	0.289879	0.284396	0.279030
(3,-1)	0.289181	0.282521	0.289238	0.286228	0.290535	0.281741	0.289879	0.284396	0.279030
(3,-1)	0.289181	0.282521	0.289238	0.286228	0.290535	0.281741	0.289879	0.284396	0.279030
(3,-1)	0.289181	0.282521	0.289238	0.286228	0.290535	0.281741	0.289879	0.284396	0.279030
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.022791	0.260148	0.024731	0.023224	0.024133	0.022712	0.023746	0.023392	0.025487
(3,-1)	0.318279	0.260148	0.316207	0.316207	0.316706	0.310844	0.315471	0.319592	0.315631
(3,-1)	0.318278	0.299606	0.316207	0.316207	0.316706	0.310844	0.315471	0.319592	0.315631
(3,-1)	0.318279	0.299606	0.316207	0.316207	0.316706	0.310844	0.315471	0.319592	0.315631
(3,-1)	0.318279		0.316207	0.316207	0.316706	0.310844	0.315471	0.319592	0.315631
(3,-1)	0.318279		0.316207	0.316207	0.316706	0.310844	0.315471	0.319592	0.315631
(3,-1)	0.318278		0.316207	0.316207	0.316706	0.310844	0.315471	0.319592	0.315631
(3,-1)	0.289181		0.285843	0.291000	0.288684	0.287410	0.282786	0.291158	0.288543
(3,-1)	0.289181		0.285843	0.291000	0.288684	0.287410	0.282786	0.291158	0.288543
(3,-1)	0.289181		0.285843	0.291000	0.288684	0.287410	0.282786	0.291158	0.288543
(3,-1)	0.289181		0.285843	0.291000	0.288684	0.287410	0.282786	0.291158	0.288543
(3,-1)	0.289181		0.285843	0.291000	0.288684	0.287410	0.282786	0.291158	0.288543
(3,-1)	0.289181		0.285843	0.291000	0.288684	0.287410	0.282786	0.291158	0.288543
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.022791	0.023467	0.023838	0.024554	0.026395	0.022804	0.022998	0.023225	0.023840
(3,-1)	0.318279	0.310912	0.318549	0.321906	0.320581	0.315234	0.316987	0.317442	0.315240
(3,-1)	0.318278	0.310912	0.318549	0.321906	0.320581	0.315234	0.316987	0.317442	0.315240
(3,-1)	0.318279	0.310912	0.318549	0.321906	0.320581	0.315234	0.316987	0.317442	0.315240
(3,-1)	0.318279	0.310912	0.318549	0.321906	0.320581	0.315234	0.316987	0.317442	0.315240
(3,-1)	0.318279	0.310912	0.318549	0.321906	0.320581	0.315234	0.316987	0.317442	0.315240
(3,-1)	0.318278	0.310912	0.318549	0.321906	0.320581	0.315234	0.316987	0.317442	0.315240
(3,-1)	0.289181	0.286378	0.292212	0.297459	0.305179	0.289852	0.289925	0.289475	0.288635
(3,-1)	0.289181	0.286378	0.292212	0.297459	0.305179	0.289852	0.289925	0.289475	0.288635
(3,-1)	0.289181	0.286378	0.292212	0.297459	0.305179	0.289852	0.289925	0.289475	0.288635
(3,-1)	0.289181	0.286378	0.292212	0.297459	0.305179	0.289852	0.289925	0.289475	0.288635
(3,-1)	0.289181	0.286378	0.292212	0.297459	0.305179	0.289852	0.289925	0.289475	0.288635
(3,-1)	0.289181	0.286378	0.292212	0.297459	0.305179	0.289852	0.289925	0.289475	0.288635
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.022791	0.259573	0.023964	0.022249	0.023525	0.024160	0.023687		
(3,-1)	0.318279	0.259573	0.317877	0.330582	0.320048	0.319007	0.317626		
(3,-1)	0.318278	0.297356	0.317877	0.330582	0.320048	0.319007	0.317633		
(3,-1)	0.318279	0.297356	0.317877	0.330582	0.320048	0.319007	0.317626		
(3,-1)	0.318279		0.317877	0.330582	0.320048	0.319007	0.317626		
(3,-1)	0.318279		0.317877	0.330582	0.320048	0.319007	0.317626		
(3,-1)	0.318278		0.317877	0.330582	0.320048	0.319007	0.317633		
(3,-1)	0.289181		0.291531	0.297424	0.291331	0.290476	0.288927		
(3,-1)	0.289181		0.291531	0.297424	0.291331	0.290476	0.288921		
(3,-1)	0.289181		0.291531	0.297424	0.291331	0.290476	0.288921		
(3,-1)	0.289181		0.291531	0.297424	0.291331	0.290476	0.288927		
(3,-1)	0.289181		0.291531	0.297424	0.291331	0.290476	0.288921		
(3,-1)	0.289181		0.291531	0.297424	0.291331	0.290476	0.288921		

Table S115: Density value (a.u.) at the considered critical points for the H<sub>2</sub>CF<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.263983	0.267238	0.267627	0.267013	0.264191	0.268198	0.262044	0.262908	0.258841
(3,-1)	0.263983	0.267238	0.267627	0.267013	0.264191	0.268198	0.262044	0.262908	0.258841
(3,-1)	0.309112	0.296194	0.304550	0.301026	0.306544	0.297527	0.305861	0.297065	0.290998
(3,-1)	0.309112	0.296194	0.304550	0.301026	0.306544	0.297527	0.305861	0.297065	0.290998
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.263983	0.308549	0.255652	0.266168	0.265125	0.259023	0.264309	0.262861	0.263393
(3,-1)	0.263983	0.282833	0.255652	0.266168	0.265125	0.259023	0.264309	0.262861	0.263393
(3,-1)	0.309112	0.282833	0.303659	0.306920	0.304358	0.303352	0.296055	0.307854	0.305421
(3,-1)	0.309112	0.282833	0.303659	0.306920	0.304358	0.303352	0.296055	0.307854	0.305421
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.263983	0.260434	0.260439	0.259928	0.256281	0.264290	0.265086	0.265251	0.263573
(3,-1)	0.263983	0.260434	0.260439	0.259928	0.256281	0.264290	0.265086	0.265251	0.263573
(3,-1)	0.309112	0.302992	0.308587	0.314270	0.320722	0.306177	0.306149	0.305544	0.304772
(3,-1)	0.309112	0.302992	0.308587	0.314270	0.320722	0.306177	0.306149	0.305544	0.304772
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.263983	0.305625	0.260356	0.257499	0.264768	0.262903	0.260035		
(3,-1)	0.263983	0.282157	0.260356	0.257499	0.264768	0.262903	0.260035		
(3,-1)	0.309112	0.282157	0.307880	0.316099	0.308187	0.307542	0.306394		
(3,-1)	0.309112	0.282157	0.307880	0.316099	0.308187	0.307542	0.306394		

Table S116: Density value (a.u.) at the considered critical points for the HCF<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.318158	0.303535	0.312479	0.308765	0.315059	0.305015	0.314080	0.304357	0.298058
(3,-1)	0.287305	0.289562	0.290741	0.289375	0.287136	0.291092	0.285330	0.284657	0.281520
(3,-1)	0.287305	0.289562	0.290741	0.289375	0.287136	0.291092	0.285330	0.284657	0.281520
(3,-1)	0.287305	0.289562	0.290741	0.289375	0.287136	0.291092	0.285330	0.284657	0.281520
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.318158	0.199285	0.313290	0.315366	0.312791	0.311812	0.303820	0.316925	0.314671
(3,-1)	0.287305	0.199285	0.277385	0.289641	0.287941	0.281073	0.286594	0.285667	0.286061
(3,-1)	0.287305	0.293372	0.277385	0.289641	0.287941	0.281073	0.286594	0.285667	0.286061
(3,-1)	0.287305	0.293372	0.277385	0.289641	0.287941	0.281073	0.286594	0.285667	0.286061
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.318158	0.311479	0.317885	0.322971	0.329058	0.314684	0.314784	0.314244	0.313483
(3,-1)	0.287305	0.282410	0.282887	0.283696	0.281369	0.287099	0.288054	0.288104	0.287211
(3,-1)	0.287305	0.282410	0.282887	0.283696	0.281369	0.287099	0.288054	0.288104	0.287211
(3,-1)	0.287305	0.282410	0.282887	0.283696	0.281369	0.287099	0.288054	0.288104	0.287211
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.318158	0.197979	0.317143	0.326356	0.316733	0.316311	0.315033		
(3,-1)	0.287305	0.197979	0.283760	0.282095	0.288111	0.285896	0.282994		
(3,-1)	0.287305	0.291713	0.283760	0.282095	0.288111	0.285896	0.282993		
(3,-1)	0.287305	0.291713	0.283760	0.282095	0.288111	0.285896	0.282993		

Table S117: Density value (a.u.) at the considered critical points for the H<sub>2</sub>CCl<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.199370	0.191440	0.194091	0.193205	0.196656	0.190807	0.190737	0.192090	0.198634
(3,-1)	0.199370	0.191440	0.194091	0.193205	0.196656	0.190807	0.190737	0.192090	0.198634
(3,-1)	0.302071	0.290748	0.298932	0.295471	0.300561	0.290287	0.299739	0.293256	0.287398
(3,-1)	0.302071	0.290748	0.298932	0.295471	0.300561	0.290287	0.299739	0.293256	0.287398
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.199370	0.299576	0.200824	0.196229	0.195822	0.186621	0.189625	0.198334	0.195914
(3,-1)	0.199370	0.204251	0.200824	0.196229	0.195822	0.186621	0.189625	0.198334	0.195914
(3,-1)	0.302071	0.204251	0.296857	0.300909	0.298303	0.297440	0.291359	0.301578	0.298844
(3,-1)	0.302071	0.204251	0.296857	0.300909	0.298303	0.297440	0.291359	0.301578	0.298844
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.199370	0.188585	0.194080	0.196695	0.197692	0.197854	0.197106	0.195181	0.194284
(3,-1)	0.199370	0.188585	0.194080	0.196695	0.197692	0.197854	0.197106	0.195181	0.194284
(3,-1)	0.302071	0.295924	0.302186	0.307706	0.314729	0.300532	0.300343	0.299580	0.298312
(3,-1)	0.302071	0.295924	0.302186	0.307706	0.314729	0.300532	0.300343	0.299580	0.298312
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.199370	0.297391	0.191158	0.204734	0.196993	0.197564	0.195900		
(3,-1)	0.199370	0.202812	0.191158	0.204734	0.196993	0.197564	0.195900		
(3,-1)	0.302071	0.202812	0.301683	0.308974	0.301549	0.300630	0.299473		
(3,-1)	0.302071	0.202812	0.301683	0.308974	0.301549	0.300630	0.299473		



Table S118: Density value (a.u.) at the considered critical points for the  $\text{HCCl}_3$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.308440	0.296196	0.304788	0.301175	0.306761	0.295986	0.305629	0.298805	0.292248
(3,-1)	0.204476	0.195653	0.198364	0.197429	0.201432	0.194652	0.195027	0.196575	0.203596
(3,-1)	0.204476	0.195653	0.198364	0.197429	0.201432	0.194652	0.195027	0.196575	0.203596
(3,-1)	0.204476	0.195653	0.198364	0.197429	0.201432	0.194652	0.195027	0.196575	0.203596
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.308440	0.267796	0.303560	0.307080	0.304430	0.303436	0.296949	0.308179	0.305341
(3,-1)	0.204476	0.275783	0.205881	0.200928	0.200561	0.190766	0.194083	0.203413	0.200770
(3,-1)	0.204476	0.334476	0.205881	0.200928	0.200561	0.190766	0.194083	0.203413	0.200770
(3,-1)	0.204476	0.334476	0.205881	0.200928	0.200561	0.190766	0.194083	0.203413	0.200770
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.308440	0.301800	0.308442	0.314023	0.320570	0.307283	0.306967	0.306011	0.304479
(3,-1)	0.204476	0.193056	0.198995	0.201801	0.202862	0.202981	0.202151	0.200034	0.198983
(3,-1)	0.204476	0.193056	0.198995	0.201801	0.202862	0.202981	0.202151	0.200034	0.198983
(3,-1)	0.204476	0.193056	0.198995	0.201801	0.202862	0.202981	0.202151	0.200034	0.198983
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.308440	0.267179	0.308416	0.316301	0.307626	0.306791	0.305637		
(3,-1)	0.204476	0.275008	0.196289	0.211195	0.201701	0.202489	0.200712		
(3,-1)	0.204476	0.337187	0.196289	0.211195	0.201701	0.202489	0.200720		
(3,-1)	0.204476	0.337187	0.196289	0.211195	0.201701	0.202489	0.200720		

Table S119: Density value (a.u.) at the considered critical points for the H<sub>3</sub>C–NH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.270904	0.263269	0.267083	0.265323	0.268685	0.262572	0.264554	0.266630	0.270879
(3,-1)	0.284331	0.274482	0.281432	0.278406	0.282607	0.274664	0.281831	0.277496	0.271930
(3,-1)	0.347445	0.338691	0.348079	0.345300	0.349317	0.339361	0.348613	0.347926	0.340519
(3,-1)	0.347445	0.338691	0.348079	0.345300	0.349317	0.339361	0.348613	0.347926	0.340519
(3,-1)	0.289683	0.279740	0.287096	0.283884	0.288131	0.279678	0.287517	0.282445	0.276942
(3,-1)	0.289683	0.279740	0.287096	0.283884	0.288131	0.279678	0.287517	0.282445	0.276942
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.270904	0.266059	0.267876	0.269009	0.267794	0.258999	0.262681	0.270163	0.266399
(3,-1)	0.284331	0.455779	0.277806	0.283033	0.280683	0.280410	0.275708	0.283041	0.280364
(3,-1)	0.347445	0.278018	0.339713	0.349006	0.346904	0.349334	0.343517	0.350625	0.342454
(3,-1)	0.347445	0.278018	0.339713	0.349006	0.346904	0.349334	0.343517	0.350625	0.342454
(3,-1)	0.289683	0.278018	0.283642	0.288619	0.286104	0.285440	0.280536	0.288516	0.285984
(3,-1)	0.289683		0.283642	0.288619	0.286104	0.285440	0.280536	0.288516	0.285984
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.270904	0.262892	0.264076	0.267357	0.263389	0.268990	0.268804	0.267733	0.265711
(3,-1)	0.284331	0.279089	0.284254	0.289454	0.297591	0.282030	0.281998	0.281444	0.280573
(3,-1)	0.347445	0.342521	0.348599	0.353568	0.357767	0.350091	0.349009	0.347506	0.345917
(3,-1)	0.347445	0.342521	0.348599	0.353568	0.357767	0.350091	0.349009	0.347506	0.345917
(3,-1)	0.289683	0.284505	0.289673	0.294946	0.302753	0.287422	0.287444	0.286970	0.286079
(3,-1)	0.289683	0.284505	0.289673	0.294946	0.302753	0.287422	0.287444	0.286970	0.286079
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.270904	0.266159	0.262585	0.276378	0.269330	0.269174	0.266830		
(3,-1)	0.284331	0.462802	0.281947	0.289017	0.283849	0.282965	0.281732		
(3,-1)	0.347445	0.277616	0.351138	0.354076	0.348014	0.346816	0.345175		
(3,-1)	0.347445	0.277616	0.351138	0.354076	0.348014	0.346816	0.345175		
(3,-1)	0.289683	0.277616	0.287991	0.294597	0.289345	0.288322	0.287144		
(3,-1)	0.289683		0.287991	0.294597	0.289345	0.288322	0.287144		

Table S120: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>-CN system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.271128	0.262562	0.267296	0.264678	0.268713	0.262453	0.264428	0.270739	0.269175
(3,-1)	0.471461	0.475039	0.476211	0.471943	0.473307	0.477838	0.475443	0.456422	0.467195
(3,-1)	0.286731	0.276367	0.284062	0.280742	0.285117	0.276249	0.284374	0.279508	0.274831
(3,-1)	0.286731	0.276367	0.284062	0.280742	0.285117	0.276249	0.284374	0.279508	0.274831
(3,-1)	0.286731	0.276367	0.284062	0.280742	0.285117	0.276249	0.284374	0.279508	0.274831
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.271128	0.251544	0.268182	0.269239	0.267328	0.265932	0.268600	0.269812	0.266452
(3,-1)	0.471461	0.282166	0.454649	0.477119	0.473168	0.463233	0.467251	0.470625	0.469267
(3,-1)	0.286731	0.287207	0.280342	0.285632	0.283031	0.282246	0.277554	0.285643	0.282967
(3,-1)	0.286731	0.287207	0.280342	0.285632	0.283031	0.282246	0.277554	0.285643	0.282967
(3,-1)	0.286731	0.495488	0.280342	0.285632	0.283031	0.282246	0.277554	0.285643	0.282967
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.271128	0.260151	0.267417	0.268711	0.263059	0.267264	0.267737	0.267241	0.265718
(3,-1)	0.471461	0.460564	0.473498	0.486663	0.491701	0.467819	0.472264	0.474565	0.475891
(3,-1)	0.286731	0.281149	0.286877	0.291976	0.300284	0.284680	0.284660	0.284093	0.282980
(3,-1)	0.286731	0.281149	0.286877	0.291976	0.300284	0.284680	0.284660	0.284093	0.282980
(3,-1)	0.286731	0.281149	0.286877	0.291976	0.300284	0.284680	0.284660	0.284093	0.282980
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.271128	0.251480	0.264638	0.277186	0.269680	0.269210	0.267521		
(3,-1)	0.471461	0.281551	0.479026	0.477235	0.474536	0.471967	0.469752		
(3,-1)	0.286731	0.286283	0.285994	0.291979	0.286253	0.285151	0.283970		
(3,-1)	0.286731	0.286283	0.285994	0.291979	0.286253	0.285151	0.283967		
(3,-1)	0.286731	0.494364	0.285994	0.291979	0.286253	0.285151	0.283967		

Table S121: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>-NO<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.256867	0.252794	0.255031	0.254388	0.255891	0.250942	0.252394	0.256432	0.258422
(3,-1)	0.291125	0.279823	0.287933	0.284456	0.289140	0.279928	0.288386	0.282610	0.277834
(3,-1)	0.295772	0.284774	0.293058	0.289512	0.294233	0.285131	0.293548	0.287201	0.282068
(3,-1)	0.295772	0.284774	0.293058	0.289512	0.294233	0.285131	0.293548	0.287201	0.282068
(3,-1)	0.497066	0.486803	0.489065	0.488394	0.495050	0.481262	0.485903	0.486257	0.496377
(3,-1)	0.497077	0.486803	0.489065	0.488394	0.495050	0.481262	0.485903	0.486257	0.496377
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.256867	0.243384	0.253770	0.255849	0.255451	0.250040	0.252301	0.256466	0.252606
(3,-1)	0.291125	0.288311	0.284462	0.289679	0.286987	0.285936	0.280904	0.289849	0.287431
(3,-1)	0.295772	0.284806	0.289961	0.294782	0.292036	0.290959	0.285385	0.294985	0.292310
(3,-1)	0.295772	0.284806	0.289961	0.294782	0.292036	0.290959	0.285385	0.294985	0.292310
(3,-1)	0.497066	0.339539	0.495102	0.493789	0.494161	0.476903	0.482030	0.499331	0.488316
(3,-1)	0.497077	0.533162	0.495102	0.493789	0.494161	0.476903	0.482030	0.499331	0.488316
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.256867	0.251476	0.250617	0.253474	0.243723	0.255931	0.255806	0.255279	0.252834
(3,-1)	0.291125	0.285137	0.290982	0.296165	0.304562	0.288904	0.288840	0.288201	0.287139
(3,-1)	0.295772	0.290133	0.296029	0.301257	0.309249	0.293648	0.293651	0.293110	0.292200
(3,-1)	0.295772	0.290133	0.296029	0.301257	0.309249	0.293648	0.293651	0.293110	0.292200
(3,-1)	0.497066	0.483320	0.494402	0.498963	0.509856	0.494543	0.494340	0.492279	0.487754
(3,-1)	0.497077	0.483320	0.494402	0.498963	0.509856	0.494543	0.494340	0.492279	0.487754
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.256867	0.243257	0.248603	0.254765	0.255988	0.255817	0.253139		
(3,-1)	0.291125	0.287015	0.290457	0.296750	0.290489	0.289388	0.288270		
(3,-1)	0.295772	0.283883	0.295471	0.302067	0.295306	0.294175	0.293055		
(3,-1)	0.295772	0.283883	0.295471	0.302067	0.295306	0.294175	0.293055		
(3,-1)	0.497066	0.337021	0.490623	0.511885	0.492884	0.495169	0.489799		
(3,-1)	0.497077	0.532537	0.490623	0.511885	0.492884	0.495169	0.489799		

Table S122: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>-O-N=O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.247823	0.246747	0.248065	0.247671	0.246425	0.246601	0.244374	0.245347	0.245507
(3,-1)	0.296511	0.285841	0.293813	0.290347	0.295030	0.285762	0.294510	0.288078	0.282712
(3,-1)	0.294146	0.282155	0.290396	0.286910	0.291937	0.282865	0.291033	0.284948	0.279638
(3,-1)	0.293642	0.282155	0.290396	0.286910	0.291937	0.282865	0.291033	0.284948	0.279638
(3,-1)	0.339027	0.327265	0.328147	0.328788	0.334549	0.324773	0.327705	0.333042	0.339183
(3,-1)	0.537408	0.526750	0.529781	0.528271	0.534767	0.522793	0.526988	0.522631	0.534300
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.247823	0.118387	0.241936	0.247305	0.246643	0.239992	0.243230	0.245987	0.244948
(3,-1)	0.296511	0.270597	0.290854	0.295550	0.292872	0.291992	0.286427	0.295674	0.293285
(3,-1)	0.294146	0.270597	0.287460	0.292388	0.289762	0.289098	0.283488	0.292713	0.290020
(3,-1)	0.293642	0.270597	0.287460	0.292388	0.289762	0.289098	0.283488	0.292713	0.290020
(3,-1)	0.339027	0.119954	0.338553	0.332806	0.334308	0.327560	0.329589	0.339454	0.331678
(3,-1)	0.537408	0.119954	0.531526	0.534336	0.533888	0.514329	0.519687	0.538323	0.527085
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.247823	0.242923	0.242131	0.242592	0.239825	0.246813	0.247004	0.246939	0.244043
(3,-1)	0.296511	0.291184	0.296817	0.302278	0.309919	0.294488	0.294485	0.293957	0.293157
(3,-1)	0.294146	0.288140	0.293795	0.299292	0.307189	0.291506	0.291449	0.290831	0.289989
(3,-1)	0.293642	0.288140	0.293795	0.299292	0.307189	0.291506	0.291449	0.290831	0.289989
(3,-1)	0.339027	0.329605	0.333009	0.331837	0.337029	0.337423	0.336154	0.334177	0.330002
(3,-1)	0.537408	0.522833	0.533818	0.540767	0.552587	0.532997	0.533658	0.532347	0.528641
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.247823	0.120682	0.240853	0.241438	0.246503	0.245273	0.242497		
(3,-1)	0.296511	0.270838	0.296108	0.302600	0.296205	0.295157	0.294031		
(3,-1)	0.294146	0.270838	0.292769	0.300277	0.293019	0.292111	0.290885		
(3,-1)	0.293642	0.270838	0.292769	0.300277	0.293019	0.292111	0.290885		
(3,-1)	0.339027	0.121708	0.328198	0.351241	0.331906	0.335104	0.329443		
(3,-1)	0.537408	0.121708	0.532025	0.551076	0.533201	0.534783	0.529608		

Table S123: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>–SiH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.122118	0.121541	0.123165	0.121328	0.122786	0.120273	0.121026	0.121874	0.125048
(3,-1)	0.279064	0.270874	0.277532	0.274605	0.278295	0.270623	0.277889	0.274170	0.269646
(3,-1)	0.279064	0.270874	0.277532	0.274605	0.278295	0.270623	0.277889	0.274170	0.269646
(3,-1)	0.279064	0.270874	0.277532	0.274605	0.278295	0.270623	0.277889	0.274170	0.269646
(3,-1)	0.121892	0.123119	0.123338	0.121991	0.122600	0.121066	0.122783	0.120575	0.119231
(3,-1)	0.121892	0.123119	0.123338	0.121991	0.122600	0.121066	0.122783	0.120575	0.119231
(3,-1)	0.121892	0.123119	0.123338	0.121991	0.122600	0.121066	0.122783	0.120575	0.119231
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.122118	0.304226	0.118161	0.123819	0.122199	0.122320	0.123249	0.123004	0.121754
(3,-1)	0.279064	0.416099	0.272779	0.278702	0.276343	0.275961	0.271997	0.278289	0.275696
(3,-1)	0.279064	0.346478	0.272779	0.278702	0.276343	0.275961	0.271997	0.278289	0.275696
(3,-1)	0.279064	0.291389	0.272779	0.278702	0.276343	0.275961	0.271997	0.278289	0.275696
(3,-1)	0.121892		0.114447	0.123671	0.122342	0.124716	0.123262	0.122395	0.120626
(3,-1)	0.121892		0.114447	0.123671	0.122342	0.124716	0.123262	0.122395	0.120626
(3,-1)	0.121892		0.114447	0.123671	0.122342	0.124716	0.123262	0.122395	0.120626
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.122118	0.119225	0.119284	0.122927	0.117008	0.125134	0.124059	0.122582	0.121740
(3,-1)	0.279064	0.273928	0.279800	0.284566	0.292897	0.277361	0.277349	0.276900	0.276057
(3,-1)	0.279064	0.273928	0.279800	0.284566	0.292897	0.277361	0.277349	0.276900	0.276057
(3,-1)	0.279064	0.273928	0.279800	0.284566	0.292897	0.277361	0.277349	0.276900	0.276057
(3,-1)	0.121892	0.121575	0.122317	0.125299	0.128128	0.124406	0.123741	0.122967	0.122522
(3,-1)	0.121892	0.121575	0.122317	0.125299	0.128128	0.124406	0.123741	0.122967	0.122522
(3,-1)	0.121892	0.121575	0.122317	0.125299	0.128128	0.124406	0.123741	0.122967	0.122522
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.122118	0.305050	0.120115	0.125666	0.123026	0.122044	0.121059		
(3,-1)	0.279064	0.419970	0.277760	0.283099	0.278984	0.277864	0.276441		
(3,-1)	0.279064	0.349822	0.277760	0.283099	0.278984	0.277864	0.276437		
(3,-1)	0.279064	0.289346	0.277760	0.283099	0.278984	0.277864	0.276437		
(3,-1)	0.121892		0.120062	0.122519	0.123164	0.122302	0.121245		
(3,-1)	0.121892		0.120062	0.122519	0.123164	0.122302	0.121245		
(3,-1)	0.121892		0.120062	0.122519	0.123164	0.122302	0.121245		

Table S124: Density value (a.u.) at the considered critical points for the HCOOH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.311758	0.309725	0.311627	0.309550	0.310234	0.309884	0.308228	0.303327	0.305332
(3,-1)	0.430258	0.430308	0.431901	0.428738	0.430838	0.430563	0.427941	0.416777	0.420269
(3,-1)	0.356226	0.349215	0.360504	0.358424	0.360398	0.355054	0.361105	0.361137	0.349471
(3,-1)	0.299655	0.286944	0.294619	0.291396	0.297261	0.287499	0.296075	0.288620	0.283190
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.311758	0.413648	0.300190	0.312530	0.310548	0.300580	0.305732	0.309903	0.308454
(3,-1)	0.430258	0.307384	0.413709	0.433520	0.430707	0.417609	0.423297	0.429359	0.426784
(3,-1)	0.356226	0.289953	0.350481	0.359810	0.358181	0.359764	0.356550	0.361768	0.354711
(3,-1)	0.299655	0.240052	0.294323	0.297448	0.295232	0.294340	0.287881	0.298896	0.296502
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.311758	0.304200	0.305393	0.310279	0.309339	0.310816	0.311481	0.310933	0.309938
(3,-1)	0.430258	0.417353	0.426718	0.437347	0.440989	0.429946	0.431054	0.429809	0.431321
(3,-1)	0.356226	0.356355	0.354272	0.357271	0.352718	0.362964	0.361470	0.360425	0.357657
(3,-1)	0.299655	0.293616	0.299410	0.305053	0.311395	0.297314	0.297183	0.296477	0.295806
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.311758	0.417452	0.307360	0.313299	0.311079	0.309649	0.306170		
(3,-1)	0.430258	0.308327	0.432958	0.437261	0.431195	0.429675	0.425702		
(3,-1)	0.356226	0.288054	0.362897	0.359582	0.357028	0.355242	0.353397		
(3,-1)	0.299655	0.240058	0.299209	0.307891	0.298193	0.298003	0.296363		

Table S125: Density value (a.u.) at the considered critical points for the HCOOCH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.423989	0.427466	0.429059	0.425954	0.428070	0.427901	0.425141	0.414145	0.417596
(3,-1)	0.310526	0.313309	0.315300	0.313058	0.313872	0.312861	0.311842	0.306731	0.308321
(3,-1)	0.295999	0.285470	0.293144	0.289888	0.295781	0.284761	0.294534	0.287284	0.281927
(3,-1)	0.238143	0.243598	0.244801	0.244240	0.242903	0.243095	0.241025	0.241164	0.240572
(3,-1)	0.295024	0.286943	0.294843	0.291440	0.296045	0.286862	0.295554	0.289017	0.283604
(3,-1)	0.292818	0.284267	0.292422	0.288982	0.293808	0.284851	0.293079	0.286787	0.281383
(3,-1)	0.292818	0.284267	0.292422	0.288982	0.293808	0.284851	0.293079	0.286787	0.281383
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.423989	0.405210	0.411059	0.430707	0.427956	0.414815	0.420617	0.426629	0.424081
(3,-1)	0.310526	0.316759	0.303517	0.316319	0.314180	0.304253	0.309347	0.313680	0.312232
(3,-1)	0.295999	0.259491	0.292673	0.296026	0.293787	0.292950	0.286647	0.297470	0.295013
(3,-1)	0.238143	0.336244	0.237696	0.244124	0.243290	0.235836	0.239517	0.242524	0.242088
(3,-1)	0.295024	0.280811	0.291968	0.296521	0.293889	0.293072	0.287347	0.296643	0.294151
(3,-1)	0.292818	0.274759	0.289411	0.294230	0.291607	0.291056	0.285185	0.294458	0.291701
(3,-1)	0.292818	0.272826	0.289411	0.294230	0.291607	0.291056	0.285185	0.294458	0.291701
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.423989	0.414742	0.423990	0.434386	0.438085	0.427175	0.428300	0.427097	0.428547
(3,-1)	0.310526	0.307897	0.309185	0.314202	0.313623	0.314640	0.315287	0.314669	0.313665
(3,-1)	0.295999	0.292219	0.297995	0.303645	0.310225	0.295929	0.295784	0.295033	0.294363
(3,-1)	0.238143	0.239962	0.239050	0.239477	0.237586	0.243473	0.243721	0.243643	0.241061
(3,-1)	0.295024	0.292229	0.297682	0.303235	0.310642	0.295356	0.295374	0.294892	0.294072
(3,-1)	0.292818	0.289864	0.295426	0.301013	0.308572	0.293176	0.293148	0.292602	0.291757
(3,-1)	0.292818	0.289864	0.295426	0.301013	0.308572	0.293176	0.293148	0.292602	0.291757
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.423989	0.408249	0.430071	0.434467	0.428352	0.426876	0.422841		
(3,-1)	0.310526	0.317706	0.311336	0.317796	0.314726	0.313225	0.309607		
(3,-1)	0.295999	0.258796	0.297651	0.306633	0.296703	0.296498	0.294840		
(3,-1)	0.238143	0.339509	0.238098	0.238426	0.243260	0.241882	0.239197		
(3,-1)	0.295024	0.280174	0.296798	0.303323	0.297250	0.296222	0.295102		
(3,-1)	0.292818	0.274539	0.294406	0.301601	0.294931	0.293957	0.292788		
(3,-1)	0.292818	0.272723	0.294406	0.301601	0.294931	0.293957	0.292788		



Table S126: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>CONH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.414002	0.417168	0.418808	0.415803	0.417999	0.417335	0.414988	0.405069	0.408740
(3,-1)	0.322092	0.319688	0.323100	0.320227	0.323515	0.318831	0.319970	0.317501	0.319961
(3,-1)	0.262199	0.252236	0.257963	0.255102	0.260893	0.251189	0.255249	0.263313	0.261257
(3,-1)	0.346190	0.341726	0.351713	0.348850	0.352481	0.343455	0.352131	0.350643	0.342279
(3,-1)	0.286332	0.279264	0.287047	0.283685	0.287957	0.279738	0.287373	0.282426	0.277047
(3,-1)	0.280629	0.273695	0.281087	0.277845	0.282016	0.274135	0.281365	0.277103	0.271927
(3,-1)	0.278704	0.271830	0.279153	0.275950	0.280066	0.272106	0.279384	0.275368	0.270371
(3,-1)	0.344841	0.340412	0.350482	0.347658	0.351199	0.342182	0.350894	0.349629	0.340688
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.414002	0.213477	0.402131	0.420562	0.417932	0.404667	0.410913	0.416800	0.414377
(3,-1)	0.322092	0.257121	0.314373	0.325433	0.323057	0.313192	0.318435	0.323863	0.321205
(3,-1)	0.262199	0.255619	0.261676	0.261188	0.259331	0.259121	0.260714	0.263397	0.258366
(3,-1)	0.346190	0.257121	0.341670	0.352229	0.349981	0.353046	0.346617	0.353689	0.345421
(3,-1)	0.286332	0.334313	0.283174	0.288483	0.285826	0.285249	0.280283	0.288330	0.285519
(3,-1)	0.280629	0.287277	0.276714	0.282549	0.279984	0.279667	0.275134	0.282290	0.279603
(3,-1)	0.278704	0.287277	0.274735	0.280587	0.278047	0.277770	0.273412	0.280340	0.277681
(3,-1)	0.344841	0.284365	0.340543	0.350917	0.348703	0.351880	0.345525	0.352484	0.344201
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.414002	0.405131	0.413838	0.423538	0.426945	0.417415	0.418522	0.417347	0.418445
(3,-1)	0.322092	0.315680	0.318732	0.325559	0.320121	0.323348	0.324069	0.323019	0.322585
(3,-1)	0.262199	0.254131	0.260625	0.261923	0.256622	0.260813	0.260876	0.259759	0.257890
(3,-1)	0.346190	0.345369	0.350821	0.356156	0.358985	0.353057	0.352047	0.350662	0.349261
(3,-1)	0.286332	0.283787	0.289514	0.294555	0.302436	0.287102	0.287133	0.286694	0.285840
(3,-1)	0.280629	0.278112	0.283749	0.288614	0.297095	0.281291	0.281310	0.280831	0.279946
(3,-1)	0.278704	0.276176	0.281817	0.286597	0.295153	0.279433	0.279426	0.278915	0.277962
(3,-1)	0.344841	0.344346	0.349225	0.354666	0.356655	0.351931	0.350878	0.349493	0.348009
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.414002	0.211942	0.419344	0.424846	0.418288	0.416918	0.412889		
(3,-1)	0.322092	0.256401	0.320582	0.331891	0.325006	0.324002	0.321592		
(3,-1)	0.262199	0.254898	0.257874	0.274928	0.262239	0.262375	0.260965		
(3,-1)	0.346190	0.256401	0.354920	0.355811	0.350886	0.349324	0.347842		
(3,-1)	0.286332	0.336837	0.288423	0.294543	0.288871	0.287677	0.286460		
(3,-1)	0.280629	0.286086	0.281995	0.288334	0.283047	0.281922	0.280640		
(3,-1)	0.278704	0.286086	0.279999	0.286212	0.281129	0.280004	0.278730		
(3,-1)	0.344841	0.283384	0.353690	0.354350	0.349542	0.347979	0.346532		

Table S127: Density value (a.u.) at the considered critical points for the CH<sub>2</sub>-NH-CH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.212967	0.208992	0.208199	0.210008	0.213558	0.206012	0.205767	0.213834	0.219522
(3,-1)	0.257437	0.252008	0.253843	0.253366	0.256174	0.250715	0.251992	0.253060	0.259216
(3,-1)	0.256074	0.248376	0.252606	0.250533	0.254253	0.247626	0.250256	0.251833	0.258937
(3,-1)	0.257472	0.252008	0.253843	0.253366	0.256174	0.250715	0.251992	0.253060	0.259216
(3,-1)	0.347421	0.338619	0.347920	0.345073	0.349117	0.339049	0.348374	0.347316	0.339589
(3,-1)	0.295146	0.285874	0.293041	0.289842	0.294231	0.285252	0.293609	0.287702	0.282281
(3,-1)	0.295176	0.285874	0.293041	0.289842	0.294231	0.285252	0.293609	0.287702	0.282281
(3,-1)	0.292174	0.283086	0.290149	0.286972	0.291319	0.282504	0.290661	0.285216	0.279906
(3,-1)	0.292096	0.283086	0.290149	0.286972	0.291319	0.282504	0.290661	0.285216	0.279906
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.212967	0.307020	0.216870	0.210165	0.212199	0.212534	0.214825	0.214840	0.210503
(3,-1)	0.257437	0.449013	0.257281	0.255606	0.255503	0.247856	0.250283	0.257512	0.255007
(3,-1)	0.256074	0.449013	0.256517	0.254351	0.252861	0.244948	0.248573	0.255484	0.252796
(3,-1)	0.257472		0.257281	0.255606	0.255503	0.247856	0.250283	0.257512	0.255007
(3,-1)	0.347421		0.339242	0.348945	0.346783	0.348892	0.343184	0.350553	0.342454
(3,-1)	0.295146		0.289549	0.294755	0.292273	0.291034	0.286119	0.294840	0.292300
(3,-1)	0.295176		0.289549	0.294755	0.292273	0.291034	0.286119	0.294840	0.292300
(3,-1)	0.292174		0.286426	0.291850	0.289379	0.288332	0.283609	0.291868	0.289284
(3,-1)	0.292096		0.286426	0.291850	0.289379	0.288332	0.283609	0.291868	0.289284
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.212967	0.190106	0.212385	0.211309	0.207409	0.213250	0.212599	0.210557	0.209037
(3,-1)	0.257437	0.252201	0.253245	0.255285	0.256414	0.256478	0.255885	0.254718	0.252960
(3,-1)	0.256074	0.246412	0.251486	0.254405	0.253810	0.253064	0.253398	0.252987	0.251234
(3,-1)	0.257472	0.252201	0.253245	0.255285	0.256414	0.256478	0.255885	0.254718	0.252960
(3,-1)	0.347421	0.342501	0.348410	0.353490	0.357622	0.350212	0.349126	0.347547	0.345874
(3,-1)	0.295146	0.290078	0.295931	0.301361	0.308979	0.293673	0.293736	0.293232	0.292309
(3,-1)	0.295176	0.290078	0.295931	0.301361	0.308979	0.293673	0.293736	0.293232	0.292309
(3,-1)	0.292174	0.287193	0.293114	0.298421	0.306368	0.290701	0.290765	0.290277	0.289365
(3,-1)	0.292096	0.287193	0.293114	0.298421	0.306368	0.290701	0.290765	0.290277	0.289365
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.212967	0.309087	0.209133	0.216846	0.211379	0.213615	0.212274		
(3,-1)	0.257437	0.455456	0.250828	0.261720	0.255715	0.256329	0.253042		
(3,-1)	0.256074	0.455456	0.249039	0.262179	0.254963	0.254711	0.252956		
(3,-1)	0.257472		0.250828	0.261720	0.255715	0.256329	0.253042		
(3,-1)	0.347421		0.351103	0.354211	0.347736	0.346492	0.344792		
(3,-1)	0.295146		0.295047	0.301217	0.295422	0.294471	0.293244		
(3,-1)	0.295176		0.295047	0.301217	0.295422	0.294471	0.293244		
(3,-1)	0.292174		0.291931	0.298222	0.292475	0.291524	0.290234		
(3,-1)	0.292096		0.291931	0.298222	0.292475	0.291524	0.290234		

Table S128: Density value (a.u.) at the considered critical points for the NCCN system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.314216	0.304564	0.309286	0.306022	0.311078	0.303248	0.307588	0.311980	0.312026
(3,-1)	0.463636	0.468009	0.469043	0.464962	0.465741	0.470400	0.468262	0.450186	0.460120
(3,-1)	0.463636	0.468009	0.469043	0.464962	0.465741	0.470400	0.468262	0.450186	0.460120
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.314216	0.274401	0.307412	0.312203	0.309862	0.309296	0.312099	0.312831	0.308267
(3,-1)	0.463636	0.274401	0.448080	0.469466	0.465589	0.456116	0.459948	0.462945	0.461766
(3,-1)	0.463636	0.272983	0.448080	0.469466	0.465589	0.456116	0.459948	0.462945	0.461766
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.314216	0.303129	0.312174	0.313926	0.311672	0.309590	0.310618	0.310648	0.308543
(3,-1)	0.463636	0.453983	0.465481	0.477850	0.481531	0.459882	0.464225	0.466678	0.468007
(3,-1)	0.463636	0.453983	0.465481	0.477850	0.481531	0.459882	0.464225	0.466678	0.468007
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.314216	0.273737	0.312507	0.323938	0.312122	0.311844	0.309466		
(3,-1)	0.463636	0.273737	0.469846	0.467906	0.467028	0.464302	0.462034		
(3,-1)	0.463636	0.272339	0.469846	0.467906	0.467028	0.464302	0.462034		

Table S129: Density value (a.u.) at the considered critical points for the  $(\text{CH}_3)_2\text{CH}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.273947	0.270133	0.273930	0.272028	0.275465	0.268320	0.271181	0.273243	0.277435
(3,-1)	0.273947	0.270133	0.273930	0.272028	0.275465	0.268320	0.271181	0.273243	0.277435
(3,-1)	0.278655	0.271460	0.278574	0.275556	0.279807	0.272564	0.279026	0.275001	0.269346
(3,-1)	0.286223	0.278971	0.286366	0.283147	0.287416	0.279017	0.286801	0.281799	0.276303
(3,-1)	0.285574	0.278297	0.285815	0.282587	0.286852	0.278941	0.286239	0.281233	0.275659
(3,-1)	0.345430	0.340355	0.349637	0.346843	0.350892	0.340537	0.350094	0.349331	0.341952
(3,-1)	0.278655	0.271460	0.278574	0.275556	0.279807	0.272564	0.279026	0.275001	0.269346
(3,-1)	0.286223	0.278971	0.286366	0.283147	0.287416	0.279017	0.286801	0.281799	0.276303
(3,-1)	0.285574	0.278297	0.285815	0.282587	0.286852	0.278941	0.286239	0.281233	0.275659
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.273947	0.250498	0.274437	0.275955	0.274608	0.265190	0.269307	0.277057	0.273225
(3,-1)	0.273947	0.268917	0.274437	0.275955	0.274608	0.265190	0.269307	0.277057	0.273225
(3,-1)	0.278655	0.274574	0.274803	0.280161	0.277834	0.277810	0.273088	0.280158	0.277268
(3,-1)	0.286223	0.274590	0.282936	0.287901	0.285386	0.284732	0.279902	0.287818	0.285244
(3,-1)	0.285574	0.274590	0.282189	0.287310	0.284790	0.284263	0.279238	0.287178	0.284438
(3,-1)	0.345430	0.281730	0.341153	0.350636	0.348528	0.350679	0.344836	0.352232	0.343877
(3,-1)	0.278655	0.281730	0.274803	0.280161	0.277834	0.277810	0.273088	0.280158	0.277268
(3,-1)	0.286223	0.332491	0.282936	0.287901	0.285386	0.284732	0.279902	0.287818	0.285244
(3,-1)	0.285574	0.332491	0.282189	0.287310	0.284790	0.284263	0.279238	0.287178	0.284438
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.273947	0.269615	0.270977	0.274499	0.270589	0.275919	0.275768	0.274641	0.272482
(3,-1)	0.273947	0.269615	0.270977	0.274499	0.270589	0.275919	0.275768	0.274641	0.272482
(3,-1)	0.278655	0.276166	0.281266	0.286356	0.294436	0.279109	0.279064	0.278561	0.277788
(3,-1)	0.286223	0.283769	0.288978	0.294184	0.301988	0.286712	0.286738	0.286281	0.285386
(3,-1)	0.285574	0.283102	0.288228	0.293447	0.301181	0.286028	0.286062	0.285630	0.284779
(3,-1)	0.345430	0.344030	0.350063	0.355216	0.359114	0.351747	0.350691	0.349169	0.347523
(3,-1)	0.278655	0.276166	0.281266	0.286356	0.294436	0.279109	0.279064	0.278561	0.277788
(3,-1)	0.286223	0.283769	0.288978	0.294184	0.301988	0.286712	0.286738	0.286281	0.285386
(3,-1)	0.285574	0.283102	0.288228	0.293447	0.301181	0.286028	0.286062	0.285630	0.284779
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.273947	0.249803	0.269787	0.283688	0.276191	0.275958	0.273591		
(3,-1)	0.273947	0.268134	0.269787	0.283688	0.276191	0.275958	0.273591		
(3,-1)	0.278655	0.274018	0.278814	0.286188	0.280838	0.279968	0.278640		
(3,-1)	0.286223	0.274036	0.287426	0.293934	0.288559	0.287532	0.286330		
(3,-1)	0.285574	0.274036	0.286445	0.293289	0.287956	0.286908	0.285688		
(3,-1)	0.345430	0.280321	0.352743	0.355957	0.349552	0.348357	0.346639		
(3,-1)	0.278655	0.280321	0.278814	0.286188	0.280838	0.279968	0.278640		
(3,-1)	0.286223	0.335324	0.287426	0.293934	0.288559	0.287532	0.286330		
(3,-1)	0.285574	0.335324	0.286445	0.293289	0.287956	0.286908	0.285688		

Table S130: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>–CH<sub>2</sub>–NH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.252014	0.243225	0.249069	0.246192	0.251365	0.242303	0.245908	0.253356	0.252487
(3,-1)	0.268116	0.264505	0.268146	0.266441	0.269747	0.263805	0.265603	0.267716	0.272090
(3,-1)	0.279820	0.273238	0.280290	0.277209	0.281288	0.273570	0.280602	0.276749	0.271409
(3,-1)	0.279967	0.273592	0.280671	0.277583	0.281540	0.274202	0.280981	0.276908	0.271447
(3,-1)	0.279967	0.273592	0.280671	0.277583	0.281540	0.274202	0.280981	0.276908	0.271447
(3,-1)	0.287237	0.280008	0.287183	0.284018	0.288313	0.280072	0.287656	0.282694	0.276788
(3,-1)	0.287237	0.280008	0.287183	0.284018	0.288313	0.280072	0.287656	0.282694	0.276788
(3,-1)	0.341955	0.336700	0.346252	0.343433	0.347494	0.337556	0.346801	0.345975	0.338608
(3,-1)	0.341955	0.336700	0.346252	0.343433	0.347494	0.337556	0.346801	0.345975	0.338608
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.252014	0.328903	0.252927	0.251722	0.249716	0.247587	0.250084	0.253494	0.248988
(3,-1)	0.268116	0.276465	0.268799	0.270074	0.268900	0.259903	0.263730	0.271154	0.267384
(3,-1)	0.279820	0.276465	0.276320	0.281741	0.279318	0.279005	0.274719	0.281532	0.278938
(3,-1)	0.279967	0.436264	0.276416	0.282003	0.279555	0.279303	0.274831	0.281669	0.278974
(3,-1)	0.279967		0.276416	0.282003	0.279555	0.279303	0.274831	0.281669	0.278974
(3,-1)	0.287237		0.283620	0.288794	0.286336	0.285602	0.280718	0.288715	0.286020
(3,-1)	0.287237		0.283620	0.288794	0.286336	0.285602	0.280718	0.288715	0.286020
(3,-1)	0.341955		0.337688	0.347172	0.345044	0.347486	0.341461	0.348687	0.340457
(3,-1)	0.341955		0.337688	0.347172	0.345044	0.347486	0.341461	0.348687	0.340457
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.252014	0.244081	0.250132	0.251703	0.247274	0.251157	0.251172	0.250031	0.248055
(3,-1)	0.268116	0.263776	0.264990	0.268351	0.264270	0.270068	0.269898	0.268829	0.266804
(3,-1)	0.279820	0.277464	0.282930	0.287753	0.295782	0.280573	0.280572	0.280104	0.279240
(3,-1)	0.279967	0.277631	0.283008	0.287855	0.295924	0.280628	0.280666	0.280261	0.279441
(3,-1)	0.279967	0.277631	0.283008	0.287855	0.295924	0.280628	0.280666	0.280261	0.279441
(3,-1)	0.287237	0.284680	0.289732	0.295056	0.302554	0.287676	0.287723	0.287260	0.286321
(3,-1)	0.287237	0.284680	0.289732	0.295056	0.302554	0.287676	0.287723	0.287260	0.286321
(3,-1)	0.341955	0.340610	0.346650	0.351577	0.355851	0.348140	0.347065	0.345602	0.344099
(3,-1)	0.341955	0.340610	0.346650	0.351577	0.355851	0.348140	0.347065	0.345602	0.344099
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.252014	0.331838	0.247319	0.263908	0.252725	0.252481	0.251420		
(3,-1)	0.268116	0.277022	0.263753	0.277130	0.270338	0.270195	0.267770		
(3,-1)	0.279820	0.277022	0.280933	0.287216	0.282259	0.281241	0.279917		
(3,-1)	0.279967	0.441384	0.280762	0.287156	0.282526	0.281446	0.280130		
(3,-1)	0.279967		0.280762	0.287156	0.282526	0.281446	0.280130		
(3,-1)	0.287237		0.288225	0.294892	0.289475	0.288510	0.287239		
(3,-1)	0.287237		0.288225	0.294892	0.289475	0.288510	0.287239		
(3,-1)	0.341955		0.349132	0.352301	0.346114	0.344896	0.343208		
(3,-1)	0.341955		0.349132	0.352301	0.346114	0.344896	0.343208		

Table S131: Density value (a.u.) at the considered critical points for the H<sub>2</sub>C=C=O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.336743	0.334704	0.337992	0.334444	0.335585	0.336196	0.336239	0.328997	0.334560
(3,-1)	0.285723	0.275318	0.282676	0.279365	0.283749	0.275086	0.283016	0.278150	0.274907
(3,-1)	0.285723	0.275318	0.282676	0.279365	0.283749	0.275086	0.283016	0.278150	0.274907
(3,-1)	0.451846	0.453311	0.453937	0.451023	0.453480	0.453572	0.450506	0.438161	0.441595
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.336743	0.215403	0.327173	0.338521	0.335254	0.328704	0.332728	0.334032	0.334514
(3,-1)	0.285723	0.251424	0.278227	0.284401	0.281799	0.280478	0.276663	0.284444	0.281810
(3,-1)	0.285723	0.264980	0.278227	0.284401	0.281799	0.280478	0.276663	0.284444	0.281810
(3,-1)	0.451846	0.251424	0.434559	0.455973	0.453474	0.440819	0.445940	0.452060	0.448143
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.336743	0.329457	0.334687	0.340232	0.338831	0.330370	0.333823	0.336233	0.335176
(3,-1)	0.285723	0.279277	0.286118	0.290884	0.300757	0.283324	0.283358	0.282791	0.281719
(3,-1)	0.285723	0.279277	0.286118	0.290884	0.300757	0.283324	0.283358	0.282791	0.281719
(3,-1)	0.451846	0.439126	0.450360	0.461884	0.467906	0.452868	0.453829	0.452218	0.454266
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.336743	0.215595	0.333847	0.337647	0.337739	0.335431	0.333184		
(3,-1)	0.285723	0.251369	0.285505	0.290848	0.284608	0.283514	0.281968		
(3,-1)	0.285723	0.263840	0.285505	0.290848	0.284608	0.283514	0.281968		
(3,-1)	0.451846	0.251369	0.458072	0.461290	0.452830	0.451732	0.447242		

Table S132: Density value (a.u.) at the considered critical points for the CH<sub>2</sub>-O-CH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.217247	0.213967	0.212795	0.214791	0.217813	0.211445	0.211247	0.217410	0.224889
(3,-1)	0.253537	0.251852	0.251935	0.252225	0.252810	0.251242	0.249869	0.251898	0.252104
(3,-1)	0.265392	0.257453	0.262082	0.259696	0.263442	0.256548	0.259975	0.261845	0.267720
(3,-1)	0.253537	0.251852	0.251935	0.252225	0.252810	0.251242	0.249869	0.251898	0.252104
(3,-1)	0.296655	0.286232	0.293532	0.290302	0.294928	0.285704	0.294274	0.288005	0.282552
(3,-1)	0.296655	0.286232	0.293532	0.290302	0.294928	0.285704	0.294274	0.288005	0.282552
(3,-1)	0.296655	0.286232	0.293532	0.290302	0.294928	0.285704	0.294274	0.288005	0.282552
(3,-1)	0.296655	0.286232	0.293532	0.290302	0.294928	0.285704	0.294274	0.288005	0.282552
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.217247	0.401782	0.220264	0.214630	0.216799	0.218246	0.219007	0.219275	0.214703
(3,-1)	0.253537	0.264379	0.249516	0.252723	0.252990	0.249041	0.251629	0.253177	0.252780
(3,-1)	0.265392	0.279261	0.265195	0.263759	0.261961	0.254785	0.258221	0.264551	0.261685
(3,-1)	0.253537	0.279577	0.249516	0.252723	0.252990	0.249041	0.251629	0.253177	0.252780
(3,-1)	0.296655	0.272315	0.290390	0.295412	0.292940	0.291912	0.286593	0.295696	0.293137
(3,-1)	0.296655	0.272315	0.290390	0.295412	0.292940	0.291912	0.286593	0.295696	0.293137
(3,-1)	0.296655		0.290390	0.295412	0.292940	0.291912	0.286593	0.295696	0.293137
(3,-1)	0.296655		0.290390	0.295412	0.292940	0.291912	0.286593	0.295696	0.293137
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.217247	0.197423	0.216116	0.216131	0.211900	0.218086	0.217433	0.215896	0.213609
(3,-1)	0.253537	0.251497	0.250533	0.249624	0.249767	0.253581	0.253312	0.252697	0.250665
(3,-1)	0.265392	0.255177	0.260435	0.263346	0.261818	0.262185	0.262506	0.262117	0.260512
(3,-1)	0.253537	0.251497	0.250533	0.249624	0.249767	0.253581	0.253312	0.252697	0.250665
(3,-1)	0.296655	0.290916	0.296645	0.302218	0.309500	0.294451	0.294463	0.293917	0.293071
(3,-1)	0.296655	0.290916	0.296645	0.302218	0.309500	0.294451	0.294463	0.293917	0.293071
(3,-1)	0.296655	0.290916	0.296645	0.302218	0.309500	0.294451	0.294463	0.293917	0.293071
(3,-1)	0.296655	0.290916	0.296645	0.302218	0.309500	0.294451	0.294463	0.293917	0.293071
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.217247	0.405046	0.216046	0.220449	0.215724	0.217985	0.216011		
(3,-1)	0.253537	0.264061	0.249014	0.252189	0.252325	0.252575	0.248589		
(3,-1)	0.265392	0.277738	0.257712	0.271486	0.264536	0.264050	0.262321		
(3,-1)	0.253537	0.278913	0.249014	0.252189	0.252325	0.252575	0.248589		
(3,-1)	0.296655	0.272181	0.295877	0.302494	0.296121	0.295265	0.293994		
(3,-1)	0.296655	0.272181	0.295877	0.302494	0.296121	0.295265	0.293994		
(3,-1)	0.296655		0.295877	0.302494	0.296121	0.295265	0.293994		
(3,-1)	0.296655		0.295877	0.302494	0.296121	0.295265	0.293994		

Table S133: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>CHO system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.414477	0.416644	0.417651	0.414946	0.416135	0.417076	0.413611	0.403138	0.405781
(3,-1)	0.270306	0.258255	0.263959	0.261035	0.266580	0.257234	0.261241	0.268416	0.266426
(3,-1)	0.287604	0.276600	0.283458	0.280576	0.285779	0.276071	0.284716	0.279043	0.272913
(3,-1)	0.287679	0.278097	0.285780	0.282480	0.286686	0.278593	0.286158	0.281290	0.275950
(3,-1)	0.280969	0.270846	0.278219	0.275013	0.279273	0.271216	0.278473	0.274636	0.269845
(3,-1)	0.280969	0.270846	0.278219	0.275013	0.279273	0.271216	0.278473	0.274636	0.269845
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.414477	0.266664	0.399592	0.418572	0.416044	0.403597	0.409078	0.414215	0.411772
(3,-1)	0.270306	0.400063	0.267061	0.266979	0.265017	0.264581	0.265936	0.268964	0.263940
(3,-1)	0.287604	0.281794	0.281523	0.285915	0.283889	0.283736	0.277880	0.286991	0.284025
(3,-1)	0.287679	0.400063	0.281890	0.287169	0.284556	0.284038	0.279104	0.286994	0.284222
(3,-1)	0.280969	0.281794	0.274117	0.279777	0.277269	0.276969	0.272739	0.279650	0.277060
(3,-1)	0.280969		0.274117	0.279777	0.277269	0.276969	0.272739	0.279650	0.277060
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.414477	0.402766	0.411124	0.421391	0.423760	0.415123	0.416191	0.415127	0.416324
(3,-1)	0.270306	0.259681	0.266278	0.267872	0.263098	0.266308	0.266471	0.265425	0.263485
(3,-1)	0.287604	0.282277	0.287306	0.293301	0.299600	0.285851	0.285629	0.284873	0.284212
(3,-1)	0.287679	0.282418	0.288118	0.293194	0.300846	0.285779	0.285804	0.285380	0.284580
(3,-1)	0.280969	0.275347	0.281101	0.285827	0.294262	0.278821	0.278769	0.278201	0.277218
(3,-1)	0.280969	0.275347	0.281101	0.285827	0.294262	0.278821	0.278769	0.278201	0.277218
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.414477	0.266342	0.417281	0.419918	0.416364	0.414749	0.410830		
(3,-1)	0.270306	0.403388	0.263541	0.280062	0.268176	0.268156	0.266938		
(3,-1)	0.287604	0.280379	0.286661	0.294665	0.286614	0.286365	0.284713		
(3,-1)	0.287679	0.403388	0.286968	0.293065	0.287533	0.286369	0.285122		
(3,-1)	0.280969	0.280379	0.279387	0.285721	0.280363	0.279317	0.278031		
(3,-1)	0.280969		0.279387	0.285721	0.280363	0.279317	0.278031		



Table S134: Density value (a.u.) at the considered critical points for the O=CH–CH=O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.274022	0.261128	0.266247	0.263632	0.269790	0.259895	0.264246	0.271919	0.268524
(3,-1)	0.413073	0.415502	0.416526	0.413804	0.414739	0.416214	0.412377	0.401712	0.403957
(3,-1)	0.290234	0.279179	0.286494	0.283479	0.288730	0.278924	0.287716	0.281268	0.275356
(3,-1)	0.413073	0.415502	0.416526	0.413804	0.414739	0.416214	0.412377	0.401712	0.403957
(3,-1)	0.290234	0.279179	0.286494	0.283479	0.288730	0.278924	0.287716	0.281268	0.275356
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.274022	0.258531	0.269601	0.269933	0.268362	0.270428	0.270158	0.272732	0.266724
(3,-1)	0.413073	0.257179	0.397968	0.417235	0.414648	0.402323	0.407659	0.412676	0.410264
(3,-1)	0.290234	0.357930	0.284772	0.288866	0.286719	0.286498	0.280096	0.289973	0.287042
(3,-1)	0.413073	0.281139	0.397968	0.417235	0.414648	0.402323	0.407659	0.412676	0.410264
(3,-1)	0.290234	0.281139	0.284772	0.288866	0.286719	0.286498	0.280096	0.289973	0.287042
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.274022	0.263523	0.270317	0.271807	0.266273	0.270139	0.270052	0.268705	0.267006
(3,-1)	0.413073	0.401527	0.409664	0.419951	0.422608	0.413573	0.414693	0.413704	0.414898
(3,-1)	0.290234	0.284675	0.290242	0.296111	0.302139	0.288662	0.288462	0.287735	0.287078
(3,-1)	0.413073	0.401527	0.409664	0.419951	0.422608	0.413573	0.414693	0.413704	0.414898
(3,-1)	0.290234	0.284675	0.290242	0.296111	0.302139	0.288662	0.288462	0.287735	0.287078
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.274022	0.257781	0.267812	0.285043	0.271318	0.271896	0.270325		
(3,-1)	0.413073	0.257081	0.415914	0.417806	0.415070	0.413342	0.409508		
(3,-1)	0.290234	0.361496	0.290163	0.297747	0.289406	0.289032	0.287464		
(3,-1)	0.413073	0.279871	0.415914	0.417806	0.415070	0.413342	0.409508		
(3,-1)	0.290234	0.279871	0.290163	0.297747	0.289406	0.289032	0.287464		

Table S135: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>CH<sub>2</sub>OH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.260584	0.251429	0.257704	0.254586	0.259849	0.250871	0.254631	0.262059	0.260257
(3,-1)	0.255211	0.258863	0.260220	0.259506	0.259436	0.259258	0.257215	0.256402	0.257843
(3,-1)	0.362742	0.360932	0.371761	0.369641	0.372156	0.365413	0.372905	0.372791	0.361724
(3,-1)	0.287368	0.279551	0.286715	0.283570	0.288065	0.279779	0.287301	0.282216	0.276093
(3,-1)	0.287368	0.279551	0.286715	0.283570	0.288065	0.279779	0.287301	0.282216	0.276093
(3,-1)	0.280384	0.273791	0.280912	0.277808	0.281868	0.274083	0.281217	0.277237	0.271946
(3,-1)	0.282907	0.276244	0.283503	0.280337	0.284419	0.276524	0.283853	0.279422	0.273947
(3,-1)	0.282907	0.276244	0.283503	0.280337	0.284419	0.276524	0.283853	0.279422	0.273947
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.260584	0.264756	0.260942	0.260339	0.258136	0.257111	0.258915	0.261961	0.257179
(3,-1)	0.255211	0.264756	0.253940	0.260470	0.259708	0.251158	0.255350	0.259314	0.258544
(3,-1)	0.362742	0.286294	0.362192	0.371572	0.369977	0.371388	0.368064	0.373901	0.366184
(3,-1)	0.287368	0.278977	0.283260	0.288509	0.286105	0.285780	0.280481	0.288646	0.285837
(3,-1)	0.287368	0.278977	0.283260	0.288509	0.286105	0.285780	0.280481	0.288646	0.285837
(3,-1)	0.280384	0.286294	0.276931	0.282328	0.279881	0.279494	0.275183	0.282065	0.279497
(3,-1)	0.282907	0.278977	0.279319	0.284893	0.282388	0.281985	0.277366	0.284625	0.282019
(3,-1)	0.282907	0.278977	0.279319	0.284893	0.282388	0.281985	0.277366	0.284625	0.282019
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.260584	0.252751	0.258980	0.260466	0.255693	0.259381	0.259537	0.258555	0.256611
(3,-1)	0.255211	0.255477	0.255260	0.256580	0.255398	0.259875	0.260249	0.260083	0.257919
(3,-1)	0.362742	0.367834	0.366885	0.369581	0.366931	0.374804	0.373301	0.372151	0.369364
(3,-1)	0.287368	0.284590	0.289579	0.295145	0.302384	0.287594	0.287567	0.287000	0.286144
(3,-1)	0.287368	0.284590	0.289579	0.295145	0.302384	0.287594	0.287567	0.287000	0.286144
(3,-1)	0.280384	0.278047	0.283474	0.288299	0.296363	0.281027	0.281051	0.280632	0.279813
(3,-1)	0.282907	0.280467	0.285961	0.290918	0.298898	0.283604	0.283627	0.283194	0.282337
(3,-1)	0.282907	0.280467	0.285961	0.290918	0.298898	0.283604	0.283627	0.283194	0.282337
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.260584	0.264934	0.256055	0.272716	0.261396	0.261025	0.260034		
(3,-1)	0.255211	0.264934	0.254557	0.257925	0.259793	0.258913	0.255814		
(3,-1)	0.362742	0.284910	0.375674	0.373003	0.368838	0.367320	0.365123		
(3,-1)	0.287368	0.278055	0.288001	0.295188	0.289336	0.288497	0.287224		
(3,-1)	0.287368	0.278055	0.288001	0.295188	0.289336	0.288497	0.287224		
(3,-1)	0.280384	0.284910	0.281483	0.287676	0.282852	0.281804	0.280476		
(3,-1)	0.282907	0.278055	0.284202	0.290333	0.285425	0.284330	0.283077		
(3,-1)	0.282907	0.278055	0.284202	0.290333	0.285425	0.284330	0.283077		

Table S136: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>-O-CH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.263785	0.267206	0.268877	0.267780	0.267801	0.266130	0.265519	0.264372	0.265125
(3,-1)	0.263785	0.267206	0.268877	0.267780	0.267801	0.266130	0.265519	0.264372	0.265125
(3,-1)	0.291958	0.284049	0.291760	0.288437	0.292942	0.283963	0.292408	0.286325	0.280825
(3,-1)	0.284979	0.277126	0.284654	0.281469	0.285964	0.278061	0.285254	0.280135	0.274441
(3,-1)	0.284979	0.277126	0.284654	0.281469	0.285964	0.278061	0.285254	0.280135	0.274441
(3,-1)	0.291958	0.284049	0.291760	0.288437	0.292942	0.283963	0.292408	0.286325	0.280825
(3,-1)	0.284979	0.277126	0.284654	0.281469	0.285964	0.278061	0.285254	0.280135	0.274441
(3,-1)	0.284979	0.277126	0.284654	0.281469	0.285964	0.278061	0.285254	0.280135	0.274441
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.263785	0.153914	0.261704	0.269224	0.268087	0.259045	0.263507	0.267854	0.267159
(3,-1)	0.263785	0.171832	0.261704	0.269224	0.268087	0.259045	0.263507	0.267854	0.267159
(3,-1)	0.291958	0.263991	0.288818	0.293410	0.290840	0.290121	0.284625	0.293511	0.291010
(3,-1)	0.284979	0.171832	0.281253	0.286345	0.283904	0.283730	0.278355	0.286439	0.283585
(3,-1)	0.284979	0.286182	0.281253	0.286345	0.283904	0.283730	0.278355	0.286439	0.283585
(3,-1)	0.291958	0.286182	0.288818	0.293410	0.290840	0.290121	0.284625	0.293511	0.291010
(3,-1)	0.284979	0.286182	0.281253	0.286345	0.283904	0.283730	0.278355	0.286439	0.283585
(3,-1)	0.284979	0.286182	0.281253	0.286345	0.283904	0.283730	0.278355	0.286439	0.283585
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.263785	0.264125	0.263862	0.265571	0.264797	0.268643	0.269001	0.268693	0.266333
(3,-1)	0.263785	0.264125	0.263862	0.265571	0.264797	0.268643	0.269001	0.268693	0.266333
(3,-1)	0.291958	0.289266	0.294484	0.299966	0.307259	0.292349	0.292337	0.291834	0.290984
(3,-1)	0.284979	0.282328	0.287422	0.292863	0.300467	0.285265	0.285227	0.284717	0.283973
(3,-1)	0.284979	0.282328	0.287422	0.292863	0.300467	0.285265	0.285227	0.284717	0.283973
(3,-1)	0.291958	0.289266	0.294484	0.299966	0.307259	0.292349	0.292337	0.291834	0.290984
(3,-1)	0.284979	0.282328	0.287422	0.292863	0.300467	0.285265	0.285227	0.284717	0.283973
(3,-1)	0.284979	0.282328	0.287422	0.292863	0.300467	0.285265	0.285227	0.284717	0.283973
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.263785	0.152815	0.263235	0.267448	0.268412	0.267274	0.264270		
(3,-1)	0.263785	0.170799	0.263235	0.267448	0.268412	0.267274	0.264270		
(3,-1)	0.291958	0.263459	0.293414	0.300009	0.294177	0.293179	0.292063		
(3,-1)	0.284979	0.170799	0.285576	0.292968	0.287085	0.286192	0.284930		
(3,-1)	0.284979	0.285083	0.285576	0.292968	0.287085	0.286192	0.284930		
(3,-1)	0.291958	0.285083	0.293414	0.300009	0.294177	0.293179	0.292063		
(3,-1)	0.284979	0.285083	0.285576	0.292968	0.287085	0.286192	0.284930		
(3,-1)	0.284979	0.285083	0.285576	0.292968	0.287085	0.286192	0.284930		

Table S137: Density value (a.u.) at the considered critical points for the CH<sub>2</sub>-S-CH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.152890	0.150342	0.149478	0.151097	0.153739	0.147946	0.147143	0.153667	0.157355
(3,-1)	0.170466	0.165911	0.167014	0.167014	0.169800	0.164763	0.164758	0.167050	0.171993
(3,-1)	0.265899	0.256929	0.262002	0.259234	0.263280	0.257059	0.260427	0.261315	0.266078
(3,-1)	0.170466	0.165911	0.167014	0.167014	0.169800	0.164763	0.164758	0.167050	0.171993
(3,-1)	0.294605	0.284704	0.291984	0.288812	0.293304	0.283845	0.292611	0.287079	0.281773
(3,-1)	0.294605	0.284704	0.291984	0.288812	0.293304	0.283845	0.292611	0.287079	0.281773
(3,-1)	0.294605	0.284704	0.291984	0.288812	0.293304	0.283845	0.292611	0.287079	0.281773
(3,-1)	0.294605	0.284704	0.291984	0.288812	0.293304	0.283845	0.292611	0.287079	0.281773
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.152890	0.274303	0.156228	0.150953	0.152692	0.153078	0.154538	0.154509	0.151865
(3,-1)	0.170466	0.199106	0.173964	0.168618	0.168914	0.163671	0.165702	0.170886	0.169884
(3,-1)	0.265899	0.199106	0.265210	0.264121	0.262111	0.254467	0.257849	0.265036	0.261586
(3,-1)	0.170466	0.276358	0.173964	0.168618	0.168914	0.163671	0.165702	0.170886	0.169884
(3,-1)	0.294605	0.278644	0.288617	0.293705	0.291257	0.290225	0.285243	0.293940	0.291266
(3,-1)	0.294605	0.275473	0.288617	0.293705	0.291257	0.290225	0.285243	0.293940	0.291266
(3,-1)	0.294605	0.278644	0.288617	0.293705	0.291257	0.290225	0.285243	0.293940	0.291266
(3,-1)	0.294605	0.275473	0.288617	0.293705	0.291257	0.290225	0.285243	0.293940	0.291266
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.152890	0.136027	0.152888	0.152441	0.149208	0.154031	0.153223	0.150985	0.151129
(3,-1)	0.170466	0.161855	0.168260	0.169272	0.171335	0.170558	0.169759	0.168050	0.167517
(3,-1)	0.265899	0.258252	0.260969	0.264212	0.263739	0.261700	0.262679	0.263167	0.260801
(3,-1)	0.170466	0.161855	0.168260	0.169272	0.171335	0.170558	0.169759	0.168050	0.167517
(3,-1)	0.294605	0.288696	0.294909	0.300253	0.307847	0.292859	0.292816	0.292212	0.291196
(3,-1)	0.294605	0.288696	0.294909	0.300253	0.307847	0.292859	0.292816	0.292212	0.291196
(3,-1)	0.294605	0.288696	0.294909	0.300253	0.307847	0.292859	0.292816	0.292212	0.291196
(3,-1)	0.294605	0.288696	0.294909	0.300253	0.307847	0.292859	0.292816	0.292212	0.291196
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.152890	0.274597	0.151209	0.156039	0.151729	0.153538	0.152688		
(3,-1)	0.170466	0.198237	0.165307	0.175043	0.168905	0.169795	0.167982		
(3,-1)	0.265899	0.198237	0.258820	0.273816	0.264474	0.264027	0.262078		
(3,-1)	0.170466	0.276280	0.165307	0.175043	0.168905	0.169795	0.167982		
(3,-1)	0.294605	0.278159	0.294109	0.300375	0.294193	0.293249	0.291942		
(3,-1)	0.294605	0.275222	0.294109	0.300375	0.294193	0.293249	0.291942		
(3,-1)	0.294605	0.278159	0.294109	0.300375	0.294193	0.293249	0.291942		
(3,-1)	0.294605	0.275222	0.294109	0.300375	0.294193	0.293249	0.291942		

Table S138: Density value (a.u.) at the considered critical points for the  $(\text{CH}_3)_2\text{SO}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.275224	0.276284	0.275702	0.274310	0.276902	0.274743	0.275168	0.268155	0.273962
(3,-1)	0.198926	0.190928	0.195064	0.193241	0.197986	0.189802	0.191801	0.197112	0.201801
(3,-1)	0.198925	0.190928	0.195064	0.193240	0.197986	0.189802	0.191801	0.197112	0.201800
(3,-1)	0.282358	0.275175	0.282862	0.279585	0.284065	0.276125	0.283376	0.278632	0.273628
(3,-1)	0.284209	0.277300	0.284826	0.281540	0.285886	0.277399	0.285303	0.280383	0.275387
(3,-1)	0.281113	0.274009	0.281538	0.278299	0.282724	0.274769	0.282017	0.277520	0.272709
(3,-1)	0.284209	0.277300	0.284826	0.281540	0.285886	0.277398	0.285303	0.280383	0.275387
(3,-1)	0.281113	0.274009	0.281538	0.278299	0.282724	0.274769	0.282017	0.277521	0.272709
(3,-1)	0.282358	0.275175	0.282862	0.279585	0.284065	0.276125	0.283376	0.278632	0.273628
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.275224	0.249143	0.268824	0.277914	0.276875	0.268741	0.275239	0.278138	0.279102
(3,-1)	0.198926	0.184397	0.202011	0.197933	0.196877	0.190358	0.194284	0.200445	0.196955
(3,-1)	0.198925	0.216471	0.202011	0.197932	0.196877	0.190358	0.194284	0.200445	0.196955
(3,-1)	0.282358	0.281630	0.278731	0.284445	0.281897	0.281456	0.276551	0.284443	0.281629
(3,-1)	0.284209	0.281630	0.281060	0.286341	0.283759	0.283055	0.278338	0.286297	0.283694
(3,-1)	0.281113	0.276266	0.277685	0.283126	0.280605	0.280163	0.275449	0.283106	0.280384
(3,-1)	0.284209	0.277519	0.281060	0.286341	0.283759	0.283055	0.278338	0.286297	0.283694
(3,-1)	0.281113	0.277519	0.277685	0.283126	0.280605	0.280163	0.275449	0.283106	0.280384
(3,-1)	0.282358	0.278731	0.284444	0.281897	0.281456	0.281456	0.276551	0.284443	0.281629
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.275224	0.268053	0.273944	0.276643	0.282922	0.278466	0.278399	0.277422	0.276713
(3,-1)	0.198926	0.190991	0.195344	0.197761	0.194062	0.199487	0.198965	0.197340	0.195542
(3,-1)	0.198925	0.190991	0.195344	0.197761	0.194062	0.199487	0.198965	0.197340	0.195542
(3,-1)	0.282358	0.279529	0.285657	0.290756	0.299084	0.283435	0.283334	0.282777	0.281904
(3,-1)	0.284209	0.281462	0.287513	0.292642	0.300819	0.285229	0.285171	0.284634	0.283760
(3,-1)	0.281113	0.278333	0.284405	0.289361	0.297703	0.282033	0.281951	0.281410	0.280598
(3,-1)	0.284209	0.281462	0.287513	0.292642	0.300819	0.285229	0.285171	0.284634	0.283760
(3,-1)	0.281113	0.278333	0.284405	0.289362	0.297703	0.282033	0.281952	0.281410	0.280598
(3,-1)	0.282358	0.279529	0.285657	0.290756	0.299084	0.283435	0.283334	0.282777	0.281903
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.275224	0.248401	0.274373	0.284109	0.275551	0.275608	0.271946		
(3,-1)	0.198926	0.183376	0.193493	0.210185	0.198943	0.199451	0.198323		
(3,-1)	0.198925	0.216942	0.193493	0.210185	0.198943	0.199451	0.198323		
(3,-1)	0.282358	0.280636	0.284381	0.290838	0.284756	0.283701	0.282336		
(3,-1)	0.284209	0.280636	0.286357	0.292422	0.286702	0.285585	0.284304		
(3,-1)	0.281113	0.275628	0.282785	0.289394	0.283477	0.282437	0.281030		
(3,-1)	0.284209	0.276823	0.286357	0.292422	0.286702	0.285585	0.284304		
(3,-1)	0.281113	0.276823	0.282785	0.289394	0.283477	0.282437	0.281030		
(3,-1)	0.282358	0.284381	0.290838	0.284756	0.283701	0.282336			

Table S139: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>-CH<sub>2</sub>-SH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.250018	0.241799	0.247600	0.244695	0.249724	0.241132	0.244450	0.251416	0.251202
(3,-1)	0.182139	0.176522	0.179938	0.178470	0.182434	0.176015	0.176829	0.179617	0.185820
(3,-1)	0.219337	0.216273	0.219915	0.217918	0.220779	0.217131	0.219472	0.218332	0.216420
(3,-1)	0.287430	0.280507	0.287637	0.284521	0.288856	0.280105	0.288168	0.283335	0.277750
(3,-1)	0.287430	0.280507	0.287637	0.284521	0.288856	0.280105	0.288168	0.283335	0.277750
(3,-1)	0.281580	0.274897	0.282041	0.278932	0.283032	0.274984	0.282328	0.278272	0.272908
(3,-1)	0.282879	0.276296	0.283569	0.280436	0.284524	0.276611	0.283946	0.279501	0.274069
(3,-1)	0.282879	0.276296	0.283569	0.280436	0.284524	0.276611	0.283946	0.279501	0.274069
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.250018	0.190075	0.251375	0.250105	0.248046	0.244872	0.247910	0.251630	0.247568
(3,-1)	0.182139	0.190075	0.187163	0.182253	0.181384	0.172799	0.176776	0.184279	0.181894
(3,-1)	0.219337	0.278466	0.217452	0.221339	0.219756	0.218969	0.217798	0.221029	0.219534
(3,-1)	0.287430	0.278073	0.283879	0.289247	0.286831	0.286141	0.281206	0.289283	0.286512
(3,-1)	0.287430	0.278073	0.283879	0.289247	0.286831	0.286141	0.281206	0.289283	0.286512
(3,-1)	0.281580	0.278466	0.278169	0.283491	0.281045	0.280603	0.276229	0.283297	0.280704
(3,-1)	0.282879	0.278073	0.279567	0.284956	0.282486	0.282095	0.277331	0.284725	0.282010
(3,-1)	0.282879	0.278073	0.279567	0.284956	0.282486	0.282095	0.277331	0.284725	0.282010
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.250018	0.242030	0.248103	0.249845	0.245725	0.249376	0.249408	0.248310	0.246393
(3,-1)	0.182139	0.174511	0.179542	0.181910	0.180551	0.183584	0.183076	0.181511	0.180087
(3,-1)	0.219337	0.217624	0.221971	0.225202	0.233190	0.220321	0.220565	0.220276	0.219613
(3,-1)	0.287430	0.284663	0.290344	0.295673	0.303273	0.288343	0.288292	0.287714	0.286713
(3,-1)	0.287430	0.284663	0.290344	0.295673	0.303273	0.288343	0.288292	0.287714	0.286713
(3,-1)	0.281580	0.279171	0.284688	0.289587	0.297707	0.282345	0.282352	0.281877	0.280953
(3,-1)	0.282879	0.280528	0.286007	0.290970	0.298934	0.283619	0.283646	0.283229	0.282410
(3,-1)	0.282879	0.280528	0.286007	0.290970	0.298934	0.283619	0.283646	0.283229	0.282410
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.250018	0.189213	0.245381	0.261737	0.250916	0.250568	0.249415		
(3,-1)	0.182139	0.189213	0.177126	0.192345	0.182889	0.183255	0.182044		
(3,-1)	0.219337	0.277820	0.219530	0.225746	0.221740	0.221252	0.219705		
(3,-1)	0.287430	0.277536	0.289014	0.295414	0.289780	0.288819	0.287481		
(3,-1)	0.287430	0.277536	0.289014	0.295414	0.289780	0.288819	0.287481		
(3,-1)	0.281580	0.277820	0.282846	0.289044	0.284035	0.282999	0.281727		
(3,-1)	0.282879	0.277536	0.284229	0.290445	0.285436	0.284357	0.283057		
(3,-1)	0.282879	0.277536	0.284229	0.290445	0.285436	0.284357	0.283057		

Table S140: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>-S-CH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.188103	0.182462	0.185890	0.184355	0.188345	0.181760	0.182865	0.185043	0.191774
(3,-1)	0.188103	0.182462	0.185890	0.184355	0.188345	0.181760	0.182865	0.185043	0.191774
(3,-1)	0.283844	0.276971	0.284362	0.281175	0.285469	0.276700	0.284887	0.280210	0.275256
(3,-1)	0.283870	0.276947	0.284271	0.281147	0.285450	0.277076	0.284805	0.280143	0.274915
(3,-1)	0.283870	0.276947	0.284271	0.281147	0.285450	0.277076	0.284805	0.280143	0.274915
(3,-1)	0.283844	0.276971	0.284362	0.281175	0.285469	0.276700	0.284887	0.280210	0.275256
(3,-1)	0.283870	0.276947	0.284271	0.281147	0.285450	0.277076	0.284805	0.280143	0.274915
(3,-1)	0.283870	0.276947	0.284271	0.281147	0.285450	0.277076	0.284805	0.280143	0.274915
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.188103	0.358044	0.192869	0.188234	0.187311	0.178252	0.182305	0.190235	0.187916
(3,-1)	0.188103	0.257003	0.192869	0.188234	0.187311	0.178252	0.182305	0.190235	0.187916
(3,-1)	0.283844	0.293487	0.280730	0.285852	0.283359	0.282824	0.278072	0.285816	0.283215
(3,-1)	0.283870	0.283023	0.280386	0.285791	0.283360	0.282907	0.278047	0.285800	0.283040
(3,-1)	0.283870	0.283225	0.280386	0.285791	0.283360	0.282907	0.278047	0.285800	0.283040
(3,-1)	0.283844		0.280730	0.285852	0.283359	0.282824	0.278072	0.285816	0.283215
(3,-1)	0.283870		0.280386	0.285791	0.283360	0.282907	0.278047	0.285800	0.283040
(3,-1)	0.283870		0.280386	0.285791	0.283360	0.282907	0.278047	0.285800	0.283040
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.188103	0.180502	0.185470	0.188075	0.186865	0.189295	0.188906	0.187488	0.186012
(3,-1)	0.188103	0.180502	0.185470	0.188075	0.186865	0.189295	0.188906	0.187488	0.186012
(3,-1)	0.283844	0.281192	0.287030	0.292174	0.300171	0.284816	0.284737	0.284203	0.283311
(3,-1)	0.283870	0.281174	0.286958	0.292131	0.300156	0.284816	0.284735	0.284194	0.283253
(3,-1)	0.283870	0.281174	0.286958	0.292131	0.300156	0.284816	0.284735	0.284194	0.283253
(3,-1)	0.283844	0.281192	0.287030	0.292174	0.300171	0.284816	0.284737	0.284203	0.283311
(3,-1)	0.283870	0.281174	0.286958	0.292131	0.300156	0.284816	0.284735	0.284194	0.283253
(3,-1)	0.283870	0.281174	0.286958	0.292131	0.300156	0.284816	0.284735	0.284194	0.283253
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.188103	0.359160	0.183173	0.198504	0.188871	0.189218	0.187955		
(3,-1)	0.188103	0.256766	0.183173	0.198504	0.188871	0.189218	0.187955		
(3,-1)	0.283844	0.292026	0.285616	0.291758	0.286334	0.285283	0.283987		
(3,-1)	0.283870	0.282444	0.285264	0.291765	0.286315	0.285324	0.284008		
(3,-1)	0.283870	0.282734	0.285264	0.291765	0.286315	0.285324	0.284008		
(3,-1)	0.283844		0.285616	0.291758	0.286334	0.285283	0.283987		
(3,-1)	0.283870		0.285264	0.291765	0.286315	0.285324	0.284008		
(3,-1)	0.283870		0.285264	0.291765	0.286315	0.285324	0.284008		

Table S141: Density value (a.u.) at the considered critical points for the H<sub>2</sub>C=CHF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.364131	0.355025	0.360671	0.356267	0.360499	0.355602	0.358829	0.358060	0.363599
(3,-1)	0.261542	0.264762	0.264154	0.263950	0.261395	0.265439	0.258411	0.259499	0.255460
(3,-1)	0.301829	0.290905	0.298356	0.295144	0.300161	0.290372	0.299374	0.292183	0.287190
(3,-1)	0.291441	0.281428	0.288737	0.285480	0.289970	0.281045	0.289426	0.283717	0.278897
(3,-1)	0.291663	0.281729	0.288894	0.285635	0.290100	0.281235	0.289512	0.283981	0.279307
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.364131	0.254642	0.356690	0.362929	0.359443	0.355194	0.359054	0.361627	0.358222
(3,-1)	0.261542	0.187526	0.252691	0.263208	0.262651	0.256192	0.261920	0.260709	0.260638
(3,-1)	0.301829	0.286624	0.296412	0.300537	0.298179	0.297102	0.291080	0.301326	0.298807
(3,-1)	0.291441	0.286624	0.284965	0.290509	0.287987	0.286783	0.282161	0.290620	0.288106
(3,-1)	0.291663	0.275321	0.285116	0.290708	0.288181	0.287007	0.282546	0.290766	0.288411
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.364131	0.356460	0.362016	0.366444	0.364927	0.356171	0.359003	0.360623	0.358495
(3,-1)	0.261542	0.257937	0.258087	0.257210	0.253914	0.261844	0.262721	0.262857	0.260565
(3,-1)	0.301829	0.296103	0.302297	0.307762	0.314778	0.299744	0.299752	0.299211	0.298361
(3,-1)	0.291441	0.285734	0.291826	0.296909	0.305223	0.289195	0.289281	0.288851	0.288082
(3,-1)	0.291663	0.286019	0.292231	0.297269	0.305818	0.289411	0.289517	0.289061	0.288248
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.364131	0.253940	0.361673	0.371828	0.363418	0.361959	0.360527		
(3,-1)	0.261542	0.186179	0.258099	0.256487	0.262043	0.260791	0.257602		
(3,-1)	0.301829	0.285267	0.302098	0.308716	0.301263	0.300629	0.299261		
(3,-1)	0.291441	0.285267	0.291212	0.297074	0.290936	0.289971	0.288520		
(3,-1)	0.291663	0.274746	0.291433	0.297281	0.291133	0.290166	0.288719		



Table S142: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>-CH<sub>2</sub>-Cl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.256213	0.247590	0.253527	0.250568	0.255713	0.246784	0.250424	0.257629	0.256564
(3,-1)	0.183621	0.180660	0.182896	0.182260	0.184889	0.180167	0.179683	0.181342	0.186931
(3,-1)	0.292501	0.284814	0.292373	0.289093	0.293726	0.284509	0.292987	0.287569	0.281711
(3,-1)	0.292501	0.284814	0.292373	0.289093	0.293726	0.284509	0.292987	0.287569	0.281711
(3,-1)	0.280699	0.273854	0.281030	0.277902	0.282052	0.273977	0.281288	0.277334	0.272031
(3,-1)	0.284088	0.277374	0.284743	0.281554	0.285689	0.277613	0.285115	0.280518	0.275115
(3,-1)	0.284088	0.277374	0.284743	0.281554	0.285689	0.277613	0.285115	0.280518	0.275115
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.256213	0.352942	0.256995	0.256114	0.254033	0.251977	0.254402	0.257729	0.253345
(3,-1)	0.183621	0.211066	0.188806	0.184469	0.184178	0.176163	0.178660	0.186180	0.184078
(3,-1)	0.292501	0.290059	0.289217	0.294135	0.291616	0.290949	0.285569	0.294346	0.291591
(3,-1)	0.292501	0.284295	0.289217	0.294135	0.291616	0.290949	0.285569	0.294346	0.291591
(3,-1)	0.280699	0.282998	0.277166	0.282523	0.280070	0.279642	0.275327	0.282353	0.279782
(3,-1)	0.284088		0.280786	0.286149	0.283633	0.283166	0.278391	0.285939	0.283246
(3,-1)	0.284088		0.280786	0.286149	0.283633	0.283166	0.278391	0.285939	0.283246
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.256213	0.248226	0.254512	0.256116	0.251575	0.255364	0.255434	0.254365	0.252375
(3,-1)	0.183621	0.177677	0.182134	0.184244	0.184875	0.185968	0.185183	0.183441	0.182609
(3,-1)	0.292501	0.289509	0.295260	0.300680	0.307921	0.293323	0.293257	0.292642	0.291583
(3,-1)	0.292501	0.289509	0.295260	0.300680	0.307921	0.293323	0.293257	0.292642	0.291583
(3,-1)	0.280699	0.278243	0.283771	0.288619	0.296806	0.281438	0.281428	0.280931	0.279993
(3,-1)	0.284088	0.281685	0.287197	0.292170	0.300081	0.284809	0.284846	0.284429	0.283569
(3,-1)	0.284088	0.281685	0.287197	0.292170	0.300081	0.284809	0.284846	0.284429	0.283569
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.256213	0.354024	0.251673	0.268072	0.257058	0.256741	0.255629		
(3,-1)	0.183621	0.210142	0.179127	0.190252	0.185132	0.185522	0.183846		
(3,-1)	0.292501	0.288742	0.294265	0.301085	0.294734	0.293782	0.292518		
(3,-1)	0.292501	0.283529	0.294265	0.301085	0.294734	0.293782	0.292518		
(3,-1)	0.280699	0.282385	0.281889	0.288213	0.283090	0.282064	0.280788		
(3,-1)	0.284088		0.285546	0.291774	0.286633	0.285532	0.284258		
(3,-1)	0.284088		0.285546	0.291774	0.286633	0.285532	0.284258		

Table S143: Density value (a.u.) at the considered critical points for the H<sub>2</sub>C=CHCl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.358488	0.349396	0.354978	0.350666	0.354966	0.349802	0.353022	0.351750	0.358448
(3,-1)	0.211956	0.204181	0.206843	0.205680	0.209008	0.203725	0.202925	0.203166	0.210332
(3,-1)	0.298217	0.287961	0.295206	0.292066	0.296823	0.287019	0.295983	0.289858	0.284612
(3,-1)	0.292638	0.282603	0.289950	0.286746	0.291280	0.282285	0.290608	0.284728	0.279729
(3,-1)	0.291528	0.281476	0.288561	0.285393	0.289919	0.280906	0.289136	0.283583	0.278669
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.358488	0.346501	0.351608	0.357265	0.353862	0.347454	0.352051	0.356115	0.352924
(3,-1)	0.211956	0.283538	0.212320	0.208960	0.208274	0.197518	0.201323	0.210604	0.208340
(3,-1)	0.298217	0.286588	0.292727	0.297192	0.294839	0.293547	0.288277	0.297810	0.295276
(3,-1)	0.292638	0.286525	0.286538	0.291755	0.289299	0.288147	0.283136	0.292001	0.289362
(3,-1)	0.291528	0.285296	0.285108	0.290447	0.288022	0.286786	0.282187	0.290683	0.288268
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.358488	0.350310	0.356134	0.360968	0.360383	0.350948	0.353610	0.355061	0.352789
(3,-1)	0.211956	0.199979	0.206615	0.209818	0.211462	0.209664	0.209396	0.207755	0.206686
(3,-1)	0.298217	0.292301	0.298732	0.304038	0.311447	0.296661	0.296576	0.295920	0.294822
(3,-1)	0.292638	0.287065	0.293082	0.298255	0.306401	0.290657	0.290678	0.290184	0.289340
(3,-1)	0.291528	0.285861	0.291998	0.297174	0.305662	0.289624	0.289613	0.289020	0.288031
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.358488	0.347677	0.356204	0.366512	0.357658	0.356274	0.354808		
(3,-1)	0.211956	0.283943	0.203903	0.217287	0.209646	0.209998	0.208407		
(3,-1)	0.298217	0.285672	0.298533	0.304642	0.297715	0.296960	0.295609		
(3,-1)	0.292638	0.285622	0.292620	0.298599	0.292196	0.291287	0.289891		
(3,-1)	0.291528	0.284302	0.291404	0.297347	0.290952	0.290088	0.288731		

Table S144: Density value (a.u.) at the considered critical points for the H<sub>2</sub>C=CHCN system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.351776	0.342541	0.348539	0.344094	0.348475	0.343130	0.346287	0.345353	0.351755
(3,-1)	0.301692	0.280728	0.285277	0.282386	0.286742	0.280466	0.282602	0.288283	0.286745
(3,-1)	0.295960	0.285028	0.292284	0.289121	0.293689	0.284470	0.293051	0.286603	0.281644
(3,-1)	0.294479	0.284988	0.292098	0.288950	0.293519	0.284288	0.292823	0.286557	0.281635
(3,-1)	0.293693	0.283607	0.290835	0.287624	0.292074	0.282729	0.291394	0.285493	0.280596
(3,-1)	0.477741	0.472417	0.473605	0.469391	0.470532	0.475228	0.472674	0.453996	0.464569
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.351776	0.400421	0.345420	0.350777	0.347260	0.340231	0.345022	0.349671	0.346274
(3,-1)	0.301692	0.260500	0.285050	0.287625	0.285512	0.284008	0.287107	0.288060	0.284476
(3,-1)	0.295960	0.260500	0.289216	0.294112	0.291700	0.290539	0.285115	0.294473	0.291862
(3,-1)	0.294479	0.279940	0.289040	0.293978	0.291580	0.290441	0.285205	0.294352	0.291817
(3,-1)	0.293693	0.279940	0.287587	0.292616	0.290138	0.288653	0.283849	0.292887	0.290277
(3,-1)	0.477741	0.272532	0.452273	0.474304	0.470361	0.460234	0.464288	0.467795	0.466392
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.351776	0.343431	0.349581	0.354259	0.353941	0.344232	0.346875	0.348285	0.346120
(3,-1)	0.301692	0.278215	0.286443	0.287922	0.283310	0.285266	0.286075	0.285753	0.283941
(3,-1)	0.295960	0.289359	0.295461	0.300865	0.308650	0.293087	0.293093	0.292591	0.291762
(3,-1)	0.294479	0.289326	0.295420	0.300808	0.308671	0.293084	0.293072	0.292507	0.291622
(3,-1)	0.293693	0.287791	0.293876	0.299051	0.306686	0.291651	0.291709	0.291178	0.290105
(3,-1)	0.477741	0.457764	0.470445	0.483444	0.487920	0.464885	0.469270	0.471551	0.472962
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.351776	0.403247	0.349490	0.360186	0.351139	0.349643	0.348205		
(3,-1)	0.301692	0.259866	0.284512	0.296827	0.288077	0.287624	0.285859		
(3,-1)	0.295960	0.259866	0.295300	0.301208	0.294419	0.293568	0.292140		
(3,-1)	0.294479	0.279287	0.295134	0.301138	0.294351	0.293527	0.292117		
(3,-1)	0.293693	0.279287	0.293818	0.299187	0.293131	0.292168	0.290839		
(3,-1)	0.477741	0.272409	0.475831	0.473978	0.471658	0.469008	0.466761		

Table S145: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>-CO-CH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.408790	0.414507	0.415389	0.412768	0.414019	0.414626	0.411410	0.401530	0.404417
(3,-1)	0.263161	0.253665	0.259307	0.256472	0.262126	0.252360	0.256579	0.264512	0.262458
(3,-1)	0.263161	0.253665	0.259307	0.256472	0.262126	0.252360	0.256579	0.264512	0.262458
(3,-1)	0.285366	0.278560	0.286216	0.282907	0.287101	0.279138	0.286567	0.281690	0.276232
(3,-1)	0.285366	0.278560	0.286216	0.282907	0.287101	0.279138	0.286567	0.281690	0.276232
(3,-1)	0.278334	0.271335	0.278698	0.275488	0.279683	0.271929	0.278962	0.274970	0.270022
(3,-1)	0.278334	0.271335	0.278698	0.275488	0.279683	0.271929	0.278962	0.274970	0.270022
(3,-1)	0.278334	0.271335	0.278698	0.275488	0.279683	0.271929	0.278962	0.274970	0.270022
(3,-1)	0.278334	0.271335	0.278698	0.275488	0.279683	0.271929	0.278962	0.274970	0.270022
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.408790	0.414128	0.397839	0.416416	0.413980	0.401474	0.407329	0.412180	0.409790
(3,-1)	0.263161	0.299374	0.262907	0.262416	0.260550	0.260149	0.261775	0.264541	0.259485
(3,-1)	0.263161	0.347792	0.262907	0.262416	0.260550	0.260149	0.261775	0.264541	0.259485
(3,-1)	0.285366	0.265649	0.282247	0.287608	0.284987	0.284465	0.279533	0.287405	0.284604
(3,-1)	0.285366	0.281604	0.282247	0.287608	0.284987	0.284465	0.279533	0.287405	0.284604
(3,-1)	0.278334	0.275326	0.274352	0.280197	0.277671	0.277396	0.273027	0.279972	0.277312
(3,-1)	0.278334	0.275326	0.274352	0.280197	0.277671	0.277396	0.273027	0.279972	0.277312
(3,-1)	0.278334		0.274352	0.280197	0.277671	0.277396	0.273027	0.279972	0.277312
(3,-1)	0.278334		0.274352	0.280197	0.277671	0.277396	0.273027	0.279972	0.277312
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.408790	0.400580	0.408879	0.418890	0.420762	0.413108	0.414193	0.413127	0.414314
(3,-1)	0.263161	0.255106	0.261583	0.263041	0.257778	0.262028	0.262091	0.260959	0.259031
(3,-1)	0.263161	0.255106	0.261583	0.263041	0.257778	0.262028	0.262091	0.260959	0.259031
(3,-1)	0.285366	0.282843	0.288561	0.293627	0.301334	0.286208	0.286242	0.285817	0.285002
(3,-1)	0.285366	0.282843	0.288561	0.293627	0.301334	0.286208	0.286242	0.285817	0.285002
(3,-1)	0.278334	0.275733	0.281401	0.286164	0.294638	0.279064	0.279053	0.278541	0.277630
(3,-1)	0.278334	0.275733	0.281401	0.286164	0.294638	0.279064	0.279053	0.278541	0.277630
(3,-1)	0.278334	0.275733	0.281401	0.286164	0.294638	0.279064	0.279053	0.278541	0.277630
(3,-1)	0.278334	0.275733	0.281401	0.286164	0.294638	0.279064	0.279053	0.278541	0.277630
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.408790	0.417537	0.414930	0.417910	0.414158	0.412624	0.408603		
(3,-1)	0.263161	0.299794	0.259028	0.275776	0.263446	0.263514	0.262151		
(3,-1)	0.263161	0.351176	0.259028	0.275776	0.263446	0.263514	0.262151		
(3,-1)	0.285366	0.264990	0.287421	0.293491	0.287949	0.286766	0.285521		
(3,-1)	0.285366	0.280866	0.287421	0.293491	0.287949	0.286766	0.285521		
(3,-1)	0.278334	0.275173	0.279555	0.285977	0.280708	0.279621	0.278305		
(3,-1)	0.278334	0.275173	0.279555	0.285977	0.280708	0.279621	0.278305		
(3,-1)	0.278334		0.279555	0.285977	0.280708	0.279621	0.278305		
(3,-1)	0.278334		0.279555	0.285977	0.280708	0.279621	0.278305		

Table S146: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>COOH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.423949	0.427507	0.429093	0.425976	0.428108	0.427699	0.425141	0.414778	0.418411
(3,-1)	0.301202	0.304164	0.305864	0.304023	0.304670	0.304361	0.302616	0.298356	0.300528
(3,-1)	0.352139	0.350619	0.361956	0.359840	0.361846	0.356461	0.362574	0.362575	0.350798
(3,-1)	0.268695	0.258894	0.264675	0.261776	0.267504	0.258293	0.262052	0.269891	0.267325
(3,-1)	0.287132	0.280079	0.287802	0.284448	0.288702	0.280248	0.288154	0.283005	0.277662
(3,-1)	0.281363	0.274187	0.281760	0.278463	0.282673	0.274336	0.281992	0.277603	0.272611
(3,-1)	0.281363	0.274187	0.281760	0.278463	0.282673	0.274336	0.281992	0.277603	0.272611
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.423949	0.430561	0.411350	0.430764	0.428004	0.415037	0.421086	0.426665	0.424094
(3,-1)	0.301202	0.259997	0.295200	0.306770	0.304996	0.295131	0.300270	0.304353	0.302898
(3,-1)	0.352139	0.267186	0.351838	0.361283	0.359626	0.361314	0.357971	0.363233	0.356048
(3,-1)	0.268695	0.282069	0.267868	0.267837	0.265957	0.266303	0.267535	0.269880	0.264902
(3,-1)	0.287132	0.275745	0.283982	0.289234	0.286580	0.285869	0.280890	0.289079	0.286331
(3,-1)	0.281363	0.275745	0.277411	0.283214	0.280602	0.280215	0.275637	0.283014	0.280365
(3,-1)	0.281363		0.277411	0.283214	0.280602	0.280215	0.275637	0.283014	0.280365
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.423949	0.414511	0.423789	0.434179	0.437054	0.427265	0.428403	0.427175	0.428672
(3,-1)	0.301202	0.298697	0.299742	0.304276	0.303072	0.305239	0.305884	0.305370	0.304293
(3,-1)	0.352139	0.357753	0.355771	0.358709	0.354245	0.364410	0.362911	0.361856	0.359100
(3,-1)	0.268695	0.260803	0.267510	0.268799	0.263410	0.267046	0.267281	0.266363	0.264600
(3,-1)	0.287132	0.284574	0.290264	0.295358	0.303216	0.287789	0.287840	0.287423	0.286592
(3,-1)	0.281363	0.278682	0.284432	0.289304	0.297699	0.282093	0.282073	0.281541	0.280563
(3,-1)	0.281363	0.278682	0.284432	0.289304	0.297699	0.282093	0.282073	0.281541	0.280563
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.423949	0.434801	0.429931	0.434567	0.428408	0.426918	0.422871		
(3,-1)	0.301202	0.258990	0.301537	0.307021	0.305466	0.304153	0.300617		
(3,-1)	0.352139	0.266733	0.364467	0.361136	0.358438	0.356633	0.354738		
(3,-1)	0.268695	0.281329	0.264568	0.281218	0.268883	0.268991	0.267500		
(3,-1)	0.287132	0.275589	0.289170	0.295213	0.289657	0.288467	0.287252		
(3,-1)	0.281363	0.275589	0.283050	0.289070	0.283772	0.282607	0.281409		
(3,-1)	0.281363		0.283050	0.289070	0.283772	0.282607	0.281409		

Table S147: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>COF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.445168	0.446365	0.447798	0.444542	0.446716	0.446373	0.443924	0.432504	0.436288
(3,-1)	0.263647	0.267032	0.267114	0.266576	0.264093	0.268720	0.262488	0.262863	0.259639
(3,-1)	0.280263	0.261107	0.266820	0.263957	0.269468	0.260594	0.264037	0.271808	0.269277
(3,-1)	0.291509	0.280449	0.288213	0.284846	0.289163	0.280464	0.288599	0.283353	0.278122
(3,-1)	0.283579	0.274405	0.282089	0.278758	0.283061	0.274475	0.282351	0.277849	0.272972
(3,-1)	0.281075	0.274405	0.282089	0.278758	0.283061	0.274475	0.282351	0.277849	0.272972
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.445168	0.262580	0.428463	0.449433	0.446535	0.434074	0.439466	0.444980	0.442020
(3,-1)	0.263647	0.188112	0.255515	0.265875	0.264868	0.260428	0.264978	0.262599	0.262405
(3,-1)	0.280263	0.425060	0.269704	0.269824	0.267967	0.268528	0.269656	0.271728	0.266850
(3,-1)	0.291509	0.280921	0.284502	0.289686	0.287026	0.286278	0.281248	0.289594	0.286865
(3,-1)	0.283579	0.276256	0.277853	0.283593	0.280963	0.280514	0.275887	0.283468	0.280810
(3,-1)	0.281075	0.276256	0.277853	0.283593	0.280963	0.280514	0.275887	0.283468	0.280810
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.445168	0.432087	0.442356	0.453886	0.456931	0.445631	0.446780	0.445427	0.447473
(3,-1)	0.263647	0.259556	0.259453	0.259118	0.253327	0.263918	0.264730	0.264944	0.263615
(3,-1)	0.280263	0.262741	0.269559	0.270783	0.265154	0.268673	0.269036	0.268251	0.266504
(3,-1)	0.291509	0.285003	0.290757	0.295865	0.303649	0.288292	0.288334	0.287904	0.287046
(3,-1)	0.283579	0.279030	0.284835	0.289736	0.298144	0.282568	0.282522	0.281962	0.280943
(3,-1)	0.281075	0.279030	0.284835	0.289736	0.298144	0.282568	0.282522	0.281962	0.280943
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.445168	0.262045	0.449682	0.452896	0.447021	0.445431	0.441371		
(3,-1)	0.263647	0.186634	0.260295	0.257370	0.264400	0.262598	0.259277		
(3,-1)	0.280263	0.428816	0.266312	0.282470	0.270889	0.270958	0.269419		
(3,-1)	0.291509	0.280192	0.289793	0.295811	0.290137	0.288959	0.287752		
(3,-1)	0.283579	0.276030	0.283652	0.289662	0.284187	0.283030	0.281850		
(3,-1)	0.281075	0.276030	0.283652	0.289662	0.284187	0.283030	0.281850		

Table S148: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>COCl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.265424	0.256414	0.261761	0.259046	0.264457	0.255468	0.258931	0.266446	0.264423
(3,-1)	0.184461	0.179981	0.182071	0.181501	0.185036	0.179054	0.179852	0.181196	0.186972
(3,-1)	0.435887	0.440475	0.441305	0.438469	0.440547	0.440334	0.437369	0.426485	0.428937
(3,-1)	0.286404	0.279323	0.287048	0.283718	0.288008	0.279320	0.287420	0.282369	0.277043
(3,-1)	0.282126	0.274751	0.282558	0.279198	0.283519	0.275010	0.282838	0.278259	0.273409
(3,-1)	0.282126	0.274751	0.282558	0.279198	0.283519	0.275010	0.282838	0.278259	0.273409
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.265424	0.255733	0.265077	0.264781	0.263025	0.262335	0.264152	0.266769	0.262248
(3,-1)	0.184461	0.246836	0.189269	0.184470	0.184341	0.176688	0.178777	0.186915	0.184129
(3,-1)	0.435887	0.276565	0.422893	0.442992	0.440470	0.427359	0.433414	0.438896	0.436165
(3,-1)	0.286404	0.278827	0.283366	0.288505	0.285876	0.285214	0.280230	0.288425	0.285671
(3,-1)	0.282126	0.278827	0.278441	0.284047	0.281398	0.281019	0.276246	0.283929	0.281183
(3,-1)	0.282126	0.187379	0.278441	0.284047	0.281398	0.281019	0.276246	0.283929	0.281183
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.265424	0.257393	0.264070	0.265520	0.260026	0.264515	0.264588	0.263448	0.261494
(3,-1)	0.184461	0.178482	0.182527	0.184932	0.186670	0.186684	0.185717	0.183747	0.183125
(3,-1)	0.435887	0.425835	0.436213	0.447076	0.450595	0.439924	0.440940	0.439460	0.441169
(3,-1)	0.286404	0.283819	0.289568	0.294658	0.302378	0.287225	0.287248	0.286801	0.285868
(3,-1)	0.282126	0.279427	0.285235	0.290084	0.298334	0.282912	0.282901	0.282390	0.281380
(3,-1)	0.282126	0.279427	0.285235	0.290084	0.298334	0.282912	0.282901	0.282390	0.281380
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.265424	0.254775	0.261145	0.277401	0.265734	0.265866	0.264393		
(3,-1)	0.184461	0.246173	0.179775	0.193558	0.184800	0.185671	0.183376		
(3,-1)	0.435887	0.275934	0.443005	0.446442	0.440515	0.439217	0.435006		
(3,-1)	0.286404	0.277848	0.288614	0.294598	0.288922	0.287750	0.286544		
(3,-1)	0.282126	0.277848	0.284076	0.290187	0.284544	0.283359	0.282136		
(3,-1)	0.282126	0.186049	0.284076	0.290187	0.284544	0.283359	0.282136		

Table S149: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>Cl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.257142	0.248661	0.254425	0.251506	0.256658	0.247810	0.251280	0.258759	0.257574
(3,-1)	0.247692	0.239274	0.245188	0.242254	0.247288	0.238905	0.241865	0.249099	0.248702
(3,-1)	0.281834	0.275297	0.282389	0.279296	0.283374	0.275384	0.282731	0.278587	0.273232
(3,-1)	0.284243	0.277619	0.284780	0.281639	0.285793	0.277861	0.285166	0.280716	0.274891
(3,-1)	0.284243	0.277619	0.284780	0.281639	0.285793	0.277861	0.285166	0.280716	0.274891
(3,-1)	0.183443	0.180487	0.182736	0.182092	0.184720	0.180037	0.179511	0.181213	0.186772
(3,-1)	0.281093	0.274706	0.281819	0.278738	0.282740	0.275160	0.282176	0.277943	0.272565
(3,-1)	0.281093	0.274706	0.281819	0.278738	0.282740	0.275160	0.282176	0.277943	0.272565
(3,-1)	0.290963	0.283299	0.291004	0.287696	0.292338	0.283549	0.291604	0.286237	0.280285
(3,-1)	0.290963	0.283299	0.291004	0.287696	0.292338	0.283549	0.291604	0.286237	0.280285
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.257142	0.255135	0.257938	0.257064	0.255021	0.252812	0.255443	0.258648	0.254252
(3,-1)	0.247692	0.356586	0.249009	0.247725	0.245645	0.242546	0.245664	0.249254	0.245103
(3,-1)	0.281834	0.256263	0.278477	0.283818	0.281382	0.280918	0.276540	0.283611	0.281040
(3,-1)	0.284243	0.281304	0.280660	0.286261	0.283794	0.283288	0.278522	0.286036	0.283175
(3,-1)	0.284243	0.259138	0.280660	0.286261	0.283794	0.283288	0.278522	0.286036	0.283175
(3,-1)	0.183443	0.275936	0.188670	0.184312	0.184011	0.176010	0.178535	0.186007	0.183916
(3,-1)	0.281093	0.276153	0.277686	0.283170	0.280733	0.280357	0.275816	0.282872	0.280201
(3,-1)	0.281093	0.277340	0.277686	0.283170	0.280733	0.280357	0.275816	0.282872	0.280201
(3,-1)	0.290963	0.273714	0.287577	0.292735	0.290195	0.289662	0.284171	0.292872	0.289981
(3,-1)	0.290963	0.275296	0.287577	0.292735	0.290195	0.289662	0.284171	0.292872	0.289981
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.257142	0.248989	0.255362	0.257008	0.252152	0.256418	0.256476	0.255366	0.253313
(3,-1)	0.247692	0.239737	0.245733	0.247337	0.243444	0.247029	0.247071	0.245947	0.244028
(3,-1)	0.281834	0.279443	0.284987	0.289898	0.297961	0.282638	0.282657	0.282209	0.281283
(3,-1)	0.284243	0.281815	0.287147	0.292196	0.299773	0.284972	0.285037	0.284624	0.283738
(3,-1)	0.284243	0.281815	0.287147	0.292196	0.299773	0.284972	0.285037	0.284624	0.283738
(3,-1)	0.183443	0.177485	0.181982	0.184076	0.184699	0.185797	0.185018	0.183272	0.182446
(3,-1)	0.281093	0.278779	0.284189	0.289101	0.297156	0.281790	0.281831	0.281438	0.280620
(3,-1)	0.281093	0.278779	0.284189	0.289101	0.297156	0.281790	0.281831	0.281438	0.280620
(3,-1)	0.290963	0.288025	0.293742	0.299142	0.306417	0.291811	0.291757	0.291186	0.290187
(3,-1)	0.290963	0.288025	0.293742	0.299142	0.306417	0.291811	0.291757	0.291186	0.290187
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.257142	0.254847	0.252757	0.269045	0.257929	0.257643	0.256464		
(3,-1)	0.247692	0.360258	0.243111	0.259493	0.248541	0.248167	0.247086		
(3,-1)	0.281834	0.255363	0.283162	0.289288	0.284325	0.283288	0.281997		
(3,-1)	0.284243	0.279791	0.285606	0.291955	0.286704	0.285650	0.284284		
(3,-1)	0.284243	0.258096	0.285606	0.291955	0.286704	0.285650	0.284284		
(3,-1)	0.183443	0.275488	0.178986	0.190111	0.184941	0.185323	0.183647		
(3,-1)	0.281093	0.275672	0.282066	0.288411	0.283667	0.282603	0.281273		
(3,-1)	0.281093	0.276761	0.282066	0.288411	0.283667	0.282603	0.281273		
(3,-1)	0.290963	0.273201	0.292670	0.299658	0.293250	0.292262	0.290960		
(3,-1)	0.290963	0.274707	0.292670	0.299658	0.293250	0.292262	0.290960		



Table S150: Density value (a.u.) at the considered critical points for the  $(\text{CH}_3)_2\text{CH-OH}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.252899	0.256669	0.257825	0.257266	0.257169	0.256912	0.254931	0.254359	0.255891
(3,-1)	0.361570	0.359586	0.370655	0.368436	0.371014	0.364654	0.371789	0.371409	0.360377
(3,-1)	0.258164	0.249033	0.254971	0.251983	0.257340	0.247726	0.251818	0.259775	0.258106
(3,-1)	0.287446	0.279673	0.286709	0.283607	0.288191	0.279717	0.287363	0.282501	0.275916
(3,-1)	0.260974	0.251897	0.257983	0.254903	0.260225	0.250880	0.254856	0.262760	0.260726
(3,-1)	0.281536	0.274855	0.282304	0.279104	0.283205	0.275773	0.282636	0.278252	0.272696
(3,-1)	0.281698	0.275059	0.282514	0.279297	0.283381	0.276000	0.282834	0.278428	0.272861
(3,-1)	0.282833	0.276209	0.283533	0.280337	0.284423	0.276595	0.283849	0.279413	0.273856
(3,-1)	0.279089	0.272705	0.279794	0.276700	0.280670	0.273375	0.280060	0.276139	0.270568
(3,-1)	0.280514	0.274034	0.281258	0.278116	0.282138	0.274744	0.281557	0.277351	0.271973
(3,-1)	0.280078	0.273489	0.280741	0.277588	0.281673	0.274263	0.281033	0.276949	0.271597
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.252899	0.262440	0.251846	0.258068	0.257448	0.249112	0.253151	0.257017	0.256154
(3,-1)	0.361570	0.264362	0.360879	0.370469	0.368796	0.370298	0.366592	0.372673	0.364819
(3,-1)	0.258164	0.286029	0.258599	0.257759	0.255685	0.254373	0.256572	0.259537	0.254758
(3,-1)	0.287446	0.258113	0.283035	0.288597	0.286251	0.285872	0.280639	0.288751	0.285778
(3,-1)	0.260974	0.279348	0.261357	0.260710	0.258549	0.257446	0.259512	0.262348	0.257580
(3,-1)	0.281536	0.279348	0.277844	0.283663	0.281133	0.280874	0.276094	0.283312	0.280546
(3,-1)	0.281698	0.279017	0.278083	0.283860	0.281311	0.281043	0.276267	0.283502	0.280725
(3,-1)	0.282833	0.279017	0.279315	0.284915	0.282384	0.281987	0.277365	0.284618	0.281981
(3,-1)	0.279089	0.277412	0.275454	0.281137	0.278683	0.278474	0.274063	0.280776	0.278072
(3,-1)	0.280514	0.277412	0.277044	0.282618	0.280130	0.279779	0.275268	0.282266	0.279600
(3,-1)	0.280078	0.275233	0.276559	0.282152	0.279664	0.279371	0.274871	0.281856	0.279172
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.252899	0.253114	0.252920	0.254117	0.252820	0.257542	0.257902	0.257766	0.255613
(3,-1)	0.361570	0.366533	0.365660	0.368270	0.365791	0.373525	0.372030	0.370910	0.368216
(3,-1)	0.258164	0.250109	0.256438	0.257941	0.252931	0.257149	0.257217	0.256099	0.254047
(3,-1)	0.287446	0.284654	0.289561	0.295166	0.302079	0.287730	0.287731	0.287203	0.286321
(3,-1)	0.260974	0.253019	0.259356	0.260817	0.255672	0.259925	0.260057	0.259008	0.256985
(3,-1)	0.281536	0.279148	0.284613	0.289545	0.297610	0.282241	0.282280	0.281891	0.281110
(3,-1)	0.281698	0.279294	0.284779	0.289707	0.297698	0.282422	0.282461	0.282063	0.281287
(3,-1)	0.282833	0.280433	0.285964	0.290919	0.298948	0.283568	0.283605	0.283187	0.282353
(3,-1)	0.279089	0.276797	0.282123	0.286959	0.295089	0.279761	0.279799	0.279391	0.278592
(3,-1)	0.280514	0.278224	0.283635	0.288486	0.296619	0.281143	0.281204	0.280835	0.280071
(3,-1)	0.280078	0.277750	0.283226	0.288047	0.296123	0.280773	0.280811	0.280404	0.279614
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.252899	0.262445	0.252351	0.255108	0.257435	0.256657	0.253462		
(3,-1)	0.361570	0.264543	0.374445	0.372049	0.367669	0.366092	0.363869		
(3,-1)	0.258164	0.284666	0.253783	0.270414	0.258753	0.258516	0.257407		
(3,-1)	0.287446	0.257430	0.288265	0.295388	0.289326	0.288555	0.287130		
(3,-1)	0.260974	0.278175	0.256668	0.273254	0.261686	0.261365	0.260287		
(3,-1)	0.281536	0.278175	0.282755	0.289093	0.284113	0.282981	0.281687		
(3,-1)	0.281698	0.278105	0.282934	0.289281	0.284299	0.283147	0.281864		
(3,-1)	0.282833	0.278105	0.284310	0.290389	0.285378	0.284253	0.282996		
(3,-1)	0.279089	0.276809	0.279925	0.286305	0.281629	0.280543	0.279213		
(3,-1)	0.280514	0.276809	0.281584	0.287887	0.283076	0.281968	0.280634		
(3,-1)	0.280078	0.274592	0.281229	0.287611	0.282598	0.281508	0.280168		

Table S151: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>-CH<sub>2</sub>-O-CH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.261276	0.264887	0.266340	0.265401	0.265339	0.263659	0.263073	0.262097	0.262890
(3,-1)	0.263290	0.266660	0.268445	0.267332	0.267429	0.265732	0.265128	0.264071	0.264618
(3,-1)	0.291668	0.283778	0.291480	0.288159	0.292661	0.283750	0.292113	0.286080	0.280608
(3,-1)	0.260165	0.251005	0.257329	0.254189	0.259485	0.250659	0.254260	0.261673	0.259805
(3,-1)	0.285314	0.277555	0.284922	0.281760	0.286286	0.278661	0.285515	0.280597	0.274438
(3,-1)	0.285314	0.277555	0.284922	0.281760	0.286286	0.278661	0.285515	0.280597	0.274438
(3,-1)	0.285014	0.277176	0.284706	0.281512	0.285997	0.278144	0.285284	0.280172	0.274491
(3,-1)	0.285014	0.277176	0.284706	0.281512	0.285997	0.278144	0.285284	0.280172	0.274491
(3,-1)	0.282944	0.276321	0.283567	0.280406	0.284471	0.276639	0.283891	0.279473	0.274036
(3,-1)	0.282944	0.276321	0.283567	0.280406	0.284471	0.276639	0.283891	0.279473	0.274036
(3,-1)	0.280319	0.273789	0.280916	0.277808	0.281846	0.274107	0.281209	0.277211	0.271964
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.261276	0.277530	0.259321	0.266642	0.265639	0.256822	0.261159	0.265342	0.264609
(3,-1)	0.263290	0.277530	0.261246	0.268814	0.267678	0.258728	0.263112	0.267468	0.266682
(3,-1)	0.291668	0.277530	0.288531	0.293133	0.290563	0.289859	0.284391	0.293233	0.290732
(3,-1)	0.260165	0.270943	0.260476	0.259984	0.257768	0.256791	0.258580	0.261572	0.256792
(3,-1)	0.285314	0.280533	0.281361	0.286684	0.284273	0.284118	0.278749	0.286777	0.283740
(3,-1)	0.285314	0.280533	0.281361	0.286684	0.284273	0.284118	0.278749	0.286777	0.283740
(3,-1)	0.285014	0.270943	0.281311	0.286392	0.283941	0.283773	0.278411	0.286479	0.283634
(3,-1)	0.285014	0.280533	0.281311	0.286392	0.283941	0.283773	0.278411	0.286479	0.283634
(3,-1)	0.282944	0.280533	0.279418	0.284948	0.282445	0.282030	0.277417	0.284679	0.282082
(3,-1)	0.282944	0.270943	0.279418	0.284948	0.282445	0.282030	0.277417	0.284679	0.282082
(3,-1)	0.280319	0.280533	0.276947	0.282312	0.279859	0.279469	0.275160	0.282037	0.279485
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.261276	0.261595	0.261336	0.262947	0.262084	0.266109	0.266451	0.266184	0.263859
(3,-1)	0.263290	0.263724	0.263468	0.265107	0.264383	0.268214	0.268565	0.268285	0.265955
(3,-1)	0.291668	0.288992	0.294206	0.299693	0.307013	0.292075	0.292062	0.291551	0.290704
(3,-1)	0.260165	0.252352	0.258634	0.260100	0.255451	0.258996	0.259159	0.258179	0.256272
(3,-1)	0.285314	0.282674	0.287617	0.293082	0.300314	0.285642	0.285631	0.285115	0.284366
(3,-1)	0.285314	0.282674	0.287617	0.293082	0.300314	0.285642	0.285631	0.285115	0.284366
(3,-1)	0.285014	0.282377	0.287472	0.292913	0.300545	0.285313	0.285273	0.284752	0.284008
(3,-1)	0.285014	0.282377	0.287472	0.292913	0.300545	0.285313	0.285273	0.284752	0.284008
(3,-1)	0.282944	0.280525	0.286017	0.290972	0.298954	0.283652	0.283673	0.283230	0.282382
(3,-1)	0.282944	0.280525	0.286017	0.290972	0.298954	0.283652	0.283673	0.283230	0.282382
(3,-1)	0.280319	0.278001	0.283451	0.288269	0.296327	0.280996	0.281025	0.280608	0.279785
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.261276	0.276697	0.260930	0.264329	0.265891	0.264836	0.261745		
(3,-1)	0.263290	0.276697	0.262885	0.267134	0.267930	0.266804	0.263720		
(3,-1)	0.291668	0.276697	0.293125	0.299738	0.293886	0.292887	0.291764		
(3,-1)	0.260165	0.270467	0.255810	0.272436	0.260970	0.260590	0.259561		
(3,-1)	0.285314	0.279521	0.285890	0.293402	0.287350	0.286487	0.285129		
(3,-1)	0.285314	0.279521	0.285890	0.293402	0.287350	0.286487	0.285129		
(3,-1)	0.285014	0.270467	0.285601	0.293008	0.287129	0.286223	0.284972		
(3,-1)	0.285014	0.279521	0.285601	0.293008	0.287129	0.286223	0.284972		
(3,-1)	0.282944	0.279521	0.284248	0.290359	0.285478	0.284377	0.283124		
(3,-1)	0.282944	0.270467	0.284248	0.290359	0.285478	0.284377	0.283124		
(3,-1)	0.280319	0.279521	0.281437	0.287626	0.282807	0.281747	0.280427		

Table S152: Density value (a.u.) at the considered critical points for the  $(\text{CH}_3)_3\text{N}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.276945	0.273130	0.276826	0.274879	0.278411	0.270266	0.273962	0.276196	0.280454
(3,-1)	0.276945	0.273130	0.276826	0.274879	0.278411	0.270266	0.273962	0.276196	0.280454
(3,-1)	0.276945	0.273130	0.276826	0.274879	0.278411	0.270266	0.273962	0.276196	0.280454
(3,-1)	0.276434	0.269340	0.276674	0.273635	0.277880	0.271226	0.277152	0.273248	0.267550
(3,-1)	0.285921	0.278690	0.286295	0.283017	0.287283	0.279447	0.286689	0.281596	0.275965
(3,-1)	0.285921	0.278690	0.286295	0.283017	0.287283	0.279447	0.286689	0.281596	0.275965
(3,-1)	0.276434	0.269340	0.276674	0.273635	0.277880	0.271226	0.277152	0.273248	0.267550
(3,-1)	0.285921	0.278690	0.286295	0.283017	0.287283	0.279447	0.286689	0.281596	0.275965
(3,-1)	0.285921	0.278690	0.286295	0.283017	0.287283	0.279447	0.286689	0.281596	0.275965
(3,-1)	0.276434	0.269340	0.276674	0.273635	0.277880	0.271226	0.277152	0.273248	0.267550
(3,-1)	0.285921	0.278690	0.286295	0.283017	0.287283	0.279447	0.286689	0.281596	0.275965
(3,-1)	0.285921	0.278690	0.286295	0.283017	0.287283	0.279447	0.286689	0.281596	0.275965
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.276945	0.056278	0.277296	0.278961	0.277580	0.267473	0.272122	0.280105	0.276300
(3,-1)	0.276945	0.281754	0.277296	0.278961	0.277580	0.267473	0.272122	0.280105	0.276300
(3,-1)	0.276945	0.281754	0.277296	0.278961	0.277580	0.267473	0.272122	0.280105	0.276300
(3,-1)	0.276434	0.334571	0.272619	0.278196	0.275855	0.276094	0.271171	0.278096	0.274972
(3,-1)	0.285921	0.334571	0.282680	0.287780	0.285212	0.284694	0.279638	0.287624	0.284836
(3,-1)	0.285921	0.293919	0.282680	0.287780	0.285212	0.284694	0.279638	0.287624	0.284836
(3,-1)	0.276434	0.292064	0.272619	0.278196	0.275855	0.276094	0.271171	0.278096	0.274972
(3,-1)	0.285921	0.292064	0.282680	0.287780	0.285212	0.284694	0.279638	0.287624	0.284836
(3,-1)	0.285921	0.285291	0.282680	0.287780	0.285212	0.284694	0.279638	0.287624	0.284836
(3,-1)	0.276434	0.285291	0.272619	0.278196	0.275855	0.276094	0.271171	0.278096	0.274972
(3,-1)	0.285921		0.282680	0.287780	0.285212	0.284694	0.279638	0.287624	0.284836
(3,-1)	0.285921		0.282680	0.287780	0.285212	0.284694	0.279638	0.287624	0.284836
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.276945	0.272578	0.274027	0.277720	0.273901	0.279078	0.278910	0.277745	0.275400
(3,-1)	0.276945	0.272578	0.274027	0.277720	0.273901	0.279078	0.278910	0.277745	0.275400
(3,-1)	0.276945	0.272578	0.274027	0.277720	0.273901	0.279078	0.278910	0.277745	0.275400
(3,-1)	0.276434	0.273969	0.279100	0.284116	0.292114	0.276986	0.276958	0.276516	0.275861
(3,-1)	0.285921	0.283535	0.288704	0.293875	0.301616	0.286447	0.286493	0.286067	0.285228
(3,-1)	0.285921	0.283535	0.288704	0.293875	0.301616	0.286447	0.286493	0.286067	0.285228
(3,-1)	0.276434	0.273969	0.279100	0.284116	0.292114	0.276986	0.276958	0.276516	0.275861
(3,-1)	0.285921	0.283535	0.288704	0.293875	0.301616	0.286447	0.286493	0.286067	0.285228
(3,-1)	0.285921	0.283535	0.288704	0.293875	0.301616	0.286447	0.286493	0.286067	0.285228
(3,-1)	0.276434	0.273969	0.279100	0.284116	0.292114	0.276986	0.276958	0.276516	0.275861
(3,-1)	0.285921	0.283535	0.288704	0.293875	0.301616	0.286447	0.286493	0.286067	0.285228
(3,-1)	0.285921	0.283535	0.288704	0.293875	0.301616	0.286447	0.286493	0.286067	0.285228
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.276945	0.057271	0.273166	0.287028	0.279089	0.278876	0.276393		
(3,-1)	0.276945	0.282546	0.273166	0.287028	0.279089	0.278876	0.276396		
(3,-1)	0.276945	0.282546	0.273166	0.287028	0.279089	0.278876	0.276396		
(3,-1)	0.276434	0.335182	0.276583	0.284178	0.278708	0.277799	0.276398		
(3,-1)	0.285921	0.335182	0.287047	0.293807	0.288341	0.287241	0.286024		
(3,-1)	0.285921	0.293949	0.287047	0.293807	0.288341	0.287241	0.286024		
(3,-1)	0.276434	0.291018	0.276583	0.284178	0.278708	0.277799	0.276398		
(3,-1)	0.285921	0.291018	0.287047	0.293807	0.288341	0.287241	0.286028		
(3,-1)	0.285921	0.284292	0.287047	0.293807	0.288341	0.287241	0.286024		
(3,-1)	0.276434	0.284292	0.276583	0.284178	0.278708	0.277799	0.276398		
(3,-1)	0.285921		0.287047	0.293807	0.288341	0.287241	0.286024		
(3,-1)	0.285921		0.287047	0.293807	0.288341	0.287241	0.286028		

Table S153: Density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>4</sub>O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.053979	0.057950	0.054626	0.056987	0.056029	0.058215	0.056251	0.055455	0.054475
(3,-1)	0.283985	0.289531	0.290074	0.288777	0.287765	0.288832	0.285969	0.282070	0.281490
(3,-1)	0.283985	0.289531	0.290074	0.288777	0.287765	0.288832	0.285969	0.282070	0.281490
(3,-1)	0.336119	0.330637	0.336172	0.332050	0.336374	0.331422	0.333674	0.333917	0.339685
(3,-1)	0.336119	0.330637	0.336172	0.332050	0.336374	0.331422	0.333674	0.333917	0.339685
(3,-1)	0.295229	0.287999	0.293558	0.289937	0.294777	0.288333	0.290417	0.292629	0.296575
(3,-1)	0.297692	0.289830	0.297079	0.293876	0.298674	0.289551	0.298005	0.290984	0.286586
(3,-1)	0.297692	0.289830	0.297079	0.293876	0.298674	0.289551	0.298005	0.290984	0.286586
(3,-1)	0.290230	0.283648	0.290545	0.287432	0.291748	0.283065	0.291220	0.285304	0.280739
(3,-1)	0.290230	0.283648	0.290545	0.287432	0.291748	0.283065	0.291220	0.285304	0.280739
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.053979	0.043574	0.058213	0.054622	0.056689	0.058204	0.056562	0.056543	0.057261
(3,-1)	0.283985	0.222465	0.278332	0.289896	0.288438	0.278494	0.283879	0.287177	0.286562
(3,-1)	0.283985	0.222465	0.278332	0.289896	0.288438	0.278494	0.283879	0.287177	0.286562
(3,-1)	0.336119	0.324128	0.333689	0.338466	0.335239	0.328858	0.333478	0.337552	0.333823
(3,-1)	0.336119	0.301566	0.333689	0.338466	0.335239	0.328858	0.333478	0.337552	0.333823
(3,-1)	0.295229	0.324128	0.294206	0.296184	0.293473	0.284997	0.290680	0.296475	0.292831
(3,-1)	0.297692	0.284953	0.294367	0.299139	0.296740	0.295402	0.290068	0.299658	0.297340
(3,-1)	0.297692	0.284953	0.294367	0.299139	0.296740	0.295402	0.290068	0.299658	0.297340
(3,-1)	0.290230	0.283753	0.287045	0.292279	0.289863	0.288267	0.283897	0.292324	0.289932
(3,-1)	0.290230	0.283753	0.287045	0.292279	0.289863	0.288267	0.283897	0.292324	0.289932
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.053979	0.058473	0.056395	0.055272	0.057958	0.055587	0.055636	0.056024	0.056776
(3,-1)	0.283985	0.283267	0.283731	0.286931	0.286925	0.288075	0.288882	0.288837	0.286888
(3,-1)	0.283985	0.283267	0.283731	0.286931	0.286925	0.288075	0.288882	0.288837	0.286888
(3,-1)	0.336119	0.329907	0.336712	0.341247	0.339586	0.332357	0.334846	0.336049	0.334083
(3,-1)	0.336119	0.329907	0.336712	0.341247	0.339586	0.332357	0.334846	0.336049	0.334083
(3,-1)	0.295229	0.286583	0.294017	0.297637	0.296611	0.292556	0.293992	0.294099	0.292032
(3,-1)	0.297692	0.294325	0.300958	0.306304	0.314157	0.298099	0.298179	0.297688	0.296960
(3,-1)	0.297692	0.294325	0.300958	0.306304	0.314157	0.298099	0.298179	0.297688	0.296960
(3,-1)	0.290230	0.287200	0.293507	0.298709	0.306542	0.290779	0.290960	0.290617	0.289911
(3,-1)	0.290230	0.287200	0.293507	0.298709	0.306542	0.290779	0.290960	0.290617	0.289911
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.053979	0.044372	0.055208	0.053453	0.055191	0.056644	0.055363		
(3,-1)	0.283985	0.222170	0.284373	0.287608	0.288600	0.287147	0.283442		
(3,-1)	0.283985	0.222170	0.284373	0.287608	0.288600	0.287147	0.283442		
(3,-1)	0.336119	0.324917	0.336572	0.347819	0.338628	0.337350	0.335895		
(3,-1)	0.336119	0.301624	0.336572	0.347819	0.338628	0.337350	0.335895		
(3,-1)	0.295229	0.324917	0.293010	0.307807	0.296450	0.295677	0.294142		
(3,-1)	0.297692	0.284187	0.300823	0.307032	0.299462	0.298712	0.297166		
(3,-1)	0.297692	0.284187	0.300823	0.307032	0.299462	0.298712	0.297166		
(3,-1)	0.290230	0.282676	0.293077	0.298522	0.292505	0.291567	0.289997		
(3,-1)	0.290230	0.282676	0.293077	0.298522	0.292505	0.291567	0.289997		

Table S154: Density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>4</sub>S system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.041602	0.044771	0.041987	0.043972	0.043141	0.044977	0.043589	0.042744	0.041976
(3,-1)	0.220739	0.215873	0.219496	0.217262	0.221193	0.215937	0.216141	0.215212	0.224477
(3,-1)	0.220739	0.215873	0.219496	0.217262	0.221193	0.215937	0.216141	0.215212	0.224477
(3,-1)	0.325527	0.319747	0.325239	0.321285	0.325812	0.320382	0.322627	0.322278	0.328740
(3,-1)	0.303460	0.295956	0.301661	0.297952	0.302930	0.296023	0.298664	0.302020	0.304269
(3,-1)	0.325527	0.319747	0.325239	0.321285	0.325812	0.320382	0.322627	0.322278	0.328740
(3,-1)	0.290318	0.283356	0.290289	0.287241	0.291775	0.282695	0.291059	0.285272	0.280864
(3,-1)	0.290318	0.283356	0.290289	0.287241	0.291775	0.282695	0.291059	0.285272	0.280864
(3,-1)	0.288850	0.282024	0.288856	0.285807	0.290222	0.281369	0.289538	0.283910	0.278948
(3,-1)	0.288850	0.282024	0.288856	0.285807	0.290222	0.281369	0.289538	0.283910	0.278948
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.041602	0.054546	0.044991	0.042049	0.043818	0.045365	0.044060	0.043772	0.044254
(3,-1)	0.220739	0.337503	0.224323	0.221891	0.220328	0.208173	0.213300	0.222910	0.221162
(3,-1)	0.220739	0.303498	0.224323	0.221891	0.220328	0.208173	0.213300	0.222910	0.221162
(3,-1)	0.325527	0.303498	0.323638	0.327655	0.324599	0.315977	0.321186	0.327070	0.323714
(3,-1)	0.303460	0.322456	0.301913	0.304368	0.301599	0.294924	0.300045	0.304684	0.300774
(3,-1)	0.325527	0.322456	0.323638	0.327655	0.324599	0.315977	0.321186	0.327070	0.323714
(3,-1)	0.290318	0.299775	0.287068	0.292155	0.289839	0.288347	0.283758	0.292544	0.290107
(3,-1)	0.290318	0.287032	0.287068	0.292155	0.289839	0.288347	0.283758	0.292544	0.290107
(3,-1)	0.288850	0.287032	0.285542	0.290692	0.288358	0.286856	0.282458	0.290882	0.288405
(3,-1)	0.288850	0.284164	0.285542	0.290692	0.288358	0.286856	0.282458	0.290882	0.288405
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.041602	0.045829	0.043703	0.042691	0.045172	0.042562	0.042768	0.043211	0.044171
(3,-1)	0.220739	0.212838	0.219095	0.222919	0.223826	0.220801	0.221361	0.220817	0.218968
(3,-1)	0.220739	0.212838	0.219095	0.222919	0.223826	0.220801	0.221361	0.220817	0.218968
(3,-1)	0.325527	0.318468	0.325813	0.330541	0.330184	0.322454	0.324608	0.325465	0.323274
(3,-1)	0.303460	0.295133	0.302780	0.306009	0.304460	0.300801	0.302200	0.302290	0.300105
(3,-1)	0.325527	0.318468	0.325813	0.330541	0.330184	0.322454	0.324608	0.325465	0.323274
(3,-1)	0.290318	0.286893	0.293742	0.298992	0.307188	0.291398	0.291347	0.290759	0.289834
(3,-1)	0.290318	0.286893	0.293742	0.298992	0.307188	0.291398	0.291347	0.290759	0.289834
(3,-1)	0.288850	0.285843	0.291961	0.297192	0.305045	0.289595	0.289674	0.289220	0.288372
(3,-1)	0.288850	0.285843	0.291961	0.297192	0.305045	0.289595	0.289674	0.289220	0.288372
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.041602	0.055629	0.042823	0.041273	0.042580	0.043861	0.042857		
(3,-1)	0.220739	0.340489	0.217522	0.232215	0.221819	0.221715	0.220045		
(3,-1)	0.220739	0.304924	0.217522	0.232215	0.221819	0.221715	0.220045		
(3,-1)	0.325527	0.304924	0.325928	0.337572	0.327760	0.326649	0.325117		
(3,-1)	0.303460	0.322914	0.301790	0.316339	0.304625	0.303837	0.302332		
(3,-1)	0.325527	0.322914	0.325928	0.337572	0.327760	0.326649	0.325117		
(3,-1)	0.290318	0.300055	0.293482	0.299188	0.292333	0.291522	0.289966		
(3,-1)	0.290318	0.286142	0.293482	0.299188	0.292333	0.291522	0.289966		
(3,-1)	0.288850	0.286142	0.291512	0.297358	0.290946	0.290105	0.288532		
(3,-1)	0.288850	0.283206	0.291512	0.297358	0.290946	0.290105	0.288532		

Table S155: Density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>4</sub>NH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.052182	0.056239	0.052839	0.055172	0.054211	0.056382	0.054517	0.053598	0.052922
(3,-1)	0.347309	0.343130	0.352791	0.350092	0.353680	0.344196	0.353188	0.351657	0.342716
(3,-1)	0.308091	0.310425	0.312555	0.310103	0.311094	0.309696	0.308892	0.303999	0.305526
(3,-1)	0.308091	0.310425	0.312555	0.310103	0.311094	0.309696	0.308892	0.303999	0.305526
(3,-1)	0.323693	0.318003	0.323522	0.319547	0.323887	0.318584	0.320753	0.321452	0.327089
(3,-1)	0.323693	0.318003	0.323522	0.319547	0.323887	0.318584	0.320753	0.321452	0.327089
(3,-1)	0.301250	0.294548	0.300019	0.296325	0.301005	0.294748	0.296909	0.298657	0.303005
(3,-1)	0.292385	0.285154	0.292103	0.288984	0.293511	0.284846	0.292828	0.286741	0.282372
(3,-1)	0.292385	0.285154	0.292103	0.288984	0.293511	0.284846	0.292828	0.286741	0.282372
(3,-1)	0.289185	0.282783	0.289506	0.286447	0.290677	0.282215	0.290158	0.284411	0.279761
(3,-1)	0.289185	0.282783	0.289506	0.286447	0.290677	0.282215	0.290158	0.284411	0.279761
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.052182	0.026683	0.056455	0.052856	0.054905	0.056597	0.055032	0.054766	0.055680
(3,-1)	0.347309	0.340413	0.342794	0.353400	0.351311	0.354063	0.347886	0.355094	0.347004
(3,-1)	0.308091	0.340413	0.301436	0.313399	0.311076	0.299814	0.305101	0.310416	0.309411
(3,-1)	0.308091	0.317501	0.301436	0.313399	0.311076	0.299814	0.305101	0.310416	0.309411
(3,-1)	0.323693	0.318879	0.321811	0.325809	0.322710	0.315385	0.320358	0.325123	0.321530
(3,-1)	0.323693	0.317501	0.321811	0.325809	0.322710	0.315385	0.320358	0.325123	0.321530
(3,-1)	0.301250	0.318879	0.300010	0.302535	0.299727	0.291386	0.296919	0.302551	0.299016
(3,-1)	0.292385	0.285341	0.288861	0.294013	0.291638	0.290220	0.285569	0.294275	0.291848
(3,-1)	0.292385	0.288924	0.288861	0.294013	0.291638	0.290220	0.285569	0.294275	0.291848
(3,-1)	0.289185	0.288924	0.285812	0.291207	0.288827	0.287319	0.283030	0.291179	0.288770
(3,-1)	0.289185	0.284354	0.285812	0.291207	0.288827	0.287319	0.283030	0.291179	0.288770
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.052182	0.056742	0.054788	0.053596	0.056559	0.053665	0.053789	0.054232	0.055052
(3,-1)	0.347309	0.347077	0.352091	0.357775	0.360224	0.354692	0.353638	0.352192	0.350553
(3,-1)	0.308091	0.304364	0.306726	0.313041	0.309666	0.309853	0.311150	0.310980	0.310432
(3,-1)	0.308091	0.304364	0.306726	0.313041	0.309666	0.309853	0.311150	0.310980	0.310432
(3,-1)	0.323693	0.316799	0.323868	0.328285	0.327035	0.320273	0.322515	0.323469	0.321424
(3,-1)	0.323693	0.316799	0.323868	0.328285	0.327035	0.320273	0.322515	0.323469	0.321424
(3,-1)	0.301250	0.292885	0.300494	0.304393	0.303520	0.298547	0.300134	0.300401	0.298299
(3,-1)	0.292385	0.289230	0.295678	0.300915	0.309167	0.292743	0.292869	0.292449	0.291678
(3,-1)	0.292385	0.289230	0.295678	0.300915	0.309167	0.292743	0.292869	0.292449	0.291678
(3,-1)	0.289185	0.286213	0.292462	0.297693	0.305734	0.289694	0.289872	0.289531	0.288831
(3,-1)	0.289185	0.286213	0.292462	0.297693	0.305734	0.289694	0.289872	0.289531	0.288831
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.052182	0.027132	0.053679	0.051695	0.053334	0.054785	0.053548		
(3,-1)	0.347309	0.342057	0.356609	0.357014	0.351885	0.350441	0.348906		
(3,-1)	0.308091	0.342057	0.307441	0.314807	0.312454	0.310826	0.308173		
(3,-1)	0.308091	0.318011	0.307441	0.314807	0.312454	0.310826	0.308173		
(3,-1)	0.323693	0.319412	0.323639	0.335404	0.325994	0.324794	0.323386		
(3,-1)	0.323693	0.318011	0.323639	0.335404	0.325994	0.324794	0.323386		
(3,-1)	0.301250	0.319412	0.299876	0.313603	0.302747	0.301846	0.300396		
(3,-1)	0.292385	0.284023	0.295145	0.301265	0.294304	0.293484	0.291873		
(3,-1)	0.292385	0.287213	0.295145	0.301265	0.294304	0.293484	0.291873		
(3,-1)	0.289185	0.287213	0.291819	0.297274	0.291468	0.290537	0.288962		
(3,-1)	0.289185	0.283195	0.291819	0.297274	0.291468	0.290537	0.288962		

Table S156: Density value (a.u.) at the considered critical points for the C<sub>5</sub>H<sub>5</sub>N system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.025074	0.027812	0.025667	0.026827	0.026018	0.029095	0.025822	0.024688	0.026483
(3,-1)	0.345744	0.344673	0.348463	0.345336	0.348271	0.344237	0.344741	0.339734	0.343660
(3,-1)	0.345744	0.344673	0.348463	0.345336	0.348271	0.344237	0.344741	0.339734	0.343660
(3,-1)	0.319902	0.313019	0.318892	0.314917	0.319662	0.313150	0.316054	0.318832	0.320821
(3,-1)	0.321622	0.314352	0.320140	0.316241	0.321152	0.314283	0.317445	0.320610	0.322360
(3,-1)	0.319902	0.313019	0.318892	0.314917	0.319662	0.313150	0.316054	0.318832	0.320821
(3,-1)	0.321622	0.314352	0.320140	0.316241	0.321152	0.314283	0.317445	0.320610	0.322360
(3,-1)	0.290605	0.283639	0.290478	0.287438	0.291903	0.282764	0.291182	0.285394	0.280100
(3,-1)	0.294163	0.286555	0.293583	0.290488	0.295168	0.285888	0.294427	0.288014	0.282452
(3,-1)	0.294163	0.286555	0.293583	0.290488	0.295168	0.285888	0.294427	0.288014	0.282452
(3,-1)	0.289463	0.282941	0.289728	0.286680	0.290912	0.282226	0.290337	0.284804	0.279436
(3,-1)	0.289463	0.282941	0.289728	0.286680	0.290912	0.282226	0.290337	0.284804	0.279436
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.025074	0.216402	0.027153	0.025546	0.026539	0.025203	0.026129	0.025769	0.027792
(3,-1)	0.345744		0.338969	0.350267	0.347626	0.334815	0.340053	0.348221	0.345221
(3,-1)	0.345744		0.338969	0.350267	0.347626	0.334815	0.340053	0.348221	0.345221
(3,-1)	0.319902		0.317752	0.321370	0.318319	0.312436	0.317067	0.321185	0.317193
(3,-1)	0.321622		0.319152	0.322780	0.319829	0.314849	0.319181	0.322824	0.318610
(3,-1)	0.319902		0.317752	0.321370	0.318319	0.312436	0.317067	0.321185	0.317193
(3,-1)	0.321622		0.319152	0.322780	0.319829	0.314849	0.319181	0.322824	0.318610
(3,-1)	0.290605		0.287376	0.292334	0.290020	0.288806	0.283887	0.292647	0.290015
(3,-1)	0.294163		0.291097	0.295593	0.293274	0.291905	0.286647	0.296092	0.293511
(3,-1)	0.294163		0.291097	0.295593	0.293274	0.291905	0.286647	0.296092	0.293511
(3,-1)	0.289463		0.286164	0.291414	0.289045	0.287704	0.283121	0.291459	0.288937
(3,-1)	0.289463		0.286164	0.291414	0.289045	0.287704	0.283121	0.291459	0.288937
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.025074	0.025803	0.026077	0.026793	0.028557	0.025029	0.025270	0.025548	0.026250
(3,-1)	0.345744	0.339333	0.344510	0.351838	0.349672	0.346409	0.347799	0.347373	0.346609
(3,-1)	0.345744	0.339333	0.344510	0.351838	0.349672	0.346409	0.347799	0.347373	0.346609
(3,-1)	0.319902	0.312543	0.320148	0.323542	0.322206	0.316774	0.318566	0.319052	0.316876
(3,-1)	0.321622	0.314255	0.321904	0.325096	0.323212	0.318338	0.320094	0.320550	0.318392
(3,-1)	0.319902	0.312543	0.320148	0.323542	0.322206	0.316774	0.318566	0.319052	0.316876
(3,-1)	0.321622	0.314255	0.321904	0.325096	0.323212	0.318338	0.320094	0.320550	0.318392
(3,-1)	0.290605	0.287678	0.293548	0.298918	0.306309	0.291421	0.291429	0.290902	0.290020
(3,-1)	0.294163	0.291211	0.296850	0.302312	0.309475	0.294800	0.294794	0.294240	0.293371
(3,-1)	0.294163	0.291211	0.296850	0.302312	0.309475	0.294800	0.294794	0.294240	0.293371
(3,-1)	0.289463	0.286650	0.292596	0.297766	0.305411	0.290083	0.290209	0.289813	0.289019
(3,-1)	0.289463	0.286650	0.292596	0.297766	0.305411	0.290083	0.290209	0.289813	0.289019
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.025074	0.217148	0.026116	0.024434	0.025920	0.026601	0.026079		
(3,-1)	0.345744		0.346038	0.355595	0.349573	0.348158	0.345643		
(3,-1)	0.345744		0.346038	0.355595	0.349573	0.348158	0.345643		
(3,-1)	0.319902		0.319468	0.332172	0.321735	0.320645	0.319286		
(3,-1)	0.321622		0.321071	0.334033	0.323204	0.322261	0.320819		
(3,-1)	0.319902		0.319468	0.332172	0.321735	0.320645	0.319286		
(3,-1)	0.321622		0.321071	0.334033	0.323204	0.322261	0.320819		
(3,-1)	0.290605		0.293139	0.299416	0.292650	0.291843	0.290283		
(3,-1)	0.294163		0.296455	0.303275	0.295995	0.295257	0.293718		
(3,-1)	0.294163		0.296455	0.303275	0.295995	0.295257	0.293718		
(3,-1)	0.289463		0.292024	0.297267	0.291739	0.290813	0.289331		
(3,-1)	0.289463		0.292024	0.297267	0.291739	0.290813	0.289331		

Table S157: Density value (a.u.) at the considered critical points for the SH<sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.220930	0.215618	0.219200	0.217442	0.220234	0.216585	0.219192	0.217673	0.216735
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.220930	0.379919	0.217930	0.220538	0.219155	0.219155	0.216840	0.220227	0.219609
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.220930	0.216414	0.222285	0.225493	0.234562	0.220003	0.219998	0.219580	0.219134
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.220930	0.382018	0.219837	0.224910	0.221022	0.220656	0.219229		



Table S158: Density value (a.u.) at the considered critical points for the  $C_2H_3^\bullet$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.384655	0.377067	0.382319	0.377823	0.381544	0.378511	0.381101	0.377132	0.385864
(3,-1)	0.282947	0.272330	0.279477	0.276680	0.281022	0.272132	0.280138	0.276898	0.271862
(3,-1)	0.288503	0.277938	0.285296	0.282280	0.286655	0.277493	0.285921	0.281183	0.276391
(3,-1)	0.290618	0.281448	0.288136	0.285513	0.289224	0.281197	0.289211	0.282969	0.279600
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.384655	0.247919	0.377888	0.384279	0.380640	0.373935	0.377912	0.381996	0.379871
(3,-1)	0.282947	0.276712	0.276849	0.281571	0.279524	0.278709	0.275070	0.281652	0.279541
(3,-1)	0.288503	0.276221	0.282290	0.287207	0.284937	0.283908	0.279476	0.287450	0.284842
(3,-1)	0.290618	0.276221	0.285291	0.289758	0.287814	0.286520	0.281839	0.289714	0.289589
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.384655	0.378930	0.384016	0.388876	0.390357	0.376646	0.379912	0.381960	0.379929
(3,-1)	0.282947	0.277170	0.283578	0.287980	0.297367	0.280927	0.280943	0.280288	0.279353
(3,-1)	0.288503	0.282655	0.288609	0.293659	0.302022	0.286283	0.286277	0.285714	0.284744
(3,-1)	0.290618	0.284605	0.292464	0.295618	0.304819	0.288542	0.288642	0.288238	0.287567
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.384655	0.247962	0.383547	0.393624	0.384428	0.382674	0.381037		
(3,-1)	0.282947	0.276446	0.282214	0.288854	0.282121	0.281739	0.280323		
(3,-1)	0.288503	0.275935	0.287866	0.293904	0.287817	0.287192	0.285853		
(3,-1)	0.290618	0.275935	0.292596	0.295603	0.290401	0.289912	0.288558		

Table S159: Density value (a.u.) at the considered critical points for the  $\text{CH}_3\text{CO}^\bullet$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.252254	0.241959	0.246681	0.244444	0.249099	0.241206	0.244255	0.250791	0.250672
(3,-1)	0.285434	0.275504	0.283034	0.279826	0.284149	0.275995	0.283467	0.278871	0.273556
(3,-1)	0.284887	0.274708	0.282329	0.279002	0.283299	0.275049	0.282634	0.277990	0.273244
(3,-1)	0.284887	0.274708	0.282329	0.279002	0.283299	0.275049	0.282634	0.277990	0.273244
(3,-1)	0.430844	0.435053	0.434836	0.432494	0.433021	0.435226	0.430989	0.420166	0.421594
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.252254	0.279299	0.250429	0.249299	0.247917	0.246369	0.247969	0.250973	0.246775
(3,-1)	0.285434	0.357782	0.278905	0.284622	0.282125	0.281651	0.276917	0.284599	0.281916
(3,-1)	0.284887	0.285913	0.278439	0.283850	0.281226	0.280725	0.276204	0.283761	0.281219
(3,-1)	0.284887	0.291844	0.278439	0.283850	0.281226	0.280725	0.276204	0.283761	0.281219
(3,-1)	0.430844		0.416002	0.435479	0.433228	0.421861	0.427003	0.430424	0.428588
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.252254	0.241972	0.247294	0.248832	0.242509	0.248646	0.248698	0.247670	0.246370
(3,-1)	0.285434	0.279989	0.285813	0.290903	0.298969	0.283611	0.283556	0.282999	0.282128
(3,-1)	0.284887	0.279244	0.285113	0.290101	0.298542	0.282850	0.282794	0.282214	0.281192
(3,-1)	0.284887	0.279244	0.285113	0.290101	0.298542	0.282850	0.282794	0.282214	0.281192
(3,-1)	0.430844	0.419509	0.428022	0.438644	0.440275	0.432439	0.433306	0.431975	0.433755
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.252254	0.279718	0.243644	0.261545	0.250260	0.250495	0.248866		
(3,-1)	0.285434	0.361322	0.284758	0.290986	0.285072	0.284077	0.282836		
(3,-1)	0.284887	0.284858	0.283890	0.289753	0.284430	0.283291	0.282137		
(3,-1)	0.284887	0.290278	0.283890	0.289753	0.284430	0.283291	0.282137		
(3,-1)	0.430844		0.435424	0.436729	0.432726	0.431220	0.426745		

Table S160: Density value (a.u.) at the considered critical points for the H<sub>2</sub>COH• system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.284074	0.283040	0.283815	0.283128	0.282384	0.282845	0.280292	0.277699	0.279589
(3,-1)	0.368347	0.361610	0.372554	0.370452	0.372616	0.366164	0.373376	0.373248	0.361244
(3,-1)	0.293081	0.283042	0.289964	0.287079	0.291152	0.282357	0.291025	0.284625	0.281222
(3,-1)	0.298885	0.288834	0.295971	0.292965	0.297094	0.288147	0.297125	0.289898	0.286606
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.284074	0.281672	0.276359	0.284109	0.283410	0.274399	0.279164	0.281836	0.282452
(3,-1)	0.368347	0.271518	0.362290	0.372054	0.370417	0.371936	0.368638	0.374238	0.366647
(3,-1)	0.293081	0.281157	0.287186	0.291683	0.289515	0.289338	0.283725	0.291609	0.291132
(3,-1)	0.298885	0.281157	0.293481	0.297639	0.295355	0.294975	0.289003	0.297557	0.297129
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.284074	0.278072	0.279582	0.282097	0.282156	0.283558	0.283851	0.283336	0.281567
(3,-1)	0.368347	0.368555	0.366882	0.370034	0.366290	0.375318	0.373799	0.372633	0.369780
(3,-1)	0.293081	0.287101	0.294031	0.298076	0.306234	0.290643	0.290595	0.290066	0.289392
(3,-1)	0.298885	0.292957	0.299920	0.304063	0.311918	0.296634	0.296589	0.296069	0.295360
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.284074	0.282887	0.279977	0.283585	0.283273	0.282579	0.278860		
(3,-1)	0.368347	0.270285	0.375526	0.372639	0.369310	0.367632	0.365647		
(3,-1)	0.293081	0.280039	0.293593	0.298115	0.292597	0.291940	0.290598		
(3,-1)	0.298885	0.280039	0.299893	0.303925	0.298546	0.297779	0.296562		

Table S161: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>O• system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.287445	0.289539	0.290288	0.289231	0.288008	0.289622	0.286630	0.283146	0.283856
(3,-1)	0.279162	0.264656	0.273350	0.270272	0.276211	0.266670	0.274956	0.271466	0.268096
(3,-1)	0.289759	0.278683	0.286284	0.283087	0.287785	0.278888	0.287017	0.281708	0.276306
(3,-1)	0.289759	0.278683	0.286284	0.283087	0.287785	0.278888	0.287017	0.281708	0.276306
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.287445	0.250450	0.280017	0.289362	0.288008	0.278703	0.282882	0.286697	0.285934
(3,-1)	0.279162	0.279426	0.272643	0.276541	0.274608	0.274314	0.269715	0.277480	0.274905
(3,-1)	0.289759	0.277746	0.283513	0.288231	0.285828	0.285305	0.280067	0.288534	0.285992
(3,-1)	0.289759	0.277746	0.283513	0.288231	0.285828	0.285305	0.280067	0.288534	0.285992
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.287445	0.282776	0.282710	0.285701	0.283443	0.287317	0.288082	0.288210	0.286278
(3,-1)	0.279162	0.273122	0.278773	0.283706	0.292287	0.276673	0.276444	0.275564	0.274805
(3,-1)	0.289759	0.284243	0.289544	0.294980	0.302609	0.287439	0.287356	0.286727	0.285936
(3,-1)	0.289759	0.284243	0.289544	0.294980	0.302609	0.287439	0.287356	0.286727	0.285936
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.287445	0.249634	0.282656	0.284023	0.288265	0.286553	0.283827		
(3,-1)	0.279162	0.280431	0.277208	0.287338	0.277856	0.277935	0.276395		
(3,-1)	0.289759	0.276326	0.288129	0.295445	0.289169	0.288405	0.287231		
(3,-1)	0.289759	0.276326	0.288129	0.295445	0.289169	0.288405	0.287232		

Table S162: Density value (a.u.) at the considered critical points for the  $\text{CH}_3\text{CH}_2\text{O}^\bullet$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.241844	0.229193	0.249174	0.246305	0.251472	0.230103	0.245999	0.253623	0.252326
(3,-1)	0.279848	0.287173	0.287977	0.287097	0.285653	0.287218	0.284302	0.281200	0.281855
(3,-1)	0.288014	0.279695	0.280419	0.277288	0.283125	0.279894	0.281889	0.277709	0.273314
(3,-1)	0.288014	0.279695	0.280419	0.277288	0.283125	0.279894	0.281889	0.277709	0.273314
(3,-1)	0.281857	0.274882	0.281528	0.278419	0.282492	0.275073	0.281897	0.278029	0.272586
(3,-1)	0.284934	0.279066	0.284248	0.281046	0.285119	0.278821	0.284569	0.280014	0.274524
(3,-1)	0.284934	0.279066	0.284248	0.281046	0.285119	0.278821	0.284569	0.280014	0.274524
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.241844	0.190608	0.253045	0.251795	0.249797	0.248356	0.250273	0.242915	0.248844
(3,-1)	0.279848	0.272914	0.277594	0.286900	0.285690	0.276604	0.280764	0.284077	0.283361
(3,-1)	0.288014	0.280234	0.279234	0.283506	0.281463	0.280930	0.275998	0.289344	0.281603
(3,-1)	0.288014	0.280234	0.279234	0.283506	0.281463	0.280930	0.275998	0.289344	0.281603
(3,-1)	0.281857		0.277317	0.282976	0.280526	0.280241	0.276019	0.283559	0.280114
(3,-1)	0.284934		0.280064	0.285622	0.283081	0.282634	0.278002	0.286888	0.282747
(3,-1)	0.284934		0.280064	0.285622	0.283081	0.282634	0.278002	0.286888	0.282747
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.241844	0.244409	0.250204	0.251771	0.246740	0.251262	0.251225	0.239120	0.248174
(3,-1)	0.279848	0.280354	0.280157	0.283083	0.280403	0.284913	0.285673	0.285642	0.283920
(3,-1)	0.288014	0.279880	0.285495	0.290661	0.298651	0.283378	0.283232	0.287614	0.281628
(3,-1)	0.288014	0.279880	0.285495	0.290661	0.298651	0.283378	0.283232	0.287614	0.281628
(3,-1)	0.281857	0.278784	0.284185	0.289008	0.297250	0.281619	0.281664	0.282158	0.280499
(3,-1)	0.284934	0.281166	0.286665	0.291626	0.299574	0.284269	0.284303	0.285451	0.283045
(3,-1)	0.284934	0.281166	0.286665	0.291626	0.299574	0.284269	0.284303	0.285451	0.283045
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.241844	0.190091	0.247206	0.264043	0.252868	0.252641	0.251630		
(3,-1)	0.279848	0.272264	0.280341	0.281205	0.285824	0.284223	0.281369		
(3,-1)	0.288014	0.279451	0.284279	0.293321	0.284761	0.284607	0.283108		
(3,-1)	0.288014	0.279451	0.284279	0.293321	0.284761	0.284607	0.283108		
(3,-1)	0.281857		0.281966	0.288348	0.283503	0.282477	0.281101		
(3,-1)	0.284934		0.284942	0.290901	0.286137	0.284998	0.283763		
(3,-1)	0.284934		0.284942	0.290901	0.286137	0.284998	0.283763		

Table S163: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>S• system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.190936	0.183049	0.186259	0.184953	0.188858	0.182526	0.183576	0.185029	0.192768
(3,-1)	0.281356	0.270117	0.277877	0.274812	0.279395	0.270065	0.278215	0.274768	0.270383
(3,-1)	0.288708	0.278815	0.286186	0.283045	0.287372	0.278329	0.286675	0.281926	0.276694
(3,-1)	0.288708	0.278815	0.286186	0.283045	0.287372	0.278329	0.286675	0.281926	0.276694
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.190936	0.262640	0.193957	0.188548	0.187829	0.179628	0.182446	0.190501	0.188717
(3,-1)	0.281356	0.269377	0.274946	0.279826	0.277548	0.277138	0.272723	0.279993	0.277522
(3,-1)	0.288708	0.276113	0.282723	0.287758	0.285316	0.284729	0.279876	0.287849	0.285250
(3,-1)	0.288708	0.276113	0.282723	0.287758	0.285316	0.284729	0.279876	0.287849	0.285250
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.190936	0.180888	0.186601	0.189190	0.189046	0.189802	0.189314	0.187854	0.186628
(3,-1)	0.281356	0.275172	0.281364	0.286005	0.294513	0.279380	0.279109	0.278339	0.277283
(3,-1)	0.288708	0.283061	0.288966	0.294147	0.302036	0.286882	0.286782	0.286167	0.285195
(3,-1)	0.288708	0.283061	0.288966	0.294147	0.302036	0.286882	0.286782	0.286167	0.285195
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.190936	0.263352	0.183971	0.198480	0.189276	0.189765	0.188482		
(3,-1)	0.281356	0.268997	0.279638	0.287153	0.280538	0.279808	0.278465		
(3,-1)	0.288708	0.275400	0.287472	0.293969	0.288338	0.287361	0.286138		
(3,-1)	0.288708	0.275400	0.287472	0.293969	0.288338	0.287361	0.286138		

Table S164: Density value (a.u.) at the considered critical points for the C<sub>2</sub>H<sub>5</sub><sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.266401	0.256114	0.261641	0.258813	0.263447	0.255692	0.258803	0.263361	0.264212
(3,-1)	0.277636	0.267163	0.274424	0.271574	0.275660	0.267368	0.274938	0.272118	0.267157
(3,-1)	0.284315	0.274861	0.281974	0.278884	0.282903	0.274805	0.282284	0.278156	0.272868
(3,-1)	0.284315	0.274861	0.281974	0.278884	0.282903	0.274805	0.282284	0.278156	0.272868
(3,-1)	0.291823	0.283200	0.289765	0.286980	0.290575	0.281816	0.290647	0.284307	0.281330
(3,-1)	0.291823	0.283200	0.289765	0.286980	0.290575	0.281816	0.290647	0.284307	0.281330
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.266401	0.263840	0.265113	0.263975	0.261950	0.258493	0.260802	0.264984	0.262189
(3,-1)	0.277636	0.263840	0.271252	0.276173	0.274033	0.273986	0.270066	0.276055	0.273556
(3,-1)	0.284315	0.283905	0.278135	0.283395	0.280958	0.280525	0.276097	0.283219	0.280575
(3,-1)	0.284315	0.276421	0.278135	0.283395	0.280958	0.280525	0.276097	0.283219	0.280575
(3,-1)	0.291823	0.276421	0.286791	0.291065	0.288857	0.288418	0.283098	0.290660	0.290586
(3,-1)	0.291823	0.268275	0.286791	0.291065	0.288857	0.288418	0.283098	0.290660	0.290586
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.266401	0.255995	0.263270	0.264975	0.263797	0.262689	0.263014	0.262213	0.260341
(3,-1)	0.277636	0.272029	0.277708	0.282038	0.290755	0.275382	0.275276	0.274686	0.273759
(3,-1)	0.284315	0.279095	0.284489	0.289421	0.297436	0.282193	0.282184	0.281706	0.280787
(3,-1)	0.284315	0.279095	0.284489	0.289421	0.297436	0.282193	0.282184	0.281706	0.280787
(3,-1)	0.291823	0.286283	0.293397	0.297224	0.306306	0.290010	0.289916	0.289440	0.288596
(3,-1)	0.291823	0.286283	0.293397	0.297224	0.306306	0.290010	0.289916	0.289440	0.288596
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.266401	0.264280	0.259724	0.274672	0.264984	0.264618	0.263581		
(3,-1)	0.277636	0.264280	0.275092	0.282707	0.276935	0.276246	0.274866		
(3,-1)	0.284315	0.283130	0.282492	0.288888	0.283998	0.282970	0.281720		
(3,-1)	0.284315	0.275711	0.282492	0.288888	0.283998	0.282970	0.281720		
(3,-1)	0.291823	0.275711	0.292900	0.295464	0.291764	0.290837	0.289619		
(3,-1)	0.291823	0.267998	0.292900	0.295464	0.291764	0.290837	0.289619		

Table S165: Density value (a.u.) at the considered critical points for the  $(\text{CH}_3)_2\text{CH}^\bullet$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.264744	0.257048	0.262542	0.259720	0.264459	0.256444	0.259630	0.264718	0.265418
(3,-1)	0.264744	0.257048	0.262542	0.259720	0.264459	0.256444	0.259630	0.264718	0.265418
(3,-1)	0.287741	0.281776	0.288163	0.285478	0.289165	0.280591	0.289060	0.283287	0.279817
(3,-1)	0.281686	0.275172	0.282266	0.279159	0.283192	0.275176	0.282578	0.278397	0.272988
(3,-1)	0.281686	0.275172	0.282266	0.279159	0.283192	0.275176	0.282578	0.278397	0.272988
(3,-1)	0.273604	0.266415	0.273519	0.270665	0.274750	0.266936	0.273898	0.271189	0.266129
(3,-1)	0.279241	0.272461	0.279718	0.276631	0.280683	0.273042	0.280035	0.276141	0.270796
(3,-1)	0.279241	0.272461	0.279718	0.276631	0.280683	0.273042	0.280035	0.276141	0.270796
(3,-1)	0.273604	0.266415	0.273519	0.270665	0.274750	0.266936	0.273898	0.271189	0.266129
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.264744	0.512531	0.266242	0.264972	0.262970	0.259498	0.262057	0.266050	0.263104
(3,-1)	0.264744	0.512531	0.266242	0.264972	0.262970	0.259498	0.262057	0.266050	0.263104
(3,-1)	0.287741		0.285099	0.289576	0.287484	0.287051	0.281972	0.289208	0.288866
(3,-1)	0.281686		0.278351	0.283663	0.281204	0.280746	0.276342	0.283482	0.280804
(3,-1)	0.281686		0.278351	0.283663	0.281204	0.280746	0.276342	0.283482	0.280804
(3,-1)	0.273604		0.269977	0.275173	0.273010	0.273092	0.269116	0.275036	0.272433
(3,-1)	0.279241		0.275692	0.281152	0.278732	0.278476	0.274005	0.280933	0.278132
(3,-1)	0.279241		0.275692	0.281152	0.278732	0.278476	0.274005	0.280933	0.278132
(3,-1)	0.273604		0.269977	0.275173	0.273010	0.273092	0.269116	0.275036	0.272433
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.264744	0.256832	0.264177	0.265910	0.264339	0.263853	0.264138	0.263258	0.261337
(3,-1)	0.264744	0.256832	0.264177	0.265910	0.264339	0.263853	0.264138	0.263258	0.261337
(3,-1)	0.287741	0.284835	0.291768	0.295692	0.304482	0.288600	0.288515	0.288043	0.287235
(3,-1)	0.281686	0.279329	0.284734	0.289687	0.297623	0.282421	0.282428	0.281980	0.281068
(3,-1)	0.281686	0.279329	0.284734	0.289687	0.297623	0.282421	0.282428	0.281980	0.281068
(3,-1)	0.273604	0.271026	0.276617	0.281019	0.289472	0.274363	0.274269	0.273697	0.272797
(3,-1)	0.279241	0.276824	0.282182	0.287029	0.295150	0.279886	0.279875	0.279427	0.278574
(3,-1)	0.279241	0.276824	0.282182	0.287029	0.295150	0.279886	0.279875	0.279427	0.278574
(3,-1)	0.273604	0.271026	0.276617	0.281019	0.289472	0.274363	0.274269	0.273697	0.272797
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.264744	0.512530	0.260742	0.275965	0.265911	0.265578	0.264477		
(3,-1)	0.264744	0.512530	0.260742	0.275965	0.265911	0.265578	0.264477		
(3,-1)	0.287741		0.291158	0.294131	0.290229	0.289423	0.288040		
(3,-1)	0.281686		0.282824	0.289051	0.284198	0.283139	0.281877		
(3,-1)	0.281686		0.282824	0.289051	0.284198	0.283139	0.281877		
(3,-1)	0.273604		0.273932	0.281353	0.275828	0.275086	0.273693		
(3,-1)	0.279241		0.279977	0.286737	0.281713	0.280700	0.279393		
(3,-1)	0.279241		0.279977	0.286737	0.281713	0.280700	0.279393		
(3,-1)	0.273604		0.273932	0.281353	0.275828	0.275086	0.273693		



Table S166: Density value (a.u.) at the considered critical points for the NO<sub>2</sub><sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.515186	0.506855	0.509088	0.508043	0.513872	0.502516	0.506087	0.503573	0.514610
(3,-1)	0.515186	0.506855	0.509088	0.508043	0.513872	0.502516	0.506087	0.503573	0.514610
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.515186		0.512170	0.513166	0.513016	0.495846	0.500534	0.517411	0.507291
(3,-1)	0.515186		0.512170	0.513166	0.513016	0.495846	0.500534	0.517411	0.507291
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.515186	0.502019	0.513624	0.518948	0.532361	0.512414	0.512761	0.511246	0.507265
(3,-1)	0.515186	0.502019	0.513624	0.518948	0.532361	0.512414	0.512761	0.511246	0.507265
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.515186		0.510120	0.528816	0.511563	0.513228	0.507926		
(3,-1)	0.515186		0.510120	0.528816	0.511563	0.513228	0.507926		

Table S167: Density value (a.u.) at the considered critical points for the [HON<sub>2</sub>]<sup>‡</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.486165	0.479583	0.481303	0.480831	0.486026	0.475637	0.478122	0.478205	0.486911
(3,-1)	0.109417	0.109712	0.110532	0.110538	0.111663	0.112394	0.109951	0.110398	0.111696
(3,-1)	0.604647	0.600500	0.603452	0.599298	0.602742	0.599181	0.602911	0.582966	0.599334
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.486165	0.485850	0.485469	0.484799	0.485060	0.469794	0.474209	0.488786	0.479314
(3,-1)	0.109417	0.111514	0.109986	0.110700	0.110585	0.109931	0.109754	0.110525	0.108989
(3,-1)	0.604647	0.592168	0.591052	0.605716	0.602229	0.582781	0.587108	0.603046	0.596688
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.486165	0.473486	0.484594	0.487897	0.498279	0.484533	0.484461	0.482783	0.479106
(3,-1)	0.109417	0.109495	0.108297	0.109882	0.106176	0.110401	0.110627	0.110813	0.111772
(3,-1)	0.604647	0.594639	0.606426	0.618341	0.636351	0.596931	0.601214	0.603791	0.600929
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.486165	0.484664	0.480229	0.496361	0.483775	0.485405	0.480497		
(3,-1)	0.109417	0.109600	0.108277	0.107619	0.108275	0.107934	0.106359		
(3,-1)	0.604647	0.597474	0.608027	0.613266	0.603811	0.602209	0.598820		

Table S168: Density value (a.u.) at the considered critical points for the  $[\text{HClH}]^\ddagger$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.150468	0.148266	0.150164	0.150067	0.151555	0.148489	0.150939	0.152195	0.152949
(3,-1)	0.150468	0.148266	0.150164	0.150067	0.151555	0.148489	0.150939	0.152195	0.152949
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.150468	0.150383	0.152270	0.150607	0.150533	0.149707	0.148844	0.151511	0.148976
(3,-1)	0.150468	0.150383	0.152270	0.150607	0.150533	0.149707	0.148844	0.151511	0.148976
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.150468	0.148966	0.147659	0.148907	0.145576	0.153030	0.152135	0.151347	0.151130
(3,-1)	0.150468	0.148966	0.147659	0.148907	0.145576	0.153030	0.152135	0.151347	0.151130
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.150468	0.151698	0.146866	0.150296	0.150694	0.150835	0.149827		
(3,-1)	0.150468	0.151698	0.146866	0.150296	0.150694	0.150835	0.149827		

Table S169: Density value (a.u.) at the considered critical points for the  $[\text{ClFCH}_3]^\ddagger$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.158682	0.155356	0.153898	0.155794	0.157158	0.156834	0.153352	0.155424	0.160045
(3,-1)	0.052660	0.052326	0.051181	0.051775	0.052357	0.051902	0.051082	0.050475	0.048265
(3,-1)	0.298363	0.291171	0.298769	0.295460	0.299717	0.291464	0.299958	0.291788	0.288235
(3,-1)	0.298380	0.291187	0.298786	0.295477	0.299734	0.291483	0.299988	0.291807	0.288251
(3,-1)	0.298379	0.291188	0.298786	0.295477	0.299734	0.291483	0.299996	0.291806	0.288254
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.158682	0.155506	0.158448	0.155543	0.157658	0.158223	0.155804	0.158640	0.155593
(3,-1)	0.052660	0.049339	0.049095	0.051839	0.052587	0.051314	0.049944	0.053032	0.050792
(3,-1)	0.298363	0.293113	0.295915	0.300001	0.297225	0.296725	0.290370	0.299807	0.298692
(3,-1)	0.298380	0.293130	0.295931	0.300018	0.297241	0.296745	0.290390	0.299823	0.298709
(3,-1)	0.298379	0.293130	0.295929	0.300019	0.297241	0.296745	0.290390	0.299823	0.298710
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.158682	0.156893	0.158770	0.158364	0.156676	0.158454	0.157936	0.157214	0.156405
(3,-1)	0.052660	0.052123	0.051220	0.052721	0.052950	0.052864	0.052672	0.052595	0.052226
(3,-1)	0.298363	0.294849	0.301677	0.306387	0.314332	0.298070	0.298127	0.297970	0.297443
(3,-1)	0.298380	0.294860	0.301699	0.306403	0.314342	0.298091	0.298150	0.297997	0.297459
(3,-1)	0.298379	0.294852	0.301699	0.306404	0.314344	0.298094	0.298154	0.298005	0.297458
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.158682	0.157676	0.158850	0.156085	0.156943	0.159951	0.158820		
(3,-1)	0.052660	0.050548	0.053726	0.053703	0.052014	0.052980	0.052023		
(3,-1)	0.298363	0.291657	0.301260	0.301401	0.300292	0.298852	0.297715		
(3,-1)	0.298380	0.291673	0.301271	0.301417	0.300309	0.298868	0.297733		
(3,-1)	0.298379	0.291673	0.301274	0.301416	0.300309	0.298868	0.297728		

Table S170: Density value (a.u.) at the considered critical points for the  $[\text{ClCH}_2\text{Cl}]^{-\ddagger}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.054571	0.056888	0.055552	0.056747	0.055897	0.058864	0.055881	0.053550	0.053565
(3,-1)	0.312934	0.298487	0.307651	0.303714	0.309948	0.298861	0.308642	0.301356	0.295914
(3,-1)	0.312951	0.298502	0.307668	0.303730	0.309964	0.298877	0.308684	0.301374	0.295929
(3,-1)	0.312922	0.298475	0.307639	0.303702	0.309935	0.298848	0.308655	0.301345	0.295903
(3,-1)	0.054597	0.056912	0.055577	0.056772	0.055923	0.058888	0.055907	0.053576	0.053597
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.054571	0.054097	0.055247	0.055247	0.056269	0.054643	0.054382	0.055698	0.053702
(3,-1)	0.312934	0.302225	0.306053	0.310461	0.307613	0.307649	0.300509	0.311634	0.309238
(3,-1)	0.312951	0.302240	0.306070	0.310478	0.307629	0.307668	0.300528	0.311650	0.309255
(3,-1)	0.312922	0.302212	0.306041	0.310448	0.307600	0.307639	0.300500	0.311621	0.309226
(3,-1)	0.054597	0.054123	0.055273	0.055272	0.056294	0.054672	0.054409	0.055724	0.053727
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.054571	0.055853	0.056680	0.056494	0.056888	0.053949	0.054563	0.055284	0.056678
(3,-1)	0.312934	0.306323	0.312674	0.318355	0.326320	0.311655	0.311079	0.309814	0.307781
(3,-1)	0.312951	0.306321	0.312696	0.318368	0.326318	0.311684	0.311111	0.309855	0.307795
(3,-1)	0.312922	0.306293	0.312666	0.318339	0.326287	0.311654	0.311082	0.309826	0.307766
(3,-1)	0.054597	0.055879	0.056705	0.056518	0.056909	0.053976	0.054590	0.055310	0.056703
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.054571	0.055467	0.056573	0.051493	0.055224	0.055665	0.054687		
(3,-1)	0.312934	0.301097	0.313094	0.321920	0.311343	0.310676	0.309809		
(3,-1)	0.312951	0.301112	0.313104	0.321938	0.311359	0.310692	0.309823		
(3,-1)	0.312922	0.301085	0.313073	0.321906	0.311330	0.310663	0.309794		
(3,-1)	0.054597	0.055494	0.056599	0.051518	0.055250	0.055691	0.054712		

Table S171: Density value (a.u.) at the considered critical points for the  $[\text{FCH}_3\text{Cl}]^{-\ddagger}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.051432	0.056432	0.054289	0.055653	0.053862	0.057446	0.053965	0.052035	0.048569
(3,-1)	0.312617	0.298373	0.307475	0.303507	0.309675	0.298719	0.308482	0.301106	0.295353
(3,-1)	0.312617	0.298373	0.307475	0.303507	0.309675	0.298718	0.308482	0.301107	0.295353
(3,-1)	0.086166	0.087256	0.086437	0.087657	0.087054	0.088083	0.087418	0.087287	0.088469
(3,-1)	0.312617	0.298373	0.307475	0.303507	0.309675	0.298718	0.308482	0.301107	0.295353
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.051432	0.051535	0.052724	0.053252	0.054244	0.050812	0.051460	0.052413	0.052758
(3,-1)	0.312617	0.301839	0.305545	0.310227	0.307346	0.307078	0.300229	0.311267	0.308815
(3,-1)	0.312617	0.301839	0.305545	0.310227	0.307346	0.307079	0.300230	0.311267	0.308815
(3,-1)	0.086166	0.087368	0.088165	0.086189	0.087244	0.088735	0.086911	0.087323	0.084748
(3,-1)	0.312617	0.301839	0.305545	0.310227	0.307346	0.307079	0.300230	0.311267	0.308815
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.051432	0.052707	0.053380	0.052692	0.055515	0.051695	0.052079	0.052778	0.053928
(3,-1)	0.312617	0.306231	0.312567	0.318317	0.326266	0.310726	0.310313	0.309235	0.307588
(3,-1)	0.312617	0.306230	0.312570	0.318318	0.326266	0.310726	0.310313	0.309235	0.307589
(3,-1)	0.086166	0.087138	0.086038	0.085016	0.082053	0.086938	0.086812	0.087109	0.087375
(3,-1)	0.312617	0.306230	0.312570	0.318318	0.326266	0.310726	0.310313	0.309235	0.307589
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.051432	0.052316	0.052277	0.047156	0.053023	0.053033	0.052194		
(3,-1)	0.312617	0.300905	0.312650	0.321010	0.311149	0.310431	0.309382		
(3,-1)	0.312617	0.300905	0.312647	0.321010	0.311149	0.310431	0.309390		
(3,-1)	0.086166	0.087179	0.086408	0.082618	0.086239	0.086742	0.085260		
(3,-1)	0.312617	0.300905	0.312647	0.321010	0.311149	0.310431	0.309390		

Table S172: Density value (a.u.) at the considered critical points for the  $[\text{HOCH}_3\text{F}]^{-\ddagger}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.100079	0.106298	0.104112	0.106032	0.103426	0.107685	0.103720	0.101786	0.100215
(3,-1)	0.313226	0.298905	0.307892	0.303891	0.310090	0.299484	0.308975	0.301347	0.295632
(3,-1)	0.312902	0.298439	0.307404	0.303383	0.309570	0.298972	0.308377	0.300993	0.295345
(3,-1)	0.312959	0.298498	0.307465	0.303443	0.309629	0.299037	0.308436	0.301044	0.295396
(3,-1)	0.069577	0.073543	0.071618	0.073199	0.071777	0.075614	0.071887	0.069405	0.066814
(3,-1)	0.375484	0.369437	0.379432	0.377434	0.380252	0.373546	0.381493	0.380228	0.370744
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.100079	0.100776	0.102593	0.102358	0.103738	0.101857	0.099909	0.101787	0.101264
(3,-1)	0.313226	0.302377	0.305765	0.310693	0.307786	0.307557	0.300714	0.311666	0.309331
(3,-1)	0.312902	0.301768	0.305087	0.310220	0.307295	0.307131	0.300377	0.311152	0.308704
(3,-1)	0.312959	0.301824	0.305149	0.310279	0.307354	0.307187	0.300429	0.311211	0.308764
(3,-1)	0.069577	0.069420	0.071107	0.070861	0.072146	0.069752	0.069080	0.070940	0.069704
(3,-1)	0.375484	0.365185	0.370691	0.379596	0.378127	0.378627	0.374845	0.381424	0.373748
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.100079	0.103044	0.104009	0.103064	0.102946	0.101714	0.101714	0.102396	0.102905
(3,-1)	0.313226	0.306987	0.312811	0.318853	0.326673	0.310889	0.310554	0.309582	0.308192
(3,-1)	0.312902	0.306549	0.312315	0.318406	0.326347	0.310375	0.310047	0.309047	0.307598
(3,-1)	0.312959	0.306605	0.312374	0.318464	0.326406	0.310433	0.310105	0.309103	0.307657
(3,-1)	0.069577	0.071655	0.072784	0.072049	0.073091	0.069788	0.070209	0.070940	0.071998
(3,-1)	0.375484	0.374809	0.376590	0.377893	0.378052	0.382298	0.380723	0.379482	0.377280
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.100079	0.101901	0.103625	0.092140	0.101996	0.101892	0.100319		
(3,-1)	0.313226	0.301325	0.312772	0.321790	0.311583	0.310924	0.309691		
(3,-1)	0.312902	0.300846	0.312077	0.321364	0.311187	0.310521	0.309295		
(3,-1)	0.312959	0.300902	0.312141	0.321420	0.311246	0.310579	0.309354		
(3,-1)	0.069577	0.070792	0.071850	0.065013	0.070705	0.071074	0.069831		
(3,-1)	0.375484	0.369505	0.384163	0.381757	0.376476	0.375265	0.372509		

Table S173: Density value (a.u.) at the considered critical points for the  $[\text{HN}_2]^\ddagger$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.665368	0.655386	0.660920	0.656434	0.661798	0.653702	0.661193	0.644953	0.661388
(3,-1)	0.115511	0.116794	0.117224	0.117428	0.118750	0.119050	0.117888	0.118388	0.119215
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.665368	0.653251	0.653038	0.664286	0.661008	0.641413	0.645195	0.663979	0.651627
(3,-1)	0.115511	0.118997	0.118863	0.117538	0.117650	0.116466	0.116808	0.117850	0.115365
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.665368	0.655853	0.664724	0.678024	0.688931	0.655296	0.659473	0.662134	0.658082
(3,-1)	0.115511	0.116014	0.113664	0.115173	0.109586	0.117939	0.118155	0.118328	0.119089
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.665368	0.656426	0.669051	0.678026	0.663982	0.663022	0.660167		
(3,-1)	0.115511	0.116465	0.113791	0.115478	0.115736	0.115730	0.114119		



Table S174: Density value (a.u.) at the considered critical points for the  $[\text{HCH}_2\text{CH}_2]^\ddagger$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.349735	0.340885	0.347084	0.342457	0.347064	0.341321	0.344228	0.344626	0.349118
(3,-1)	0.035096	0.037245	0.036417	0.036803	0.036506	0.038250	0.035167	0.036009	0.033797
(3,-1)	0.295528	0.285980	0.293460	0.289932	0.294510	0.285474	0.293638	0.287944	0.282439
(3,-1)	0.295541	0.285992	0.293472	0.289943	0.294522	0.285486	0.293650	0.287955	0.282451
(3,-1)	0.294641	0.285373	0.292427	0.289182	0.293510	0.284487	0.292809	0.286905	0.282100
(3,-1)	0.294641	0.285372	0.292426	0.289182	0.293509	0.284486	0.292808	0.286905	0.282099
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.349735	0.343975	0.343381	0.349154	0.345469	0.340250	0.343535	0.347774	0.343937
(3,-1)	0.035096	0.034254	0.034568	0.036265	0.036596	0.036012	0.034784	0.035558	0.033632
(3,-1)	0.295528	0.287186	0.289607	0.295032	0.292239	0.291497	0.286260	0.294906	0.292258
(3,-1)	0.295541	0.287198	0.289619	0.295045	0.292251	0.291509	0.286272	0.294918	0.292270
(3,-1)	0.294641	0.286409	0.288608	0.294005	0.291441	0.290498	0.285311	0.293935	0.291498
(3,-1)	0.294641	0.286408	0.288607	0.294004	0.291440	0.290497	0.285311	0.293934	0.291497
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.349735	0.341473	0.347594	0.352623	0.351716	0.342710	0.345239	0.346531	0.344345
(3,-1)	0.035096	0.035515	0.035116	0.036500	0.034704	0.034762	0.035310	0.035714	0.036297
(3,-1)	0.295528	0.290184	0.296012	0.301594	0.309058	0.293639	0.293764	0.293314	0.292340
(3,-1)	0.295541	0.290196	0.296025	0.301606	0.309071	0.293651	0.293776	0.293326	0.292353
(3,-1)	0.294641	0.289376	0.295342	0.300803	0.308586	0.292762	0.292845	0.292392	0.291381
(3,-1)	0.294641	0.289375	0.295341	0.300802	0.308585	0.292761	0.292844	0.292391	0.291380
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.349735	0.345334	0.347713	0.358555	0.349133	0.347481	0.346169		
(3,-1)	0.035096	0.033214	0.036107	0.035391	0.035234	0.035395	0.034680		
(3,-1)	0.295528	0.286178	0.295355	0.300326	0.295496	0.294411	0.293356		
(3,-1)	0.295541	0.286190	0.295367	0.300338	0.295509	0.294424	0.293368		
(3,-1)	0.294641	0.285446	0.294694	0.298822	0.294673	0.293694	0.292617		
(3,-1)	0.294641	0.285445	0.294693	0.298821	0.294672	0.293693	0.292616		

Table S175: Density value (a.u.) at the considered critical points for the [HCN]<sup>‡</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.481462	0.486616	0.487667	0.483748	0.484045	0.489394	0.485044	0.468869	0.470246
(3,-1)	0.204455	0.200308	0.203758	0.202878	0.205258	0.200578	0.203271	0.207243	0.207736
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.481462	0.464067	0.464062	0.487544	0.483679	0.472323	0.477651	0.479970	0.478193
(3,-1)	0.204455	0.203082	0.205667	0.204500	0.203840	0.204073	0.204274	0.205471	0.203179
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.481462	0.467049	0.480159	0.493487	0.491387	0.478433	0.482384	0.483734	0.486620
(3,-1)	0.204455	0.197578	0.202795	0.202617	0.198471	0.205804	0.204608	0.203193	0.202815
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.481462	0.468470	0.487828	0.484007	0.484949	0.482009	0.480339		
(3,-1)	0.204455	0.203317	0.200182	0.209787	0.203308	0.203003	0.200163		

Table S176: Density value (a.u.) at the considered critical points for the  $[\text{HOCH}_4]^\ddagger$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.142715	0.143324	0.144597	0.144717	0.144138	0.146921	0.143752	0.141775	0.144845
(3,-1)	0.191373	0.182434	0.189359	0.187154	0.190954	0.183954	0.189803	0.196567	0.195060
(3,-1)	0.289724	0.280363	0.287607	0.284483	0.288586	0.279953	0.288071	0.282705	0.277637
(3,-1)	0.289255	0.280061	0.287258	0.284145	0.288181	0.279714	0.287709	0.282353	0.277225
(3,-1)	0.289340	0.279930	0.287182	0.284060	0.288195	0.279417	0.287656	0.282366	0.277317
(3,-1)	0.372674	0.365453	0.376357	0.374437	0.377140	0.370623	0.378068	0.377978	0.367064
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.142715	0.143071	0.145318	0.143791	0.143688	0.143474	0.142219	0.143103	0.141951
(3,-1)	0.191373	0.187739	0.189990	0.190806	0.189388	0.192319	0.191987	0.192440	0.188231
(3,-1)	0.289724	0.280759	0.283635	0.288968	0.286476	0.285947	0.280900	0.288734	0.286404
(3,-1)	0.289255	0.280330	0.283228	0.288564	0.286069	0.285558	0.280523	0.288242	0.285916
(3,-1)	0.289340	0.280373	0.283224	0.288566	0.286083	0.285571	0.280555	0.288360	0.286029
(3,-1)	0.372674	0.361771	0.367057	0.376274	0.374936	0.377912	0.373744	0.378817	0.370793
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.142715	0.142074	0.141997	0.143328	0.141279	0.143345	0.143352	0.143617	0.143960
(3,-1)	0.191373	0.187916	0.188125	0.188093	0.180505	0.191349	0.190734	0.189833	0.188821
(3,-1)	0.289724	0.284255	0.290397	0.295606	0.303700	0.288056	0.287919	0.287330	0.286407
(3,-1)	0.289255	0.283883	0.289924	0.295166	0.303273	0.287535	0.287419	0.286872	0.285984
(3,-1)	0.289340	0.283871	0.290025	0.295214	0.303328	0.287700	0.287555	0.286957	0.286026
(3,-1)	0.372674	0.372692	0.371538	0.374530	0.370473	0.379517	0.378003	0.376933	0.374209
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.142715	0.141492	0.143789	0.137061	0.143860	0.143336	0.143040		
(3,-1)	0.191373	0.190464	0.185536	0.202525	0.189962	0.189854	0.187725		
(3,-1)	0.289724	0.280646	0.289537	0.293473	0.289681	0.288575	0.287567		
(3,-1)	0.289255	0.280173	0.288870	0.292796	0.289266	0.288136	0.287100		
(3,-1)	0.289340	0.280296	0.289194	0.293154	0.289276	0.288190	0.287173		
(3,-1)	0.372674	0.365588	0.379934	0.377905	0.373627	0.372451	0.370059		

Table S177: Density value (a.u.) at the considered critical points for the [HHO]<sup>‡</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.187897	0.187715	0.189828	0.190405	0.188270	0.190335	0.189191	0.190663	0.191142
(3,-1)	0.158458	0.153767	0.158863	0.157414	0.161015	0.156014	0.162840	0.162276	0.163254
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.187897	0.190992	0.192366	0.189076	0.189636	0.189031	0.189341	0.189474	0.189556
(3,-1)	0.158458	0.156374	0.154326	0.159327	0.158120	0.164576	0.161201	0.159393	0.158182
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.187897	0.187037	0.185108	0.184587	0.178062	0.188257	0.188099	0.188431	0.188526
(3,-1)	0.158458	0.158485	0.159506	0.160467	0.153351	0.161067	0.160539	0.160409	0.160003
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.187897	0.187093	0.185989	0.183689	0.189365	0.189413	0.188004		
(3,-1)	0.158458	0.161046	0.156597	0.162622	0.158205	0.157666	0.156479		

Table S178: Density value (a.u.) at the considered critical points for the  $[\text{HH}_2\text{S}]^\ddagger$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.222650	0.217007	0.221007	0.218848	0.221762	0.217865	0.220413	0.219250	0.217092
(3,-1)	0.177419	0.170351	0.174246	0.173145	0.175314	0.172642	0.174094	0.176628	0.180753
(3,-1)	0.085110	0.087072	0.088369	0.087892	0.088040	0.089507	0.087505	0.087751	0.088013
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.222650	0.217153	0.218524	0.222311	0.220556	0.220104	0.218577	0.221761	0.220505
(3,-1)	0.177419	0.171995	0.174590	0.175511	0.174884	0.174775	0.174502	0.176506	0.173609
(3,-1)	0.085110	0.087377	0.088361	0.087613	0.086872	0.084976	0.085726	0.086072	0.085569
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.222650	0.218305	0.222989	0.226280	0.234288	0.221148	0.221371	0.221082	0.220385
(3,-1)	0.177419	0.170237	0.175040	0.176235	0.172174	0.175768	0.175478	0.174580	0.174410
(3,-1)	0.085110	0.085877	0.084034	0.084701	0.082109	0.086011	0.086523	0.087118	0.087573
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.222650	0.217593	0.220745	0.226559	0.222588	0.221925	0.220460		
(3,-1)	0.177419	0.176120	0.173409	0.182612	0.176714	0.177034	0.175990		
(3,-1)	0.085110	0.084807	0.084407	0.082149	0.086217	0.085155	0.084662		

Table S179: Density value (a.u.) at the considered critical points for the  $(\text{NH}_3)_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.017358	0.019006	0.018495	0.018619	0.018022	0.017633	0.018138	0.017856	0.016742
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.017358	0.017120	0.017032	0.018154	0.018183	0.017593	0.017671	0.017910	0.017282
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.017358	0.017816	0.017261	0.017480	0.017605	0.017520	0.017640	0.017869	0.017940
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.017358	0.016980	0.017385	0.017021	0.017852	0.017727	0.017422		

Table S180: Density value (a.u.) at the considered critical points for the (HF)<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.017459	0.019094	0.018535	0.018567	0.017918	0.017025	0.018049	0.017700	0.017040
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.017459	0.017153	0.016948	0.018162	0.018096	0.017719	0.017874	0.017791	0.017548
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.017459	0.017738	0.017344	0.017608	0.017991	0.017687	0.017767	0.017942	0.017812
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.017459	0.017185	0.017649	0.016952	0.017893	0.017690	0.017486		

Table S181: Density value (a.u.) at the considered critical points for the  $(\text{H}_2\text{O})_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.026411	0.028311	0.027655	0.027845	0.027102	0.026886	0.027160	0.026509	0.025024
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.026411	0.025357	0.025532	0.027186	0.027239	0.026347	0.026216	0.026753	0.026418
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.026411	0.026476	0.026197	0.026522	0.027172	0.026774	0.026793	0.026934	0.026764
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.026411	0.025425	0.026318	0.025499	0.026906	0.026731	0.026450		



Table S182: Density value (a.u.) at the considered critical points for the  $\text{NH}_3 \cdots \text{H}_2\text{O}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.013366	0.014540	0.014011	0.014102	0.013639	0.012996	0.013655	0.013648	0.013144
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.013366	0.013020	0.012909	0.013789	0.013811	0.013652	0.013739	0.013691	0.013284
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.013366	0.013530	0.013326	0.013542	0.013704	0.013573	0.013590	0.013662	0.013551
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.013366	0.012994	0.013363	0.013060	0.013660	0.013580	0.013415		

Table S183: Density value (a.u.) at the considered critical points for the (HCONH<sub>2</sub>)<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.022387	0.024882	0.024277	0.024267	0.023076	0.021946	0.023351	0.023218	0.021956
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.022387	0.022064	0.021934	0.023488	0.023265	0.023308	0.023314	0.023267	0.023203
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.022387	0.022867	0.022413	0.022670	0.022394	0.023718	0.023495	0.023412	0.022822
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.022387	0.022273	0.023114	0.020877	0.023104	0.022576	0.022653		

Table S184: Density value (a.u.) at the considered critical points for the (HCOOH)<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.001283	0.001585	0.001574	0.001555	0.001382	0.002130	0.001448	0.001202	0.001036
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.001283	0.001151	0.001333	0.001471	0.001425	0.001442	0.001299	0.001331	0.001388
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.001283	0.001287	0.001348	0.001359	0.001377	0.001465	0.001394	0.001327	0.001383
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.001283	0.001196	0.001352	0.001195	0.001402	0.001306	0.001373		

Table S185: Density value (a.u.) at the considered critical points for the C<sub>2</sub>H<sub>4</sub>...F<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.001749	0.002152	0.002012	0.002005	0.001792	0.002047	0.001863	0.001573	0.001651
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.001749	0.001688	0.001853	0.001917	0.001872	0.001906	0.001726	0.001765	0.001928
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.001749	0.001809	0.001825	0.001872	0.001949	0.001969	0.001910	0.001791	0.001877
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.001749	0.001780	0.001832	0.001610	0.001873	0.001776	0.001879		

Table S186: Density value (a.u.) at the considered critical points for the  $\text{NH}_3 \cdots \text{F}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.007000	0.008477	0.007719	0.007870	0.007285	0.005805	0.007444	0.007600	0.007452
(3,-1)	0.042061	0.046341	0.045658	0.045928	0.044589	0.044945	0.044656	0.043603	0.040767
(3,-1)	0.042061	0.046341	0.045658	0.045928	0.044589	0.044945	0.044656	0.043603	0.040767
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.007000	0.007792	0.007863	0.007448	0.007484	0.006929	0.007818	0.007433	0.008103
(3,-1)	0.042061	0.041487	0.042160	0.044663	0.044668	0.042607	0.042444	0.043632	0.043601
(3,-1)	0.042061	0.041487	0.042160	0.044663	0.044668	0.042607	0.042444	0.043632	0.043601
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.007000	0.007560	0.007743	0.007804	0.007761	0.007846	0.007680	0.007572	0.007126
(3,-1)	0.042061	0.043387	0.043866	0.044108	0.045741	0.043964	0.043910	0.044092	0.044015
(3,-1)	0.042061	0.043387	0.043866	0.044108	0.045741	0.043964	0.043910	0.044092	0.044015
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.007000	0.007522	0.007734	0.006431	0.007551	0.007439	0.007507		
(3,-1)	0.042061	0.041994	0.043899	0.041190	0.044187	0.043744	0.043425		
(3,-1)	0.042061	0.041994	0.043899	0.041190	0.044187	0.043744	0.043425		

Table S187: Density value (a.u.) at the considered critical points for the C<sub>2</sub>H<sub>2</sub>···ClF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.022956	0.024849	0.024308	0.024521	0.023813	0.024258	0.023927	0.023312	0.021851
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.022956	0.022439	0.022491	0.023884	0.023981	0.022781	0.022844	0.023431	0.022590
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.022956	0.023430	0.023041	0.023257	0.023536	0.022878	0.023103	0.023449	0.023716
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.022956	0.022436	0.023014	0.022430	0.023544	0.023434	0.022994		

Table S188: Density value (a.u.) at the considered critical points for the HCN...ClF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.054407	0.057774	0.056255	0.057372	0.056427	0.059998	0.056130	0.054344	0.051622
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.054407	0.054169	0.055408	0.055833	0.056745	0.054236	0.053660	0.055665	0.053931
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.054407	0.055835	0.056278	0.056872	0.057896	0.054216	0.054761	0.055450	0.056817
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.054407	0.054642	0.055994	0.052413	0.055649	0.055951	0.054982		

Table S189: Density value (a.u.) at the considered critical points for the  $\text{NH}_3 \cdots \text{Cl}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.023848	0.026309	0.025248	0.025653	0.024888	0.025261	0.024929	0.024175	0.023198
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.023848	0.023529	0.023597	0.024848	0.025104	0.024148	0.023924	0.024225	0.024088
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.023848	0.024163	0.023953	0.024741	0.025433	0.023926	0.024060	0.024403	0.024704
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.023848	0.023520	0.024321	0.022975	0.024604	0.024569	0.024105		



Table S190: Density value (a.u.) at the considered critical points for the H<sub>2</sub>O...ClF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.018141	0.020306	0.019389	0.019758	0.019258	0.019363	0.019354	0.018342	0.017840
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.018141	0.018366	0.018530	0.019191	0.019481	0.018636	0.018696	0.018892	0.018812
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.018141	0.018740	0.018508	0.019291	0.020015	0.018487	0.018590	0.018855	0.019163
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.018141	0.018301	0.018624	0.018161	0.018826	0.018924	0.018442		

Table S191: Density value (a.u.) at the considered critical points for the  $\text{NH}_3 \cdots \text{ClF}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.002076	0.002402	0.002422	0.002362	0.002136	0.002755	0.002206	0.001915	0.001815
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.002076	0.001979	0.002161	0.002292	0.002202	0.002231	0.002049	0.002096	0.002185
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.002076	0.002111	0.002125	0.002175	0.002205	0.002247	0.002196	0.002108	0.002189
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.002076	0.002051	0.002159	0.001971	0.002224	0.002084	0.002205		

Table S192: Density value (a.u.) at the considered critical points for the  $(\text{H}_2\text{S})_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.004601	0.005181	0.004869	0.004828	0.004631	0.003610	0.004687	0.004667	0.004714
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.004601	0.004881	0.004776	0.004802	0.004732	0.004542	0.004854	0.004996	0.004911
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.004601	0.005004	0.004815	0.004768	0.004669	0.004957	0.004880	0.004795	0.004728
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.004601	0.004868	0.004673	0.004549	0.004782	0.004688	0.004692		

Table S193: Density value (a.u.) at the considered critical points for the (HCl)<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.022874	0.025524	0.024191	0.024610	0.023624	0.023374	0.023874	0.023288	0.022198
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.022874	0.022353	0.022590	0.023652	0.023877	0.023474	0.023418	0.023122	0.023539
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.022874	0.023158	0.023080	0.023625	0.023872	0.023263	0.023238	0.023410	0.023524
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.022874	0.022551	0.023376	0.021485	0.023460	0.023384	0.023068		

Table S194: Density value (a.u.) at the considered critical points for the HCl...H<sub>2</sub>S system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+3)	0.002698	0.003290	0.002919	0.002953	0.002763	0.002250	0.002837	0.002618	0.002633
(3,+1)	0.003436	0.004020	0.003672	0.003677	0.003497	0.002825	0.003543	0.003444	0.003555
(3,+1)	0.003436	0.004020	0.003672	0.003677	0.003497	0.002825	0.003543	0.003444	0.003555
(3,+1)	0.003436	0.004020	0.003672	0.003677	0.003497	0.002825	0.003543	0.003444	0.003555
(3,+1)	0.003436	0.004020	0.003672	0.003677	0.003497	0.002825	0.003543	0.003444	0.003555
(3,-1)	0.003952	0.004514	0.004178	0.004163	0.003981	0.003227	0.004023	0.004032	0.004207
(3,-1)	0.003952	0.004514	0.004178	0.004163	0.003981	0.003227	0.004023	0.004032	0.004207
(3,-1)	0.003956	0.004519	0.004183	0.004168	0.003985	0.003231	0.004027	0.004037	0.004212
(3,-1)	0.003956	0.004519	0.004183	0.004168	0.003985	0.003231	0.004027	0.004037	0.004212
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+3)	0.002698	0.002968	0.003035	0.002870	0.002868	0.002722	0.002949	0.002988	0.003185
(3,+1)	0.003436	0.003812	0.003823	0.003631	0.003607	0.003494	0.003768	0.003804	0.003931
(3,+1)	0.003436	0.003812	0.003823	0.003631	0.003607	0.003494	0.003768	0.003804	0.003931
(3,+1)	0.003436	0.003812	0.003823	0.003631	0.003607	0.003494	0.003768	0.003804	0.003931
(3,+1)	0.003436	0.003812	0.003823	0.003631	0.003607	0.003494	0.003768	0.003804	0.003931
(3,-1)	0.003952	0.004401	0.004360	0.004139	0.004095	0.004039	0.004349	0.004357	0.004421
(3,-1)	0.003952	0.004401	0.004360	0.004139	0.004095	0.004039	0.004349	0.004357	0.004421
(3,-1)	0.003956	0.004406	0.004364	0.004144	0.004100	0.004044	0.004354	0.004362	0.004426
(3,-1)	0.003956	0.004406	0.004364	0.004144	0.004100	0.004044	0.004354	0.004362	0.004426
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+3)	0.002698	0.003064	0.003094	0.002988	0.003120	0.003123	0.003044	0.002944	0.002868
(3,+1)	0.003436	0.003879	0.003844	0.003742	0.003834	0.003902	0.003812	0.003694	0.003609
(3,+1)	0.003436	0.003879	0.003844	0.003742	0.003834	0.003902	0.003812	0.003694	0.003609
(3,+1)	0.003436	0.003879	0.003844	0.003742	0.003834	0.003902	0.003812	0.003694	0.003609
(3,+1)	0.003436	0.003879	0.003844	0.003742	0.003834	0.003902	0.003812	0.003694	0.003609
(3,-1)	0.003952	0.004434	0.004364	0.004228	0.004280	0.004447	0.004344	0.004207	0.004103
(3,-1)	0.003952	0.004434	0.004364	0.004228	0.004280	0.004447	0.004344	0.004207	0.004103
(3,-1)	0.003956	0.004439	0.004369	0.004233	0.004284	0.004452	0.004349	0.004212	0.004108
(3,-1)	0.003956	0.004439	0.004369	0.004233	0.004284	0.004452	0.004349	0.004212	0.004108
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+3)	0.002698	0.002913	0.002942	0.002619	0.002884	0.002845	0.002887		
(3,+1)	0.003436	0.003765	0.003728	0.003447	0.003648	0.003598	0.003646		
(3,+1)	0.003436	0.003765	0.003728	0.003447	0.003648	0.003598	0.003646		
(3,+1)	0.003436	0.003765	0.003728	0.003447	0.003648	0.003598	0.003646		
(3,+1)	0.003436	0.003765	0.003728	0.003447	0.003648	0.003598	0.003646		
(3,-1)	0.003952	0.004373	0.004257	0.003971	0.004166	0.004101	0.004162		
(3,-1)	0.003952	0.004373	0.004257	0.003971	0.004166	0.004101	0.004162		
(3,-1)	0.003956	0.004378	0.004261	0.003975	0.004171	0.004105	0.004167		
(3,-1)	0.003956	0.004378	0.004261	0.003975	0.004171	0.004105	0.004167		

Table S195: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>Cl···HCl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.001983	0.002383	0.002427	0.002378	0.002095	0.003001	0.002190	0.001882	0.001648
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.001983	0.001937	0.002082	0.002250	0.002161	0.002188	0.001984	0.002025	0.002128
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.001983	0.001999	0.002033	0.002054	0.002067	0.002249	0.002140	0.002033	0.002127
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.001983	0.001963	0.002098	0.001786	0.002169	0.002008	0.002144		

Table S196: Density value (a.u.) at the considered critical points for the HCN $\cdots$ CH<sub>3</sub>SH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.004271	0.005242	0.004740	0.004780	0.004389	0.003112	0.004527	0.004612	0.004469
(3,-1)	0.030146	0.033294	0.032522	0.032661	0.031681	0.031024	0.031841	0.031113	0.029648
(3,-1)	0.030146	0.033294	0.032522	0.032661	0.031681	0.031024	0.031841	0.031113	0.029648
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.004271	0.004869	0.005045	0.004564	0.004531	0.004327	0.005013	0.004721	0.005040
(3,-1)	0.030146	0.029873	0.029937	0.031887	0.031844	0.030930	0.030889	0.031253	0.031344
(3,-1)	0.030146	0.029873	0.029937	0.031887	0.031844	0.030930	0.030889	0.031253	0.031344
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.004271	0.004891	0.004917	0.004712	0.004707	0.004974	0.004818	0.004688	0.004381
(3,-1)	0.030146	0.030928	0.030644	0.030903	0.031997	0.031529	0.031481	0.031612	0.031349
(3,-1)	0.030146	0.030928	0.030644	0.030903	0.031997	0.031529	0.031481	0.031612	0.031349
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.004271	0.004664	0.004708	0.003930	0.004634	0.004514	0.004601		
(3,-1)	0.030146	0.030142	0.031328	0.029617	0.031615	0.031306	0.031106		
(3,-1)	0.030146	0.030142	0.031328	0.029617	0.031615	0.031306	0.031106		

Table S197: Density value (a.u.) at the considered critical points for the CH<sub>3</sub>SH...HCl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.024236	0.027415	0.026173	0.026572	0.025379	0.025297	0.025767	0.024949	0.024040
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.024236	0.024335	0.024303	0.025449	0.025610	0.024942	0.024794	0.024763	0.025100
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.024236	0.024666	0.024491	0.025168	0.025795	0.024867	0.024882	0.025132	0.025247
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.024236	0.024377	0.025181	0.022670	0.025093	0.024871	0.024564		



Table S198: Density value (a.u.) at the considered critical points for the HeNe system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.012580	0.013940	0.013486	0.013445	0.012910	0.011487	0.013056	0.013054	0.012542
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.012580	0.012655	0.012376	0.013189	0.013068	0.013010	0.013258	0.013117	0.012831
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.012580	0.013048	0.012598	0.012760	0.012638	0.012993	0.013007	0.013085	0.012932
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.012580	0.012629	0.012797	0.012244	0.012955	0.012735	0.012646		

Table S199: Density value (a.u.) at the considered critical points for the HeAr system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.009689	0.010714	0.010338	0.010321	0.009955	0.008485	0.009986	0.010178	0.009771
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.009689	0.009847	0.009532	0.010143	0.010074	0.010074	0.010269	0.010186	0.009811
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.009689	0.009960	0.009723	0.009879	0.009744	0.009983	0.009974	0.010032	0.009923
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.009689	0.009715	0.009886	0.009555	0.009984	0.009852	0.009741		

Table S200: Density value (a.u.) at the considered critical points for the Ne<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.001245	0.001475	0.001459	0.001428	0.001301	0.001809	0.001353	0.001133	0.001033
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.001245	0.001088	0.001281	0.001390	0.001340	0.001357	0.001244	0.001268	0.001328
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.001245	0.001260	0.001307	0.001336	0.001361	0.001349	0.001322	0.001272	0.001322
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.001245	0.001161	0.001295	0.001224	0.001333	0.001252	0.001309		

Table S201: Density value (a.u.) at the considered critical points for the NeAr system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.022604	0.024572	0.023927	0.023967	0.023107	0.022038	0.023306	0.022944	0.022021
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.022604	0.022097	0.021944	0.023381	0.023268	0.023090	0.023061	0.023115	0.023056
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.022604	0.022717	0.022340	0.022591	0.022862	0.023335	0.023234	0.023263	0.022872
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.022604	0.022200	0.022948	0.021494	0.023113	0.022784	0.022683		

Table S202: Density value (a.u.) at the considered critical points for the CH<sub>4</sub>···Ne system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.007025	0.008152	0.007879	0.007761	0.007410	0.006661	0.007637	0.007178	0.006822
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.007025	0.007239	0.007196	0.007717	0.007557	0.007087	0.007249	0.007574	0.007474
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.007025	0.007703	0.007564	0.007622	0.008035	0.007493	0.007448	0.007392	0.007570
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.007025	0.007249	0.007432	0.007499	0.007462	0.007320	0.007287		

Table S203: Density value (a.u.) at the considered critical points for the  $(\text{CH}_4)_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.002756	0.003314	0.002895	0.002933	0.002733	0.002138	0.002787	0.002569	0.002882
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.002756	0.002917	0.002934	0.002852	0.002850	0.002781	0.003021	0.003063	0.003069
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.002756	0.003203	0.003099	0.002990	0.003234	0.003115	0.003037	0.002913	0.002882
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.002756	0.003052	0.002911	0.002594	0.002842	0.002801	0.002857		

Table S204: Density value (a.u.) at the considered critical points for the  $(\text{C}_2\text{H}_2)_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.011983	0.013997	0.013525	0.013394	0.012665	0.011752	0.013104	0.012993	0.011840
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.011983	0.012272	0.012126	0.013090	0.012823	0.012327	0.012566	0.012811	0.012596
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.011983	0.012962	0.012718	0.012779	0.013092	0.012718	0.012673	0.012701	0.012793
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.011983	0.012327	0.012916	0.011901	0.012658	0.012297	0.012276		

Table S205: Density value (a.u.) at the considered critical points for the  $(C_2H_4)_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.014387	0.015574	0.015044	0.015059	0.014585	0.013105	0.014701	0.014735	0.014128
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.014387	0.014098	0.013904	0.014797	0.014734	0.014681	0.014808	0.014832	0.014532
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.014387	0.014607	0.014312	0.014452	0.014588	0.014897	0.014813	0.014816	0.014506
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.014387	0.014118	0.014614	0.013926	0.014662	0.014501	0.014407		



Table S206: Laplacian of the density value (a.u.) at the considered critical points for the SiH<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.197984	0.074095	0.113201	0.123944	0.153519	0.173892	0.129609	0.180569	0.226824
(3,-1)	0.197980	0.074092	0.113196	0.123940	0.153516	0.173909	0.129594	0.180573	0.226885
(3,-1)	0.197988	0.074098	0.113204	0.123950	0.153522	0.173901	0.129654	0.180625	0.226909
(3,-1)	0.197988	0.074098	0.113204	0.123950	0.153522	0.173901	0.129654	0.180625	0.226909
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.197984	0.211112	0.227465	0.128251	0.144627	0.146781	0.123390	0.184276	0.140130
(3,-1)	0.197980	0.211118	0.227482	0.128246	0.144624	0.146773	0.123401	0.184274	0.140140
(3,-1)	0.197988	0.211140	0.227485	0.128254	0.144633	0.146824	0.123432	0.184281	0.140146
(3,-1)	0.197988	0.211140	0.227485	0.128254	0.144633	0.146824	0.123432	0.184281	0.140146
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.197984	0.192541	0.192836	0.157170	0.271192	0.130959	0.136407	0.145851	0.144591
(3,-1)	0.197980	0.192520	0.192851	0.157163	0.271186	0.130946	0.136395	0.145842	0.144592
(3,-1)	0.197988	0.192517	0.192893	0.157163	0.271109	0.130979	0.136432	0.145897	0.144602
(3,-1)	0.197988	0.192517	0.192893	0.157163	0.271109	0.130979	0.136432	0.145897	0.144602
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.197984	0.210360	0.102212	0.215060	0.156573	0.178538	0.130958		
(3,-1)	0.197980	0.210367	0.102233	0.215056	0.156569	0.178536	0.109456		
(3,-1)	0.197988	0.210391	0.102232	0.215063	0.156576	0.178544	0.109789		
(3,-1)	0.197988	0.210391	0.102232	0.215063	0.156576	0.178544	0.109789		

Table S207: Laplacian of the density value (a.u.) at the considered critical points for the S<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.308550	-0.259128	-0.279587	-0.267815	-0.291135	-0.305319	-0.249819	-0.214925	-0.305825
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.308550	-0.327046	-0.351705	-0.295241	-0.287728	-0.179640	-0.207890	-0.326617	-0.303955
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.308550	-0.197627	-0.296338	-0.338331	-0.410673	-0.284011	-0.295212	-0.298494	-0.282430
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.308550	-0.321762	-0.256314	-0.362189	-0.296990	-0.298508	-0.840109		

Table S208: Laplacian of the density value (a.u.) at the considered critical points for the SiO system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	1.607927	1.424111	1.467401	1.475747	1.530020	1.559989	1.440087	1.569823	1.727246
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	1.607927	1.568133	1.672807	1.501762	1.520639	1.459560	1.454291	1.597998	1.482876
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	1.607927	1.518293	1.593449	1.549983	1.625850	1.488442	1.500172	1.502890	1.456790
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	1.607927	1.566965	1.517336	1.652260	1.540190	1.572351	1.488442		

Table S209: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>3</sub>H<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.308255	-1.259446	-1.295039	-1.257526	-1.258157	-1.280961	-1.305741	-1.154483	-1.296756
(3,-1)	-0.792153	-0.680523	-0.732637	-0.703477	-0.756412	-0.777131	-0.686510	-0.759884	-0.747047
(3,-1)	-1.276215	-1.194626	-1.233212	-1.195054	-1.246124	-1.260938	-1.210821	-1.076919	-1.051798
(3,-1)	-1.140325	-1.048544	-1.098108	-1.060424	-1.106821	-1.114925	-1.071524	-0.987804	-0.890841
(3,-1)	-1.140332	-1.048550	-1.098114	-1.060430	-1.106826	-1.114930	-1.071369	-0.987794	-0.890837
(3,-1)	-1.140332	-1.048550	-1.098114	-1.060430	-1.106826	-1.114930	-1.071369	-0.987794	-0.890837
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.308255	-1.259353	-0.930899	-1.299379	-1.269767	-1.241162	-1.197880	-1.303282	-1.201802
(3,-1)	-0.792153	-0.703279	-0.742614	-0.761357	-0.742191	-0.711564	-0.734504	-0.823473	-0.718327
(3,-1)	-1.276215	-1.147911	-1.203636	-1.260264	-1.230876	-1.183187	-1.056264	-1.299961	-1.223322
(3,-1)	-1.140325	-1.007228	-1.063323	-1.118924	-1.088767	-1.051133	-0.957648	-1.147253	-1.077804
(3,-1)	-1.140332	-1.007240	-1.063328	-1.118930	-1.088773	-1.051107	-0.957624	-1.147259	-1.077809
(3,-1)	-1.140332	-1.007240	-1.063328	-1.118930	-1.088773	-1.051107	-0.957624	-1.147259	-1.077809
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.308255	-1.459381	-1.326769	-1.452729	-1.498917	-1.136151	-1.209490	-1.296756	-1.243008
(3,-1)	-0.792153	-0.639630	-0.773535	-0.803776	-0.784657	-0.743594	-0.749515	-0.740785	-0.715220
(3,-1)	-1.276215	-1.163592	-1.345004	-1.440967	-1.671623	-1.241061	-1.242257	-1.232297	-1.203249
(3,-1)	-1.140325	-1.050028	-1.177741	-1.267955	-1.457324	-1.101826	-1.100814	-1.089090	-1.063694
(3,-1)	-1.140332	-1.050166	-1.177681	-1.267982	-1.457481	-1.101766	-1.100731	-1.088947	-1.063711
(3,-1)	-1.140332	-1.050166	-1.177681	-1.267982	-1.457481	-1.101766	-1.100731	-1.088947	-1.063711
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.308255	-1.305216	-1.274534	-1.344068	-1.304346	-1.285678	-1.136151		
(3,-1)	-0.792153	-0.724105	-0.765237	-0.902716	-0.772542	-0.772501	-0.743594		
(3,-1)	-1.276215	-1.121988	-1.369822	-1.358585	-1.271629	-1.264178	-1.241060		
(3,-1)	-1.140325	-0.978669	-1.165465	-1.202402	-1.134228	-1.122696	-1.101826		
(3,-1)	-1.140332	-0.978678	-1.165556	-1.202408	-1.134234	-1.122702	-1.101766		
(3,-1)	-1.140332	-0.978678	-1.165556	-1.202408	-1.134234	-1.122702	-1.101766		

Table S210: Laplacian of the density value (a.u.) at the considered critical points for the HCOCOH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.768703	-0.638020	-0.683636	-0.660222	-0.727860	-0.765086	-0.646871	-0.751880	-0.687886
(3,-1)	0.026255	-0.332868	-0.309268	-0.210896	-0.088301	0.100241	-0.200417	0.242241	0.568954
(3,-1)	-1.210864	-1.112213	-1.157128	-1.120438	-1.177809	-1.200833	-1.142078	-1.013962	-0.885621
(3,-1)	0.026255	-0.332868	-0.309268	-0.210896	-0.088301	0.100241	-0.200417	0.242241	0.568954
(3,-1)	-1.210864	-1.112213	-1.157128	-1.120438	-1.177809	-1.200833	-1.142078	-1.013962	-0.885621
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.768703	-0.650410	-0.710243	-0.726040	-0.714125	-0.756988	-0.741806	-0.814119	-0.690988
(3,-1)	0.026255	0.421449	0.660385	-0.234807	-0.117617	-0.033590	-0.183308	0.041052	-0.090666
(3,-1)	-1.210864	-1.076122	-1.157587	-1.188743	-1.161069	-1.123468	-0.997756	-1.238137	-1.166906
(3,-1)	0.026255	0.421449	0.660385	-0.234807	-0.117617	-0.033590	-0.183308	0.041052	-0.090666
(3,-1)	-1.210864	-1.076122	-1.157587	-1.188743	-1.161069	-1.123468	-0.997756	-1.238137	-1.166906
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.768703	-0.639416	-0.761818	-0.783670	-0.731550	-0.736049	-0.731870	-0.712111	-0.687394
(3,-1)	0.026255	0.222502	0.030958	-0.239870	-0.117613	-0.050570	-0.113840	-0.121747	-0.321115
(3,-1)	-1.210864	-1.119188	-1.246160	-1.348274	-1.494168	-1.187740	-1.182566	-1.165627	-1.141462
(3,-1)	0.026255	0.222502	0.030958	-0.239870	-0.117613	-0.050570	-0.113840	-0.121747	-0.321115
(3,-1)	-1.210864	-1.119188	-1.246160	-1.348274	-1.494168	-1.187740	-1.182566	-1.165627	-1.141462
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.768703	-0.671085	-0.741443	-0.897811	-0.741153	-0.751632	-0.736048		
(3,-1)	0.026255	0.317786	-0.230534	0.136727	-0.141337	-0.016676	-0.050570		
(3,-1)	-1.210864	-1.030894	-1.263707	-1.302858	-1.202551	-1.197557	-1.187739		
(3,-1)	0.026255	0.317786	-0.230534	0.136727	-0.141337	-0.016676	-0.050570		
(3,-1)	-1.210864	-1.030894	-1.263707	-1.302858	-1.202551	-1.197557	-1.187739		

Table S211: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>8</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.337807	0.314638	0.330606	0.318734	0.326969	0.323584	0.304109	0.315966	0.405126
(3,-1)	-0.585674	-0.501898	-0.545415	-0.522486	-0.567212	-0.588761	-0.501159	-0.570025	-0.574426
(3,-1)	-0.585674	-0.501898	-0.545415	-0.522486	-0.567212	-0.588761	-0.501159	-0.570025	-0.574426
(3,-1)	-0.585674	-0.501898	-0.545415	-0.522486	-0.567212	-0.588761	-0.501159	-0.570025	-0.574426
(3,-1)	-0.585674	-0.501898	-0.545415	-0.522486	-0.567212	-0.588761	-0.501159	-0.570025	-0.574426
(3,-1)	-1.146476	-1.060251	-1.103983	-1.069004	-1.114642	-1.124006	-1.079880	-0.999096	-0.886296
(3,-1)	-1.127242	-1.041252	-1.085437	-1.050630	-1.095685	-1.102990	-1.060866	-0.986124	-0.872250
(3,-1)	-1.146476	-1.060251	-1.103983	-1.069004	-1.114642	-1.124006	-1.079880	-0.999096	-0.886296
(3,-1)	-1.127242	-1.041252	-1.085437	-1.050630	-1.095685	-1.102990	-1.060866	-0.986124	-0.872250
(3,-1)	-1.146476	-1.060251	-1.103983	-1.069004	-1.114642	-1.124006	-1.079880	-0.999096	-0.886296
(3,-1)	-1.127242	-1.041252	-1.085437	-1.050630	-1.095685	-1.102990	-1.060866	-0.986124	-0.872250
(3,-1)	-1.146476	-1.060251	-1.103983	-1.069004	-1.114642	-1.124006	-1.079880	-0.999096	-0.886296
(3,-1)	-1.127242	-1.041252	-1.085437	-1.050630	-1.095685	-1.102990	-1.060866	-0.986124	-0.872250
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.337807	0.354369	0.336960	0.331633	0.321542	0.290639	0.318498	0.330663	0.337761
(3,-1)	-0.585674	-0.549668	-0.583478	-0.569497	-0.554280	-0.509265	-0.547356	-0.619355	-0.541153
(3,-1)	-0.585674	-0.549668	-0.583478	-0.569497	-0.554280	-0.509265	-0.547356	-0.619355	-0.541153
(3,-1)	-0.585674	-0.549668	-0.583478	-0.569497	-0.554280	-0.509265	-0.547356	-0.619355	-0.541153
(3,-1)	-0.585674	-0.549668	-0.583478	-0.569497	-0.554280	-0.509265	-0.547356	-0.619355	-0.541153
(3,-1)	-1.146476	-1.022339	-1.068214	-1.125297	-1.097651	-1.060962	-0.973807	-1.154926	-1.085556
(3,-1)	-1.127242	-1.000750	-1.047188	-1.106046	-1.078398	-1.044369	-0.958937	-1.134273	-1.065272
(3,-1)	-1.146476	-1.022339	-1.068214	-1.125297	-1.097651	-1.060962	-0.973807	-1.154926	-1.085556
(3,-1)	-1.127242	-1.000750	-1.047188	-1.106046	-1.078398	-1.044369	-0.958937	-1.134273	-1.065272
(3,-1)	-1.146476	-1.022339	-1.068214	-1.125297	-1.097651	-1.060962	-0.973807	-1.154926	-1.085556
(3,-1)	-1.127242	-1.000750	-1.047188	-1.106046	-1.078398	-1.044369	-0.958937	-1.134273	-1.065272
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.337807	0.282195	0.304156	0.316402	0.298638	0.308727	0.314147	0.313210	0.310710
(3,-1)	-0.585674	-0.465405	-0.553057	-0.584382	-0.546260	-0.558313	-0.560763	-0.548704	-0.534926
(3,-1)	-0.585674	-0.465405	-0.553057	-0.584382	-0.546260	-0.558313	-0.560763	-0.548704	-0.534926
(3,-1)	-0.585674	-0.465405	-0.553057	-0.584382	-0.546260	-0.558313	-0.560763	-0.548704	-0.534926
(3,-1)	-0.585674	-0.465405	-0.553057	-0.584382	-0.546260	-0.558313	-0.560763	-0.548704	-0.534926
(3,-1)	-1.146476	-1.058989	-1.181787	-1.274732	-1.460112	-1.109095	-1.107891	-1.097504	-1.073363
(3,-1)	-1.127242	-1.040893	-1.163236	-1.253687	-1.442853	-1.089477	-1.088105	-1.077609	-1.053239
(3,-1)	-1.146476	-1.058989	-1.181787	-1.274732	-1.460112	-1.109095	-1.107891	-1.097504	-1.073363
(3,-1)	-1.127242	-1.040893	-1.163236	-1.253687	-1.442853	-1.089477	-1.088105	-1.077609	-1.053239
(3,-1)	-1.146476	-1.058989	-1.181787	-1.274732	-1.460112	-1.109095	-1.107891	-1.097504	-1.073363
(3,-1)	-1.127242	-1.040893	-1.163236	-1.253687	-1.442853	-1.089477	-1.088105	-1.077609	-1.053239
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.337807	0.339122	0.295348	0.342449	0.332617	0.326490	0.308727		
(3,-1)	-0.585674	-0.549348	-0.528686	-0.680707	-0.575883	-0.575709	-0.558313		
(3,-1)	-0.585674	-0.549348	-0.528686	-0.680707	-0.575883	-0.575709	-0.558313		
(3,-1)	-0.585674	-0.549348	-0.528686	-0.680707	-0.575883	-0.575709	-0.558313		
(3,-1)	-0.585674	-0.549348	-0.528686	-0.680707	-0.575883	-0.575709	-0.558313		
(3,-1)	-1.146476	-0.989655	-1.171864	-1.206985	-1.140149	-1.130588	-1.109095		
(3,-1)	-1.127242	-0.969980	-1.145658	-1.185529	-1.120839	-1.110912	-1.089477		
(3,-1)	-1.146476	-0.989655	-1.171864	-1.206985	-1.140149	-1.130588	-1.109095		
(3,-1)	-1.127242	-0.969980	-1.145658	-1.185529	-1.120839	-1.110912	-1.089477		
(3,-1)	-1.146476	-0.989655	-1.171864	-1.206985	-1.140149	-1.130588	-1.109095		
(3,-1)	-1.127242	-0.969980	-1.145658	-1.185529	-1.120839	-1.110912	-1.089477		
(3,-1)	-1.146476	-0.989655	-1.171864	-1.206985	-1.140149	-1.130588	-1.109095		
(3,-1)	-1.127242	-0.969980	-1.145658	-1.185529	-1.120839	-1.110912	-1.089477		

Table S212: Laplacian of the density value (a.u.) at the considered critical points for the [H<sub>3</sub>CHOH]<sup>‡</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.041461	-0.079506	-0.051172	-0.062195	-0.051120	-0.041298	-0.046564	-0.016166	-0.102890
(3,-1)	-0.532584	-0.486611	-0.517180	-0.500240	-0.529941	-0.534017	-0.504453	-0.592026	-0.571377
(3,-1)	-1.159192	-1.072103	-1.119432	-1.081720	-1.126933	-1.132381	-1.093090	-0.998501	-0.905950
(3,-1)	-1.154224	-1.067649	-1.115205	-1.077725	-1.122434	-1.126759	-1.088571	-0.995320	-0.901420
(3,-1)	-1.156452	-1.069357	-1.116520	-1.078849	-1.124188	-1.129831	-1.090285	-0.996876	-0.904797
(3,-1)	-2.742307	-2.658606	-2.625695	-2.618292	-2.702899	-2.822519	-2.695198	-2.707308	-2.793892
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.041461	-0.056811	-0.050463	-0.048158	-0.055131	-0.048801	-0.039259	-0.041298	-0.013172
(3,-1)	-0.532584	-0.430960	-0.480521	-0.530537	-0.518118	-0.565066	-0.546750	-0.534017	-0.469102
(3,-1)	-1.159192	-1.021258	-1.081624	-1.138772	-1.108114	-1.071483	-0.969699	-1.132381	-1.102144
(3,-1)	-1.154224	-1.016436	-1.077177	-1.134062	-1.103548	-1.066977	-0.966294	-1.126759	-1.096879
(3,-1)	-1.156452	-1.018767	-1.078458	-1.135992	-1.105395	-1.069200	-0.967997	-1.129831	-1.099433
(3,-1)	-2.742307	-2.608395	-2.547137	-2.707046	-2.713845	-2.700287	-2.601793	-2.822519	-2.429466
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.041461	-0.031578	-0.018058	-0.048402	-0.009833	-0.042335	-0.046831	-0.053373	-0.057457
(3,-1)	-0.532584	-0.480181	-0.520991	-0.543745	-0.457290	-0.532174	-0.525887	-0.515036	-0.500109
(3,-1)	-1.159192	-1.065163	-1.202321	-1.292463	-1.480369	-1.123845	-1.120966	-1.107865	-1.082959
(3,-1)	-1.154224	-1.061515	-1.196957	-1.287447	-1.475726	-1.118262	-1.115518	-1.102742	-1.078099
(3,-1)	-1.156452	-1.062502	-1.199626	-1.289479	-1.477322	-1.121377	-1.118457	-1.105312	-1.080437
(3,-1)	-2.742307	-2.671278	-2.641572	-2.728786	-2.807134	-2.786824	-2.777104	-2.756110	-2.695213
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.041461	-0.023681	-0.059535	0.020410	-0.055794	-0.057645	-0.042335		
(3,-1)	-0.532584	-0.500607	-0.508851	-0.600467	-0.530614	-0.528385	-0.532173		
(3,-1)	-1.159192	-0.995304	-1.197489	-1.208166	-1.156046	-1.143522	-1.123845		
(3,-1)	-1.154224	-0.990329	-1.188092	-1.201798	-1.151214	-1.138556	-1.118262		
(3,-1)	-1.156452	-0.993288	-1.195199	-1.205734	-1.153208	-1.140815	-1.121376		
(3,-1)	-2.742307	-2.657748	-2.982714	-2.993784	-2.729331	-2.773087	-2.786823		

Table S213: Laplacian of the density value (a.u.) at the considered critical points for the [HHO]<sup>‡</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.310732	-0.339017	-0.319584	-0.331042	-0.312529	-0.330607	-0.301484	-0.348794	-0.379383
(3,-1)	-0.480377	-0.467233	-0.482688	-0.474005	-0.496887	-0.503154	-0.509662	-0.526093	-0.582024
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.310732	-0.337728	-0.345425	-0.322157	-0.333172	-0.321885	-0.331523	-0.330607	-0.278413
(3,-1)	-0.480377	-0.466000	-0.412346	-0.488797	-0.480432	-0.569828	-0.510406	-0.503154	-0.474453
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.310732	-0.287450	-0.245920	-0.253336	-0.144461	-0.314469	-0.318331	-0.324584	-0.319513
(3,-1)	-0.480377	-0.483951	-0.499645	-0.526658	-0.417520	-0.518864	-0.508862	-0.504079	-0.483795
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.310732	-0.291104	-0.275150	-0.274627	-0.333760	-0.342331	-0.314469		
(3,-1)	-0.480377	-0.521159	-0.499980	-0.503962	-0.484628	-0.481494	-0.518864		



Table S214: Laplacian of the density value (a.u.) at the considered critical points for the [HSHH]<sup>‡</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.689293	-0.633051	-0.658572	-0.636194	-0.664978	-0.667804	-0.630702	-0.645911	-0.569292
(3,-1)	-0.419163	-0.374940	-0.392912	-0.379943	-0.403451	-0.398039	-0.357936	-0.412796	-0.440889
(3,-1)	-0.072510	-0.096815	-0.085603	-0.091701	-0.089179	-0.086571	-0.084863	-0.076353	-0.103984
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.689293	-0.619495	-0.648917	-0.674528	-0.656685	-0.648191	-0.627012	-0.667804	-0.650385
(3,-1)	-0.419163	-0.325024	-0.365358	-0.405501	-0.396286	-0.399741	-0.390245	-0.398039	-0.347654
(3,-1)	-0.072510	-0.104363	-0.107109	-0.084495	-0.088108	-0.051742	-0.058414	-0.086571	-0.083634
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.689293	-0.630194	-0.700760	-0.742289	-0.831406	-0.657780	-0.661321	-0.656122	-0.643457
(3,-1)	-0.419163	-0.323519	-0.416368	-0.442121	-0.397700	-0.393848	-0.398416	-0.388724	-0.377249
(3,-1)	-0.072510	-0.080058	-0.056349	-0.064739	-0.055076	-0.083682	-0.086477	-0.088884	-0.089293
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.689293	-0.611941	-0.673053	-0.738156	-0.683984	-0.678378	-0.657779		
(3,-1)	-0.419163	-0.378749	-0.392693	-0.463943	-0.416404	-0.416915	-0.393847		
(3,-1)	-0.072510	-0.070586	-0.064149	-0.056927	-0.079405	-0.079905	-0.083681		

Table S215: Laplacian of the density value (a.u.) at the considered critical points for the water...water  $0.90R_e$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.113185	0.102057	0.110152	0.106938	0.110233	0.112025	0.109245	0.122077	0.133034
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.113185	0.126566	0.121870	0.111263	0.108939	0.114183	0.112839	0.112025	0.110587
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.113185	0.114169	0.120223	0.116447	0.108537	0.111201	0.111487	0.111153	0.113389
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.113185	0.123196	0.119294	0.118072	0.110980	0.109933	0.111201		

Table S216: Laplacian of the density value (a.u.) at the considered critical points for the water...water  $1.00R_e$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.075922	0.068539	0.072574	0.071197	0.073520	0.074054	0.071663	0.078982	0.083258
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.075922	0.080393	0.078929	0.073566	0.072755	0.071971	0.071917	0.074054	0.072988
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.075922	0.075307	0.080716	0.078440	0.081866	0.073065	0.073214	0.073260	0.073889
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.075922	0.080759	0.084489	0.078376	0.073873	0.073858	0.073065		

Table S217: Laplacian of the density value (a.u.) at the considered critical points for the water...water  $1.50R_e$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.008376	0.008104	0.008254	0.008173	0.008120	0.008395	0.007973	-2.756975	0.007762
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.008376	0.008700	0.008419	0.008208	0.008130	0.008042	-2.637906	0.008395	0.008100
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.008376	0.008359	0.008261	0.008206	0.007633	0.008230	0.008212	0.008265	0.008064
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.008376	0.008600	0.008611	0.008128	0.008259	0.008178	0.008229		

Table S218: Laplacian of the density value (a.u.) at the considered critical points for the methane···methane  $0.90R_e$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.021371	0.021302	0.020686	0.020850	0.020933	0.020977	0.020248	0.021230	0.021793
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.021371	0.021015	0.021374	0.020899	0.021094	0.021199	0.020351	0.020977	0.020885
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.021371	0.020363	0.020583	0.021017	0.021554	0.020905	0.020889	0.020802	0.020681
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.021371	0.020999	-1.125715	0.021455	0.021102	0.021365	0.020905		

Table S219: Laplacian of the density value (a.u.) at the considered critical points for the methane...methane  $1.00R_e$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.010076	0.010347	0.009934	0.009978	0.009905	0.009788	0.009653	0.010569	0.009389
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.010076	0.009871	0.009801	0.009983	0.010030	0.009781	0.010204	0.009788	0.009976
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.010076	0.009493	0.009865	0.010176	0.010163	0.009918	0.009932	0.009948	0.009734
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.010076	0.009873	-1.125124	0.010048	0.010041	0.010106	0.009917		

Table S220: Laplacian of the density value (a.u.) at the considered critical points for the methane...methane  $1.50R_e$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.000223	0.000266	0.000254	0.000250	0.000225	0.000218	0.000245	0.000173	0.000195
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.000223	0.000197	0.000231	0.000242	0.000234	0.000238	0.000210	0.000218	0.000243
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.000223	0.000225	0.000239	0.000237	0.000271	0.000230	0.000232	0.000224	0.000233
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.000223	0.000210	0.000217	0.000211	0.000238	0.000224	0.000230		

Table S221: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.372582	-1.318920	-1.382715	-1.342239	-1.372807	-1.199577	-1.400865	-1.233529	-1.353988
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.372582	-1.362661	-1.551050	-1.388006	-1.351924	-1.497895	-1.284578	-1.386898	-1.449510
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.372582	-1.355133	-1.514022	-1.517495	-1.621304	-1.411257	-1.392551	-1.377652	-1.341253
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.372582	-1.228481	-1.424755	-1.398537	-1.392087	-1.370150	-1.373684		



Table S222: Laplacian of the density value (a.u.) at the considered critical points for the LiH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.151444	0.125947	0.135532	0.133569	0.142818	0.125046	0.139703	0.142877	0.180482
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.151444	0.169543	0.153069	0.138029	0.137352	0.134035	0.136990	0.144899	0.139571
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.151444	0.129983	0.137240	0.139902	0.145829	0.142227	0.142573	0.143108	0.141606
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.151444	0.178407	0.155695	0.150884	0.143643	0.145534	0.143714		

Table S223: Laplacian of the density value (a.u.) at the considered critical points for the BeH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.228297	0.137260	0.164887	0.167606	0.206995	0.230646	0.190743	0.224227	0.337615
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.228297	0.283795	0.254857	0.175978	0.184114	0.216779	0.213298	0.200485	0.211051
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.228297	0.168888	0.205306	0.201762	0.184918	0.198294	0.202015	0.203161	0.205755
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.228297	0.286670	0.197711	0.231531	0.197172	0.211673	0.209632		

Table S224: Laplacian of the density value (a.u.) at the considered critical points for the  ${}^2\text{CH}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.118767	-1.063848	-1.104108	-1.072099	-1.111009	-0.997620	-1.089860	-1.005712	-0.858854
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.118767	-1.067912	-1.096666	-1.120962	-1.094550	-1.162706	-1.058396	-1.118017	-1.151388
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.118767	-1.054685	-1.196485	-1.233132	-1.350789	-1.124359	-1.115292	-1.096003	-1.078622
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.118767	-0.966148	-1.255023	-1.182031	-1.132325	-1.121443	-1.133021		

Table S225: Laplacian of the density value (a.u.) at the considered critical points for the  $^3\text{CH}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.178065	-1.112091	-1.150175	-1.118048	-1.150336	-1.008457	-1.132528	-1.103438	-1.088704
(3,-1)	-1.178065	-1.112091	-1.150175	-1.118048	-1.150336	-1.008457	-1.132528	-1.103438	-1.088704
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.178065	-1.170525	-1.108405	-1.165281	-1.138751	-1.191503	-1.112579	-1.158301	-1.228615
(3,-1)	-1.178065	-1.170525	-1.108405	-1.165281	-1.138751	-1.191503	-1.112579	-1.158301	-1.228615
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.178065	-1.065452	-1.258975	-1.257513	-1.420767	-1.150706	-1.145889	-1.133572	-1.110686
(3,-1)	-1.178065	-1.065452	-1.258975	-1.257513	-1.420767	-1.150706	-1.145889	-1.133572	-1.110686
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.178065	-1.041310	-1.350384	-1.224691	-1.179790	-1.168726	-1.176436		
(3,-1)	-1.178065	-1.041310	-1.350384	-1.224691	-1.179790	-1.168726	-1.176436		

Table S226: Laplacian of the density value (a.u.) at the considered critical points for the  $^1\text{CH}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.132256	-1.066337	-1.112024	-1.076298	-1.117422	-0.999591	-1.092995	-0.988774	-0.853863
(3,-1)	-1.132256	-1.066337	-1.112024	-1.076298	-1.117422	-0.999591	-1.092995	-0.988774	-0.853863
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.132256	-1.013418	-1.083833	-1.129117	-1.099895	-1.088996	-0.966381	-1.125894	-1.094543
(3,-1)	-1.132256	-1.013418	-1.083833	-1.129117	-1.099895	-1.088996	-0.966381	-1.125894	-1.094543
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.132256	-1.066693	-1.182467	-1.288343	-1.439986	-1.122702	-1.117019	-1.101399	-1.078817
(3,-1)	-1.132256	-1.066693	-1.182467	-1.288343	-1.439986	-1.122702	-1.117019	-1.101399	-1.078817
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.132256	-0.972164	-1.179053	-1.195066	-1.140817	-1.128423	-1.139779		
(3,-1)	-1.132256	-0.972164	-1.179053	-1.195066	-1.140817	-1.128423	-1.139779		

Table S227: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub><sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.184642	-1.106753	-1.150473	-1.114058	-1.154809	-1.020498	-1.128869	-1.013562	-0.956033
(3,-1)	-1.184642	-1.106753	-1.150473	-1.114058	-1.154809	-1.020498	-1.128869	-1.013562	-0.956033
(3,-1)	-1.184642	-1.106753	-1.150473	-1.114058	-1.154809	-1.020498	-1.128869	-1.013562	-0.956033
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.184642	-1.088149	-1.119506	-1.167232	-1.137228	-1.107760	-0.991451	-1.160078	-1.166783
(3,-1)	-1.184642	-1.088149	-1.119506	-1.167232	-1.137228	-1.107760	-0.991451	-1.160078	-1.166783
(3,-1)	-1.184642	-1.088149	-1.119506	-1.167232	-1.137228	-1.107760	-0.991451	-1.160078	-1.166783
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.184642	-1.086757	-1.238507	-1.307077	-1.495435	-1.153669	-1.149122	-1.136088	-1.111686
(3,-1)	-1.184642	-1.086757	-1.238507	-1.307077	-1.495435	-1.153669	-1.149122	-1.136088	-1.111686
(3,-1)	-1.184642	-1.086757	-1.238507	-1.307077	-1.495435	-1.153669	-1.149122	-1.136088	-1.111686
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.184642	-1.044702	-1.261127	-1.232112	-1.183217	-1.170237	-1.180299		
(3,-1)	-1.184642	-1.044702	-1.261127	-1.232112	-1.183217	-1.170237	-1.180229		
(3,-1)	-1.184642	-1.044702	-1.261127	-1.232112	-1.183217	-1.170237	-1.180230		

Table S228: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.110257	-1.019528	-1.069862	-1.032481	-1.076975	-0.944852	-1.041297	-0.967668	-0.872661
(3,-1)	-1.110257	-1.019528	-1.069862	-1.032481	-1.076975	-0.944852	-1.041297	-0.967668	-0.872661
(3,-1)	-1.110257	-1.019528	-1.069862	-1.032481	-1.076975	-0.944852	-1.041297	-0.967668	-0.872661
(3,-1)	-1.110257	-1.019528	-1.069862	-1.032481	-1.076975	-0.944852	-1.041297	-0.967668	-0.872661
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.110257	-0.980720	-1.034171	-1.088773	-1.058731	-1.025424	-0.936788	-1.082694	-1.050079
(3,-1)	-1.110257	-0.980720	-1.034171	-1.088773	-1.058731	-1.025424	-0.936788	-1.082694	-1.050079
(3,-1)	-1.110257	-0.980720	-1.034171	-1.088773	-1.058731	-1.025424	-0.936788	-1.082694	-1.050079
(3,-1)	-1.110257	-0.980720	-1.034171	-1.088773	-1.058731	-1.025424	-0.936788	-1.082694	-1.050079
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.110257	-1.022759	-1.147874	-1.233733	-1.420515	-1.070018	-1.068519	-1.057108	-1.032790
(3,-1)	-1.110257	-1.022759	-1.147874	-1.233733	-1.420515	-1.070018	-1.068519	-1.057108	-1.032790
(3,-1)	-1.110257	-1.022759	-1.147874	-1.233733	-1.420515	-1.070018	-1.068519	-1.057108	-1.032790
(3,-1)	-1.110257	-1.022759	-1.147874	-1.233733	-1.420515	-1.070018	-1.068519	-1.057108	-1.032790
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.110257	-0.954080	-1.120596	-1.167177	-1.104442	-1.092410	-1.102147		
(3,-1)	-1.110257	-0.954080	-1.120596	-1.167177	-1.104442	-1.092410	-1.102148		
(3,-1)	-1.110257	-0.954080	-1.120596	-1.167177	-1.104442	-1.092410	-1.102148		
(3,-1)	-1.110257	-0.954080	-1.120596	-1.167177	-1.104442	-1.092410	-1.102149		

Table S229: Laplacian of the density value (a.u.) at the considered critical points for the  $^3\text{NH}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.730200	-1.685532	-1.671198	-1.656431	-1.705052	-1.502213	-1.653958	-1.444859	-1.349708
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.730200	-1.358085	-1.563683	-1.715356	-1.708172	-1.670764	-1.439298	-1.751466	-1.539798
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.730200	-1.647136	-1.802250	-1.857013	-2.065452	-1.743429	-1.729032	-1.697474	-1.663810
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.730200	-1.548178	-1.783001	-1.846924	-1.743402	-1.760994	-1.750715		



Table S230: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{NH}_2^\bullet$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.786407	-1.733855	-1.715475	-1.696214	-1.755811	-1.536248	-1.704316	-1.675321	-1.613409
(3,-1)	-1.786407	-1.733855	-1.715475	-1.696214	-1.755811	-1.536248	-1.704316	-1.675321	-1.613409
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.786407	-1.526048	-1.615116	-1.760402	-1.749480	-1.768859	-1.594150	-1.796453	-1.579023
(3,-1)	-1.786407	-1.526048	-1.615116	-1.760402	-1.749480	-1.768859	-1.594150	-1.796453	-1.579023
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.786407	-1.672090	-1.821715	-1.946596	-2.162724	-1.783842	-1.769727	-1.737623	-1.703382
(3,-1)	-1.786407	-1.672090	-1.821715	-1.946596	-2.162724	-1.783842	-1.769727	-1.737623	-1.703382
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.786407	-1.559952	-1.858921	-1.904108	-1.789826	-1.805809	-1.793616		
(3,-1)	-1.786407	-1.559952	-1.858921	-1.904108	-1.789826	-1.805809	-1.793616		

Table S231: Laplacian of the density value (a.u.) at the considered critical points for the NH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.827132	-1.764477	-1.748514	-1.727862	-1.791507	-1.554708	-1.732334	-1.733621	-1.741398
(3,-1)	-1.827132	-1.764477	-1.748514	-1.727862	-1.791507	-1.554708	-1.732334	-1.733621	-1.741398
(3,-1)	-1.827132	-1.764477	-1.748514	-1.727862	-1.791507	-1.554708	-1.732334	-1.733621	-1.741398
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.827132	-1.573651	-1.648521	-1.793089	-1.781810	-1.776471	-1.628002	-1.827775	-1.593517
(3,-1)	-1.827132	-1.573651	-1.648521	-1.793089	-1.781810	-1.776471	-1.628002	-1.827775	-1.593517
(3,-1)	-1.827132	-1.573651	-1.648521	-1.793089	-1.781810	-1.776471	-1.628002	-1.827775	-1.593517
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.827132	-1.678229	-1.854633	-1.979185	-2.214303	-1.808284	-1.795283	-1.763132	-1.725511
(3,-1)	-1.827132	-1.678229	-1.854633	-1.979185	-2.214303	-1.808284	-1.795283	-1.763132	-1.725511
(3,-1)	-1.827132	-1.678229	-1.854633	-1.979185	-2.214303	-1.808284	-1.795283	-1.763132	-1.725511
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.827132	-1.587078	-1.915283	-1.943589	-1.822985	-1.838806	-1.822877		
(3,-1)	-1.827132	-1.587078	-1.915283	-1.943589	-1.822985	-1.838806	-1.822943		
(3,-1)	-1.827132	-1.587078	-1.915283	-1.943589	-1.822985	-1.838806	-1.822944		

Table S232: Laplacian of the density value (a.u.) at the considered critical points for the OH<sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-2.637956	-2.578389	-2.540463	-2.532973	-2.609153	-2.367481	-2.602001	-2.627551	-2.673382
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-2.637956	-2.510780	-2.473520	-2.616700	-2.620686	-2.655059	-2.537785	-2.730653	-2.337420
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-2.637956	-2.603713	-2.553810	-2.651598	-2.695226	-2.693368	-2.686745	-2.669419	-2.611432
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-2.637956	-2.569561	-2.863368	-2.851884	-2.646723	-2.684609	-2.655876		

Table S233: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>2</sub>O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-2.693243	-2.633585	-2.601771	-2.591420	-2.666270	-2.415351	-2.662535	-2.668292	-2.765233
(3,-1)	-2.693243	-2.633585	-2.601771	-2.591420	-2.666270	-2.415351	-2.662535	-2.668292	-2.765233
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-2.693243	-2.575798	-2.522541	-2.671661	-2.672531	-2.642236	-2.548630	-2.776512	-2.388373
(3,-1)	-2.693243	-2.575798	-2.522541	-2.671661	-2.672531	-2.642236	-2.548630	-2.776512	-2.388373
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-2.693243	-2.630046	-2.600339	-2.690767	-2.780324	-2.748793	-2.737857	-2.717347	-2.652577
(3,-1)	-2.693243	-2.630046	-2.600339	-2.690767	-2.780324	-2.748793	-2.737857	-2.717347	-2.652577
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-2.693243	-2.622755	-2.958320	-2.894866	-2.693880	-2.726205	-2.697695		
(3,-1)	-2.693243	-2.622755	-2.958320	-2.894866	-2.693880	-2.726205	-2.697694		

Table S234: Laplacian of the density value (a.u.) at the considered critical points for the HF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-3.476079	-3.382270	-3.230091	-3.241768	-3.361340	-3.209715	-3.352374	-3.460237	-3.772480
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-3.476079	-4.094033	-3.550618	-3.367427	-3.408707	-3.332360	-3.452735	-3.566138	-3.133313
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-3.476079	-3.454243	-3.197828	-3.189925	-3.146644	-3.424455	-3.466989	-3.484724	-3.479733
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-3.476079	-3.868406	-3.614161	-3.957031	-3.426038	-3.546657	-3.480292		

Table S235: Laplacian of the density value (a.u.) at the considered critical points for the Li<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.007788	0.000666	0.001132	0.002832	0.005951	0.004470	0.004093	0.011284	0.017284
(3,-1)	0.007788	0.000666	0.001132	0.002832	0.005951	0.004470	0.004093	0.011284	0.017284
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.007788	0.743263	0.016590	0.002482	0.004480	0.005953	0.008273	0.004329	0.001240
(3,-1)	0.007788		0.016590	0.002482	0.004480	0.005953	0.008273	0.004329	0.001240
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.007788	0.004577	0.006878	0.006382	0.009879	0.004816	0.006272	0.007595	0.005502
(3,-1)	0.007788	0.004577	0.006878	0.006382	0.009879	0.004816	0.006272	0.007595	0.005502
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.007788	0.735407	0.010949	0.007953	0.004388	0.006790	0.005594		
(3,-1)	0.007788		0.010949	0.007953	0.004388	0.006790	0.005594		

Table S236: Laplacian of the density value (a.u.) at the considered critical points for the LiF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.734547	0.692082	0.697948	0.700298	0.715694	0.717666	0.699727	0.712635	0.766574
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.734547	-1.223871	0.738289	0.707761	0.712880	0.717562	0.706965	0.721187	0.704994
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.734547	0.711222	0.720090	0.716361	0.715532	0.706590	0.710764	0.712134	0.709617
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.734547	-1.241302	0.704326	0.747139	0.717446	0.726635	0.719260		

Table S237: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>2</sub>H<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.264093	-1.220833	-1.254383	-1.216285	-1.216446	-1.302296	-1.257665	-1.109884	-1.048517
(3,-1)	-1.276909	-1.200148	-1.237862	-1.199593	-1.250491	-1.105322	-1.215815	-1.073398	-1.048517
(3,-1)	-1.276909	-1.200148	-1.237862	-1.199593	-1.250491	-1.105322	-1.215815	-1.073398	-1.048517
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.264093	-1.084525	-1.188419	-1.258455	-1.227530	-1.197426	-1.152918	-1.227532	-1.154205
(3,-1)	-1.276909	-1.054987	-1.218597	-1.265065	-1.235528	-1.185327	-1.054794	-1.267213	-1.231710
(3,-1)	-1.276909	-1.054987	-1.218597	-1.265065	-1.235528	-1.185327	-1.054794	-1.267213	-1.231710
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.264093	-1.368001	-1.282692	-1.410644	-1.445324	-1.097072	-1.169659	-1.252261	-1.199856
(3,-1)	-1.276909	-1.166559	-1.346762	-1.441403	-1.661923	-1.247004	-1.248047	-1.237585	-1.208834
(3,-1)	-1.276909	-1.166559	-1.346762	-1.441403	-1.661923	-1.247004	-1.248047	-1.237585	-1.208834
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.264093	-1.103749	-1.245763	-1.286884	-1.262297	-1.241336	-1.242267		
(3,-1)	-1.276909	-1.021018	-1.376422	-1.364782	-1.274708	-1.267288	-1.273935		
(3,-1)	-1.276909	-1.021018	-1.376422	-1.364782	-1.274708	-1.267288	-1.273935		



Table S238: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{H}_2\text{C}=\text{CH}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.161883	-1.033641	-1.099060	-1.055964	-1.106376	-1.034201	-1.059139	-1.072901	-1.183381
(3,-1)	-1.182700	-1.094737	-1.140108	-1.102749	-1.150911	-0.998298	-1.115773	-1.014619	-0.921833
(3,-1)	-1.182700	-1.094737	-1.140108	-1.102749	-1.150911	-0.998298	-1.115773	-1.014619	-0.921833
(3,-1)	-1.182700	-1.094737	-1.140108	-1.102749	-1.150911	-0.998298	-1.115773	-1.014619	-0.921833
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.161883	-0.595237	-1.084641	-1.126441	-1.095358	-1.037668	-1.061734	-1.134933	-1.059031
(3,-1)	-1.182700	-0.981127	-1.113320	-1.163308	-1.133860	-1.092318	-0.988280	-1.162776	-1.129793
(3,-1)	-1.182700	-0.981127	-1.113320	-1.163308	-1.133860	-1.092318	-0.988280	-1.162776	-1.129793
(3,-1)	-1.182700	-0.981127	-1.113320	-1.163308	-1.133860	-1.092318	-0.988280	-1.162776	-1.129793
(3,-1)	-1.182700	-0.981127	-1.113320	-1.163308	-1.133860	-1.092318	-0.988280	-1.162776	-1.129793
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.161883	-1.054049	-1.152069	-1.223732	-1.209578	-1.046280	-1.081154	-1.105431	-1.060423
(3,-1)	-1.182700	-1.091556	-1.226649	-1.320907	-1.507258	-1.148742	-1.146757	-1.134555	-1.107434
(3,-1)	-1.182700	-1.091556	-1.226649	-1.320907	-1.507258	-1.148742	-1.146757	-1.134555	-1.107434
(3,-1)	-1.182700	-1.091556	-1.226649	-1.320907	-1.507258	-1.148742	-1.146757	-1.134555	-1.107434
(3,-1)	-1.182700	-1.091556	-1.226649	-1.320907	-1.507258	-1.148742	-1.146757	-1.134555	-1.107434
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.161883	-0.603114	-1.156945	-1.259194	-1.140689	-1.131172	-1.152615		
(3,-1)	-1.182700	-0.952127	-1.226866	-1.252339	-1.178207	-1.168245	-1.177243		
(3,-1)	-1.182700	-0.952127	-1.226866	-1.252339	-1.178207	-1.168245	-1.177243		
(3,-1)	-1.182700	-0.952127	-1.226866	-1.252339	-1.178207	-1.168245	-1.177244		
(3,-1)	-1.182700	-0.952127	-1.226866	-1.252339	-1.178207	-1.168245	-1.177244		

Table S239: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>3</sub>C–CH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.650899	-0.552250	-0.604044	-0.577083	-0.625665	-0.529263	-0.558146	-0.636626	-0.623310
(3,-1)	-1.107936	-1.019126	-1.066148	-1.030409	-1.074921	-0.942385	-1.038908	-0.967314	-0.861257
(3,-1)	-1.107936	-1.019126	-1.066148	-1.030409	-1.074921	-0.942385	-1.038908	-0.967314	-0.861257
(3,-1)	-1.107936	-1.019126	-1.066148	-1.030409	-1.074921	-0.942385	-1.038908	-0.967314	-0.861257
(3,-1)	-1.107936	-1.019126	-1.066148	-1.030409	-1.074921	-0.942385	-1.038908	-0.967314	-0.861257
(3,-1)	-1.107936	-1.019126	-1.066148	-1.030409	-1.074921	-0.942385	-1.038908	-0.967314	-0.861257
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.650899	1.170223	-0.635941	-0.628841	-0.610365	-0.584059	-0.613196	-0.648264	-0.597430
(3,-1)	-1.107936		-1.030785	-1.085917	-1.057373	-1.024557	-0.939043	-1.082281	-1.046969
(3,-1)	-1.107936		-1.030785	-1.085917	-1.057373	-1.024557	-0.939043	-1.082281	-1.046969
(3,-1)	-1.107936		-1.030785	-1.085917	-1.057373	-1.024557	-0.939043	-1.082281	-1.046969
(3,-1)	-1.107936		-1.030785	-1.085917	-1.057373	-1.024557	-0.939043	-1.082281	-1.046969
(3,-1)	-1.107936		-1.030785	-1.085917	-1.057373	-1.024557	-0.939043	-1.082281	-1.046969
(3,-1)	-1.107936		-1.030785	-1.085917	-1.057373	-1.024557	-0.939043	-1.082281	-1.046969
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.650899	-0.523211	-0.627121	-0.654735	-0.622376	-0.617982	-0.619169	-0.606356	-0.587726
(3,-1)	-1.107936	-1.022772	-1.142703	-1.229338	-1.414774	-1.069177	-1.067587	-1.056142	-1.032192
(3,-1)	-1.107936	-1.022772	-1.142703	-1.229338	-1.414774	-1.069177	-1.067587	-1.056142	-1.032192
(3,-1)	-1.107936	-1.022772	-1.142703	-1.229338	-1.414774	-1.069177	-1.067587	-1.056142	-1.032192
(3,-1)	-1.107936	-1.022772	-1.142703	-1.229338	-1.414774	-1.069177	-1.067587	-1.056142	-1.032192
(3,-1)	-1.107936	-1.022772	-1.142703	-1.229338	-1.414774	-1.069177	-1.067587	-1.056142	-1.032192
(3,-1)	-1.107936	-1.022772	-1.142703	-1.229338	-1.414774	-1.069177	-1.067587	-1.056142	-1.032192
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.650899	1.117195	-0.604442	-0.747427	-0.639325	-0.637293	-0.654257		
(3,-1)	-1.107936		-1.117255	-1.165197	-1.101463	-1.090661	-1.099794		
(3,-1)	-1.107936		-1.117255	-1.165197	-1.101463	-1.090661	-1.099739		
(3,-1)	-1.107936		-1.117255	-1.165197	-1.101463	-1.090661	-1.099738		
(3,-1)	-1.107936		-1.117255	-1.165197	-1.101463	-1.090661	-1.099794		
(3,-1)	-1.107936		-1.117255	-1.165197	-1.101463	-1.090661	-1.099738		
(3,-1)	-1.107936		-1.117255	-1.165197	-1.101463	-1.090661	-1.099738		

Table S240: Laplacian of the density value (a.u.) at the considered critical points for the CN<sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.907235	0.410235	0.564358	0.624684	0.778378	0.141750	0.492278	0.982180	1.527979
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.907235	0.146788	1.503968	0.633995	0.697136	0.644117	0.356340	1.015933	0.674557
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.907235	1.092735	0.727476	0.658203	0.570933	0.803792	0.662934	0.589736	0.351526
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.907235	0.048991	0.606308	0.680457	0.827845	0.863205	0.846537		

Table S241: Laplacian of the density value (a.u.) at the considered critical points for the HCN system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.228995	-0.692900	-0.590245	-0.510236	-0.356825	-0.925747	-0.631285	-0.075735	0.336830
(3,-1)	-1.300616	-1.219494	-1.257241	-1.218198	-1.273416	-1.117150	-1.237738	-1.083741	-1.066187
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.228995	0.854217	0.410205	-0.512178	-0.408810	-0.552449	-0.646371	-0.167668	-0.408834
(3,-1)	-1.300616		-1.261106	-1.287615	-1.257811	-1.210146	-1.070104	-1.297675	-1.261094
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.228995	-0.108952	-0.265952	-0.460579	-0.236965	-0.300241	-0.419172	-0.506952	-0.691986
(3,-1)	-1.300616	-1.180725	-1.365807	-1.454953	-1.652238	-1.274519	-1.274574	-1.262578	-1.232796
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.228995	0.749216	-0.462295	-0.088454	-0.426268	-0.309399	-0.362497		
(3,-1)	-1.300616		-1.411830	-1.397911	-1.297309	-1.291644	-1.296128		

Table S242: Laplacian of the density value (a.u.) at the considered critical points for the CO system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.492577	0.004990	0.068816	0.160516	0.284445	-0.124517	0.178384	0.571321	1.044980
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.492577	0.699905	1.087545	0.141151	0.254093	0.285914	0.145463	0.502017	0.321592
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.492577	0.654592	0.482238	0.186132	0.419227	0.279326	0.250907	0.285949	0.016574
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.492577	0.605045	0.056701	0.495630	0.299233	0.420980	0.420956		

Table S243: Laplacian of the density value (a.u.) at the considered critical points for the HCO<sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.336865	-0.067672	-0.022089	0.066680	0.203860	-0.207967	0.085692	0.487365	0.878372
(3,-1)	-1.024481	-0.951629	-0.985044	-0.955366	-1.001518	-0.886058	-0.971417	-0.898241	-0.794750
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.336865	0.277182	0.921788	0.057690	0.165441	0.207372	0.057754	0.400111	0.204899
(3,-1)	-1.024481	-1.054884	-0.938412	-1.010662	-0.987885	-0.988516	-0.882102	-1.014441	-0.987208
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.336865	0.501979	0.328730	0.074732	0.255541	0.220122	0.168690	0.169627	-0.035422
(3,-1)	-1.024481	-0.945295	-1.055512	-1.136572	-1.275773	-1.011745	-1.005659	-0.988277	-0.971856
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.336865	0.163188	0.057065	0.395875	0.167187	0.286356	0.273790		
(3,-1)	-1.024481	-1.010864	-1.080762	-1.106034	-1.019259	-1.015497	-1.019226		

Table S244: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>2</sub>C=O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.121633	-0.443272	-0.434259	-0.334395	-0.223976	-0.591491	-0.327002	0.114082	0.403667
(3,-1)	-1.186761	-1.087899	-1.134635	-1.097834	-1.153170	-1.012110	-1.117811	-0.994475	-0.865447
(3,-1)	-1.186761	-1.087899	-1.134635	-1.097834	-1.153170	-1.012110	-1.117811	-0.994475	-0.865447
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.121633	-0.469565	0.497411	-0.367651	-0.251187	-0.149764	-0.290647	-0.045608	-0.230328
(3,-1)	-1.186761	-1.073334	-1.133936	-1.164587	-1.136597	-1.101594	-0.978003	-1.174337	-1.142666
(3,-1)	-1.186761	-2.559520	-1.133936	-1.164587	-1.136597	-1.101594	-0.978003	-1.174337	-1.142666
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.121633	0.065339	-0.123256	-0.398483	-0.304064	-0.183710	-0.247989	-0.259168	-0.438472
(3,-1)	-1.186761	-1.099860	-1.218657	-1.321931	-1.465577	-1.162518	-1.156902	-1.139386	-1.116287
(3,-1)	-1.186761	-1.099860	-1.218657	-1.321931	-1.465577	-1.162518	-1.156902	-1.139386	-1.116287
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.121633	-0.552623	-0.363996	-0.031676	-0.283046	-0.162031	-0.191143		
(3,-1)	-1.186761	-1.029504	-1.228960	-1.274695	-1.179673	-1.173729	-1.181786		
(3,-1)	-1.186761	-2.605197	-1.228960	-1.274695	-1.179673	-1.173729	-1.181787		

Table S245: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>-OH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.691728	-0.632749	-0.678524	-0.656522	-0.655514	-0.656583	-0.643736	-0.560375	-0.399582
(3,-1)	-1.206645	-1.107367	-1.162007	-1.121604	-1.171393	-1.028156	-1.138739	-1.021550	-0.899394
(3,-1)	-2.672908	-2.622538	-2.579659	-2.574889	-2.649883	-2.407752	-2.645006	-2.647626	-2.747259
(3,-1)	-1.156703	-1.057145	-1.108529	-1.070588	-1.120084	-0.986539	-1.084200	-0.987393	-0.863035
(3,-1)	-1.156703	-1.057145	-1.108529	-1.070588	-1.120084	-0.986539	-1.084200	-0.987393	-0.863035
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.691728	-2.211590	-0.364282	-0.693509	-0.662610	-0.498633	-0.582560	-0.605941	-0.677683
(3,-1)	-1.206645		-1.144966	-1.184451	-1.152241	-1.107868	-0.997978	-1.182467	-1.153978
(3,-1)	-2.672908		-2.498637	-2.651852	-2.657686	-2.625252	-2.531501	-2.759683	-2.368681
(3,-1)	-1.156703		-1.083376	-1.131918	-1.102001	-1.067297	-0.964532	-1.131342	-1.099192
(3,-1)	-1.156703		-1.083376	-1.131918	-1.102001	-1.067297	-0.964532	-1.131342	-1.099192
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.691728	-0.606955	-0.601188	-0.652672	-0.657913	-0.629574	-0.657597	-0.667411	-0.664864
(3,-1)	-1.206645	-1.117013	-1.238841	-1.333480	-1.502064	-1.169474	-1.167162	-1.153984	-1.129656
(3,-1)	-2.672908	-2.609020	-2.587852	-2.679459	-2.774322	-2.730084	-2.720502	-2.701393	-2.637578
(3,-1)	-1.156703	-1.069032	-1.186453	-1.281531	-1.451438	-1.119341	-1.116312	-1.102288	-1.078946
(3,-1)	-1.156703	-1.069032	-1.186453	-1.281531	-1.451438	-1.119341	-1.116312	-1.102288	-1.078946
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.691728	-2.299239	-0.575155	-0.481185	-0.693873	-0.646314	-0.648414		
(3,-1)	-1.206645		-1.231539	-1.274792	-1.201676	-1.189599	-1.200976		
(3,-1)	-2.672908		-2.937763	-2.874791	-2.672889	-2.708942	-2.677526		
(3,-1)	-1.156703		-1.171556	-1.223788	-1.149575	-1.139320	-1.149948		
(3,-1)	-1.156703		-1.171556	-1.223788	-1.149575	-1.139320	-1.149949		



Table S246: Laplacian of the density value (a.u.) at the considered critical points for the N<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-2.479160	-2.296581	-2.383535	-2.318875	-2.393847	-2.253594	-2.324999	-2.039829	-2.438913
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-2.479160	-0.591010	-2.267641	-2.428056	-2.383281	-2.046470	-2.018068	-2.452221	-2.144733
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-2.479160	-2.315853	-2.483356	-2.829454	-2.990153	-2.264262	-2.345258	-2.407693	-2.283320
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-2.479160	-0.559966	-2.603482	-2.630952	-2.444710	-2.431012	-2.496867		

Table S247: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>2</sub>N–NH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.562680	-0.470243	-0.496878	-0.488336	-0.547190	-0.393122	-0.460935	-0.494860	-0.563503
(3,-1)	-1.839449	-1.771166	-1.752367	-1.733580	-1.800725	-1.555132	-1.741527	-1.734630	-1.709744
(3,-1)	-1.931207	-1.860727	-1.841101	-1.820900	-1.890257	-1.641150	-1.831383	-1.819140	-1.795909
(3,-1)	-1.839449	-1.771166	-1.752367	-1.733580	-1.800725	-1.555132	-1.741527	-1.734630	-1.709744
(3,-1)	-1.931207	-1.860727	-1.841101	-1.820900	-1.890257	-1.641150	-1.831383	-1.819140	-1.795909
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.562680	-2.402650	-0.603987	-0.536362	-0.537591	-0.378210	-0.436348	-0.588129	-0.509863
(3,-1)	-1.839449		-1.642152	-1.801518	-1.792629	-1.801746	-1.643596	-1.840710	-1.602674
(3,-1)	-1.931207		-1.732139	-1.892054	-1.882183	-1.889831	-1.722906	-1.935720	-1.683194
(3,-1)	-1.839449		-1.642152	-1.801518	-1.792629	-1.801746	-1.643596	-1.840710	-1.602674
(3,-1)	-1.931207		-1.732139	-1.892054	-1.882183	-1.889831	-1.722906	-1.935720	-1.683194
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.562680	-0.435297	-0.496583	-0.544153	-0.569603	-0.568744	-0.550624	-0.517821	-0.493527
(3,-1)	-1.839449	-1.696732	-1.863170	-1.997931	-2.219501	-1.820327	-1.808027	-1.775873	-1.740194
(3,-1)	-1.931207	-1.785694	-1.947001	-2.088080	-2.300434	-1.911097	-1.899610	-1.867106	-1.828290
(3,-1)	-1.839449	-1.696732	-1.863170	-1.997931	-2.219501	-1.820327	-1.808027	-1.775873	-1.740194
(3,-1)	-1.931207	-1.785694	-1.947001	-2.088080	-2.300434	-1.911097	-1.899610	-1.867106	-1.828290
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.562680	-2.396243	-0.465412	-0.703596	-0.544542	-0.562615	-0.570434		
(3,-1)	-1.839449		-1.918510	-1.963602	-1.833237	-1.852590	-1.836761		
(3,-1)	-1.931207		-2.017321	-2.061713	-1.925709	-1.945466	-1.928871		
(3,-1)	-1.839449		-1.918510	-1.963602	-1.833237	-1.852590	-1.836761		
(3,-1)	-1.931207		-2.017321	-2.061713	-1.925709	-1.945466	-1.928870		

Table S248: Laplacian of the density value (a.u.) at the considered critical points for the NO• system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-2.489144	-2.215771	-2.293924	-2.262010	-2.404777	-2.122376	-2.214671	-2.007605	-2.497274
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-2.489144	-0.727487	-2.420856	-2.387049	-2.384872	-1.829823	-1.897267	-2.504157	-2.151982
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-2.489144	-2.136104	-2.427025	-2.690148	-3.045187	-2.310361	-2.346495	-2.340640	-2.243064
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-2.489144	-0.680769	-2.406088	-2.827904	-2.398935	-2.439847	-2.467583		

Table S249: Laplacian of the density value (a.u.) at the considered critical points for the O<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.638847	-0.564318	-0.571215	-0.570949	-0.662530	-0.425225	-0.516763	-0.538375	-0.666877
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.638847	-0.018980	-0.719160	-0.642985	-0.658150	-0.385208	-0.464215	-0.740084	-0.567910
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.638847	-0.502977	-0.667701	-0.730432	-0.973893	-0.674723	-0.658861	-0.616473	-0.566877
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.638847	0.011961	-0.580181	-0.932281	-0.603210	-0.644013	-0.662238		

Table S250: Laplacian of the density value (a.u.) at the considered critical points for the HO–OH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.055252	0.103692	0.111250	0.098829	0.046312	0.130060	0.097638	0.025771	-0.002599
(3,-1)	-2.758626	-2.684349	-2.648579	-2.638495	-2.724306	-2.477498	-2.720783	-2.715753	-2.805093
(3,-1)	-2.758626	-2.684349	-2.648579	-2.638495	-2.724306	-2.477498	-2.720783	-2.715753	-2.805093
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.055252	0.489581	-0.014369	0.061769	0.038765	0.035415	0.016031	-0.012746	0.057333
(3,-1)	-2.758626		-2.561282	-2.731421	-2.734814	-2.724111	-2.623882	-2.851145	-2.449046
(3,-1)	-2.758626		-2.561282	-2.731421	-2.734814	-2.724111	-2.623882	-2.851145	-2.449046
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.055252	0.057420	0.071156	0.101598	0.165501	-0.001762	0.011399	0.026258	0.055851
(3,-1)	-2.758626	-2.719508	-2.646827	-2.767623	-2.786520	-2.810640	-2.804800	-2.786393	-2.731851
(3,-1)	-2.758626	-2.719508	-2.646827	-2.767623	-2.786520	-2.810640	-2.804800	-2.786393	-2.731851
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.055252	0.454756	0.098695	-0.130026	0.069082	0.030002	0.026115		
(3,-1)	-2.758626		-3.009073	-2.998344	-2.754032	-2.794116	-2.762300		
(3,-1)	-2.758626		-3.009073	-2.998344	-2.754032	-2.794116	-2.762297		

Table S251: Laplacian of the density value (a.u.) at the considered critical points for the F<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.515059	0.529430	0.544312	0.528922	0.466940	0.504448	0.543073	0.507549	0.420671
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.515059	0.492962	0.436949	0.482683	0.452848	0.420909	0.429192	0.401924	0.479442
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.515059	0.454402	0.443797	0.447348	0.494502	0.448230	0.445938	0.452034	0.461781
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.515059	0.331802	0.452643	0.239554	0.508512	0.457178	0.445894		

Table S252: Laplacian of the density value (a.u.) at the considered critical points for the CO<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.002370	-0.172513	-0.159982	-0.053196	-0.028662	-0.401843	-0.098700	0.427709	0.598624
(3,-1)	0.002370	-0.172513	-0.159982	-0.053196	-0.028662	-0.401843	-0.098700	0.427709	0.598624
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.002370	0.147273	0.779344	-0.169456	-0.063213	0.035230	-0.089429	0.112254	-0.046376
(3,-1)	0.002370	0.147273	0.779344	-0.169456	-0.063213	0.035230	-0.089429	0.112254	-0.046376
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.002370	0.311348	-0.015483	-0.301464	-0.342362	-0.021017	-0.084983	-0.081154	-0.297676
(3,-1)	0.002370	0.311348	-0.015483	-0.301464	-0.342362	-0.021017	-0.084983	-0.081154	-0.297676
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.002370	0.154597	-0.262612	-0.109435	-0.039294	0.039384	0.028849		
(3,-1)	0.002370	0.154597	-0.262612	-0.109435	-0.039294	0.039384	0.028850		

Table S253: Laplacian of the density value (a.u.) at the considered critical points for the  $^1\text{SiH}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.140772	0.017756	0.054408	0.063521	0.093885	0.063984	0.066756	0.130476	0.182134
(3,-1)	0.140772	0.017756	0.054408	0.063521	0.093885	0.063984	0.066756	0.130476	0.182134
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.140772	0.187249	0.157573	0.070259	0.085598	0.104135	0.080499	0.114833	0.076181
(3,-1)	0.140772	0.187249	0.157573	0.070259	0.085598	0.104135	0.080499	0.114833	0.076181
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.140772	0.133426	0.128378	0.089916	0.085924	0.080845	0.082175	0.089315	0.083069
(3,-1)	0.140772	0.133426	0.128378	0.089916	0.085924	0.080845	0.082175	0.089315	0.083069
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.140772	0.164844	0.070993	0.159021	0.099148	0.121465	0.117602		
(3,-1)	0.140772	0.164844	0.070993	0.159021	0.099148	0.121465	0.117602		



Table S254: Laplacian of the density value (a.u.) at the considered critical points for the  $^3\text{SiH}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.181843	0.059830	0.103601	0.110215	0.136566	0.126052	0.109730	0.179154	0.191606
(3,-1)	0.181843	0.059830	0.103601	0.110215	0.136566	0.126052	0.109730	0.179154	0.191606
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.181843	0.193060	0.195199	0.116868	0.129670	0.140250	0.112918	0.153097	0.124897
(3,-1)	0.181843	0.193060	0.195199	0.116868	0.129670	0.140250	0.112918	0.153097	0.124897
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.181843	0.174923	0.163470	0.124700	0.121023	0.118311	0.120479	0.127191	0.115686
(3,-1)	0.181843	0.174923	0.163470	0.124700	0.121023	0.118311	0.120479	0.127191	0.115686
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.181843	0.185551	0.102387	0.198508	0.143167	0.162530	0.157158		
(3,-1)	0.181843	0.185551	0.102387	0.198508	0.143167	0.162530	0.157158		

Table S255: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{SiH}_3^\bullet$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.184221	0.060550	0.101556	0.110934	0.138705	0.123606	0.114974	0.172094	0.203640
(3,-1)	0.184221	0.060550	0.101556	0.110934	0.138705	0.123606	0.114974	0.172094	0.203640
(3,-1)	0.184221	0.060550	0.101556	0.110934	0.138705	0.123606	0.114974	0.172094	0.203640
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.184221	0.203204	0.205526	0.116193	0.131562	0.137273	0.109853	0.158756	0.125511
(3,-1)	0.184221	0.203204	0.205526	0.116193	0.131562	0.137273	0.109853	0.158756	0.125511
(3,-1)	0.184221	0.203204	0.205526	0.116193	0.131562	0.137273	0.109853	0.158756	0.125511
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.184221	0.180158	0.172168	0.135433	0.163565	0.119880	0.123387	0.132041	0.124750
(3,-1)	0.184221	0.180158	0.172168	0.135433	0.163565	0.119880	0.123387	0.132041	0.124750
(3,-1)	0.184221	0.180158	0.172168	0.135433	0.163565	0.119880	0.123387	0.132041	0.124750
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.184221	0.202701	0.098179	0.201888	0.143909	0.165294	0.160576		
(3,-1)	0.184221	0.202701	0.098179	0.201888	0.143909	0.165294	0.160594		
(3,-1)	0.184221	0.202701	0.098179	0.201888	0.143909	0.165294	0.160594		

Table S256: Laplacian of the density value (a.u.) at the considered critical points for the SiH<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.189062	0.066535	0.104898	0.115869	0.145213	0.125208	0.121747	0.172584	0.219743
(3,-1)	0.189062	0.066535	0.104898	0.115869	0.145213	0.125208	0.121747	0.172584	0.219743
(3,-1)	0.189062	0.066535	0.104898	0.115869	0.145213	0.125208	0.121747	0.172584	0.219743
(3,-1)	0.189062	0.066535	0.104898	0.115869	0.145213	0.125208	0.121747	0.172584	0.219743
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.189062	-0.097224	0.218911	0.119915	0.136477	0.139036	0.115700	0.165993	0.131688
(3,-1)	0.189062	-0.097224	0.218911	0.119915	0.136477	0.139036	0.115700	0.165993	0.131688
(3,-1)	0.189062		0.218911	0.119915	0.136477	0.139036	0.115700	0.165993	0.131688
(3,-1)	0.189062		0.218911	0.119915	0.136477	0.139036	0.115700	0.165993	0.131688
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.189062	0.184678	0.183665	0.147877	0.260343	0.123364	0.128568	0.137921	0.136747
(3,-1)	0.189062	0.184678	0.183665	0.147877	0.260343	0.123364	0.128568	0.137921	0.136747
(3,-1)	0.189062	0.184678	0.183665	0.147877	0.260343	0.123364	0.128568	0.137921	0.136747
(3,-1)	0.189062	0.184678	0.183665	0.147877	0.260343	0.123364	0.128568	0.137921	0.136747
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.189062	-0.121101	0.094668	0.206525	0.148024	0.170111	0.167335		
(3,-1)	0.189062	-0.121101	0.094668	0.206525	0.148024	0.170111	0.167335		
(3,-1)	0.189062		0.094668	0.206525	0.148024	0.170111	0.167335		
(3,-1)	0.189062		0.094668	0.206525	0.148024	0.170111	0.167335		

Table S257: Laplacian of the density value (a.u.) at the considered critical points for the PH<sub>2</sub><sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.102742	-0.282380	-0.217928	-0.202738	-0.157618	-0.232357	-0.219210	-0.066025	-0.156358
(3,-1)	-0.102742	-0.282380	-0.217928	-0.202738	-0.157618	-0.232357	-0.219210	-0.066025	-0.156358
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.102742	-0.064730	-0.023406	-0.196281	-0.170535	-0.128410	-0.192141	-0.118069	-0.208828
(3,-1)	-0.102742	-0.064730	-0.023406	-0.196281	-0.170535	-0.128410	-0.192141	-0.118069	-0.208828
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.102742	-0.045526	-0.122196	-0.156442	-0.097518	-0.147876	-0.167374	-0.181743	-0.184222
(3,-1)	-0.102742	-0.045526	-0.122196	-0.156442	-0.097518	-0.147876	-0.167374	-0.181743	-0.184222
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.102742	-0.086273	-0.230444	-0.054477	-0.158170	-0.123367	-0.129389		
(3,-1)	-0.102742	-0.086273	-0.230444	-0.054477	-0.158170	-0.123367	-0.129389		

Table S258: Laplacian of the density value (a.u.) at the considered critical points for the PH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.092390	-0.264089	-0.205346	-0.185552	-0.143249	-0.231766	-0.184236	-0.037321	-0.130861
(3,-1)	-0.092390	-0.264089	-0.205346	-0.185552	-0.143249	-0.231766	-0.184236	-0.037321	-0.130861
(3,-1)	-0.092390	-0.264089	-0.205346	-0.185552	-0.143249	-0.231766	-0.184236	-0.037321	-0.130861
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.092390	-0.618477	0.013679	-0.184963	-0.156181	-0.091304	-0.178404	-0.103832	-0.186096
(3,-1)	-0.092390	-0.618477	0.013679	-0.184963	-0.156181	-0.091304	-0.178404	-0.103832	-0.186096
(3,-1)	-0.092390		0.013679	-0.184963	-0.156181	-0.091304	-0.178404	-0.103832	-0.186096
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.092390	0.006200	-0.091086	-0.138738	-0.056468	-0.118931	-0.143690	-0.156872	-0.162343
(3,-1)	-0.092390	0.006200	-0.091086	-0.138738	-0.056468	-0.118931	-0.143690	-0.156872	-0.162343
(3,-1)	-0.092390	0.006200	-0.091086	-0.138738	-0.056468	-0.118931	-0.143690	-0.156872	-0.162343
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.092390	-0.610848	-0.213974	-0.049982	-0.148317	-0.112929	-0.121266		
(3,-1)	-0.092390	-0.610848	-0.213974	-0.049982	-0.148317	-0.112929	-0.121195		
(3,-1)	-0.092390		-0.213974	-0.049982	-0.148317	-0.112929	-0.121195		

Table S259: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>2</sub>S system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.688491	-0.630160	-0.656451	-0.634033	-0.662880	-0.616019	-0.629453	-0.645006	-0.566749
(3,-1)	-0.688491	-0.630160	-0.656451	-0.634033	-0.662880	-0.616019	-0.629453	-0.645006	-0.566749
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.688491	-0.748990	-0.647518	-0.672870	-0.655160	-0.646024	-0.626036	-0.667183	-0.648979
(3,-1)	-0.688491		-0.647518	-0.672870	-0.655160	-0.646024	-0.626036	-0.667183	-0.648979
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.688491	-0.630999	-0.698939	-0.739795	-0.828061	-0.655952	-0.659685	-0.654699	-0.642264
(3,-1)	-0.688491	-0.630999	-0.698939	-0.739795	-0.828061	-0.655952	-0.659685	-0.654699	-0.642264
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.688491	-0.774802	-0.673782	-0.739433	-0.683150	-0.677907	-0.683196		
(3,-1)	-0.688491		-0.673782	-0.739433	-0.683150	-0.677907	-0.683196		

Table S260: Laplacian of the density value (a.u.) at the considered critical points for the HCl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.884399	-0.836860	-0.850377	-0.822984	-0.862836	-0.755513	-0.806981	-0.820400	-0.836350
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.884399	-0.288913	-0.775120	-0.872246	-0.850880	-0.846201	-0.793745	-0.868302	-0.793636
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.884399	-0.706683	-0.938603	-1.005486	-1.225499	-0.856410	-0.859971	-0.845656	-0.826912
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.884399	-0.281742	-0.941109	-0.951527	-0.884216	-0.880481	-0.893373		

Table S261: Laplacian of the density value (a.u.) at the considered critical points for the S<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.267723	-0.221786	-0.240051	-0.230224	-0.253528	-0.221197	-0.209333	-0.182899	-0.264624
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.267723	-0.102091	-0.313148	-0.255325	-0.249439	-0.149087	-0.177181	-0.266809	-0.265200
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.267723	-0.156900	-0.257445	-0.295041	-0.363030	-0.248243	-0.257366	-0.257426	-0.244237
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.267723	-0.077577	-0.216055	-0.320136	-0.256440	-0.258929	-0.272513		



Table S262: Laplacian of the density value (a.u.) at the considered critical points for the Cl<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.078345	-0.023835	-0.030479	-0.033457	-0.061437	-0.008625	-0.017980	-0.053816	-0.048796
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.078345	0.198559	-0.109419	-0.053153	-0.061054	-0.032657	-0.047358	-0.086056	-0.061757
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.078345	-0.025435	-0.057845	-0.049527	-0.063499	-0.090888	-0.077020	-0.056434	-0.052109
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.078345	0.192560	-0.023608	-0.146924	-0.060585	-0.076228	-0.079035		

Table S263: Laplacian of the density value (a.u.) at the considered critical points for the NaCl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.194706	0.177004	0.178682	0.180519	0.187018	0.175720	0.181647	0.190298	0.193334
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.194706	1.395805	0.197828	0.182842	0.185576	0.189524	0.188171	0.188765	0.185833
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.194706	0.184300	0.185801	0.183887	0.179478	0.187500	0.187216	0.186884	0.187552
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.194706	1.390759	0.188189	0.196753	0.187506	0.191640	0.186347		

Table S264: Laplacian of the density value (a.u.) at the considered critical points for the SiO system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	1.423144	1.252647	1.292002	1.301235	1.352227	1.281384	1.267654	1.390228	1.538403
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	1.423144	0.142195	1.491654	1.324369	1.343426	1.289047	1.282225	1.381581	1.310786
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	1.423144	1.341143	1.408538	1.364560	1.433147	1.312015	1.323256	1.326498	1.286933
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	1.423144	0.077948	1.338712	1.466183	1.359633	1.390879	1.378056		

Table S265: Laplacian of the density value (a.u.) at the considered critical points for the CS system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.108551	-0.344336	-0.188562	-0.169960	-0.005919	-0.330448	-0.301054	0.137445	0.158754
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.108551	0.704738	0.436889	-0.094027	-0.048169	-0.218050	-0.206110	0.076185	-0.112487
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.108551	-0.060019	0.003089	-0.051056	-0.150800	0.035153	-0.024946	-0.119872	-0.144928
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.108551	0.654400	-0.080876	0.331782	-0.051617	0.027526	0.001288		

Table S266: Laplacian of the density value (a.u.) at the considered critical points for the SO system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.634199	0.387146	0.437660	0.477941	0.564689	0.408241	0.465818	0.740199	0.738793
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.634199	-0.439560	0.896349	0.498979	0.555063	0.600377	0.498754	0.646394	0.503357
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.634199	0.694611	0.629621	0.522703	0.546870	0.576163	0.560536	0.551208	0.487249
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.634199	-0.388158	0.513855	0.775565	0.532681	0.599654	0.573374		

Table S267: Laplacian of the density value (a.u.) at the considered critical points for the ClO• system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.380319	-0.242646	-0.259785	-0.265451	-0.336117	-0.227768	-0.241839	-0.329239	-0.365758
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.380319	-0.209321	-0.463730	-0.319577	-0.341249	-0.276411	-0.315168	-0.403635	-0.336657
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.380319	-0.259363	-0.341788	-0.319765	-0.359516	-0.374202	-0.365609	-0.343495	-0.316781
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.380319	-0.184979	-0.262255	-0.592787	-0.322503	-0.375126	-0.366856		

Table S268: Laplacian of the density value (a.u.) at the considered critical points for the CIF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.196364	-0.081760	-0.085357	-0.096835	-0.151282	-0.089828	-0.068770	-0.144382	-0.190563
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.196364	-0.337038	-0.227397	-0.132204	-0.154974	-0.147444	-0.157017	-0.200759	-0.156198
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.196364	-0.107681	-0.161567	-0.138881	-0.111852	-0.176666	-0.167823	-0.149995	-0.141646
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.196364	-0.315880	-0.122532	-0.301570	-0.143152	-0.181500	-0.174959		

Table S269: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>Cl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.319684	-0.245293	-0.268167	-0.259587	-0.297212	-0.227712	-0.239275	-0.241246	-0.318036
(3,-1)	-1.195145	-1.099573	-1.150489	-1.112003	-1.162417	-1.011596	-1.127764	-1.021657	-0.912903
(3,-1)	-1.195145	-1.099573	-1.150489	-1.112003	-1.162417	-1.011596	-1.127764	-1.021657	-0.912903
(3,-1)	-1.195145	-1.099573	-1.150489	-1.112003	-1.162417	-1.011596	-1.127764	-1.021657	-0.912903
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.319684	-0.329661	-0.354652	-0.291140	-0.288478	-0.185335	-0.221883	-0.316633	-0.293980
(3,-1)	-1.195145	-0.621834	-1.129092	-1.173683	-1.143296	-1.104784	-0.994721	-1.173751	-1.140953
(3,-1)	-1.195145	-1.008339	-1.129092	-1.173683	-1.143296	-1.104784	-0.994721	-1.173751	-1.140953
(3,-1)	-1.195145	-1.016271	-1.129092	-1.173683	-1.143296	-1.104784	-0.994721	-1.173751	-1.140953
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.319684	-0.204263	-0.265195	-0.301649	-0.314666	-0.308954	-0.300117	-0.279470	-0.275385
(3,-1)	-1.195145	-1.100809	-1.234946	-1.328992	-1.508640	-1.161723	-1.158561	-1.144641	-1.118420
(3,-1)	-1.195145	-1.100809	-1.234946	-1.328992	-1.508640	-1.161723	-1.158561	-1.144641	-1.118420
(3,-1)	-1.195145	-1.100809	-1.234946	-1.328992	-1.508640	-1.161723	-1.158561	-1.144641	-1.118420
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.319684	-0.324952	-0.233723	-0.393053	-0.301148	-0.309714	-0.318645		
(3,-1)	-1.195145	-0.612767	-1.229618	-1.265321	-1.190223	-1.179712	-1.189582		
(3,-1)	-1.195145	-0.977983	-1.229618	-1.265321	-1.190223	-1.179712	-1.189560		
(3,-1)	-1.195145	-0.985967	-1.229618	-1.265321	-1.190223	-1.179712	-1.189560		



Table S270: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>3</sub>C–SH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.339352	-0.268976	-0.297214	-0.284676	-0.318170	-0.256307	-0.263680	-0.283051	-0.340592
(3,-1)	-0.690687	-0.632076	-0.655243	-0.634695	-0.663576	-0.614880	-0.629451	-0.646487	-0.564828
(3,-1)	-1.140308	-1.051556	-1.098823	-1.062431	-1.109211	-0.964832	-1.075148	-0.989159	-0.888755
(3,-1)	-1.151212	-1.060486	-1.108058	-1.071694	-1.119161	-0.973074	-1.083821	-0.996599	-0.892893
(3,-1)	-1.151212	-1.060486	-1.108058	-1.071694	-1.119161	-0.973074	-1.083821	-0.996599	-0.892893
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.339352	-0.206825	-0.360529	-0.317308	-0.310251	-0.221184	-0.263243	-0.335426	-0.310911
(3,-1)	-0.690687	-2.616071	-0.650245	-0.672568	-0.656647	-0.647199	-0.629394	-0.669413	-0.649240
(3,-1)	-1.140308		-1.067053	-1.119576	-1.090636	-1.056950	-0.959549	-1.116912	-1.082953
(3,-1)	-1.151212		-1.076120	-1.129566	-1.100776	-1.067292	-0.968137	-1.128211	-1.093127
(3,-1)	-1.151212		-1.076120	-1.129566	-1.100776	-1.067292	-0.968137	-1.128211	-1.093127
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.339352	-0.232321	-0.294009	-0.325988	-0.314327	-0.325709	-0.322654	-0.308461	-0.299294
(3,-1)	-0.690687	-0.633339	-0.696849	-0.737813	-0.821367	-0.658055	-0.661459	-0.656102	-0.643896
(3,-1)	-1.140308	-1.049099	-1.180901	-1.271618	-1.458405	-1.105177	-1.102515	-1.090056	-1.065437
(3,-1)	-1.151212	-1.059522	-1.191030	-1.283310	-1.469471	-1.116579	-1.113655	-1.100520	-1.075105
(3,-1)	-1.151212	-1.059522	-1.191030	-1.283310	-1.469471	-1.116579	-1.113655	-1.100520	-1.075105
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.339352	-0.171026	-0.275946	-0.407079	-0.325310	-0.328953	-0.339930		
(3,-1)	-0.690687	-2.650721	-0.670650	-0.739756	-0.683439	-0.679780	-0.684451		
(3,-1)	-1.140308		-1.166301	-1.201846	-1.134969	-1.124392	-1.133299		
(3,-1)	-1.151212		-1.177900	-1.214543	-1.145488	-1.135260	-1.144531		
(3,-1)	-1.151212		-1.177900	-1.214543	-1.145488	-1.135260	-1.144531		

Table S271: Laplacian of the density value (a.u.) at the considered critical points for the HOCl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.163733	-0.080520	-0.086344	-0.093277	-0.138493	-0.072204	-0.070993	-0.135723	-0.146840
(3,-1)	-2.691307	-2.623911	-2.585876	-2.579684	-2.662581	-2.414024	-2.661832	-2.668999	-2.767575
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.163733	0.911236	-0.212002	-0.125086	-0.140791	-0.113951	-0.137937	-0.182211	-0.137093
(3,-1)	-2.691307	0.911236	-2.529539	-2.666247	-2.672874	-2.654122	-2.561366	-2.788578	-2.392755
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.163733	-0.088185	-0.134544	-0.112789	-0.102495	-0.170790	-0.160009	-0.140493	-0.129684
(3,-1)	-2.691307	-2.654321	-2.577212	-2.681757	-2.704749	-2.746507	-2.740917	-2.724315	-2.668563
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.163733	0.862857	-0.088593	-0.286830	-0.132253	-0.161644	-0.164609		
(3,-1)	-2.691307	0.862857	-2.943274	-2.924777	-2.684858	-2.725369	-2.690729		

Table S272: Laplacian of the density value (a.u.) at the considered critical points for the SO<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.834585	0.584709	0.638138	0.686807	0.751685	0.592514	0.658483	0.962715	0.983131
(3,-1)	0.834585	0.584709	0.638138	0.686807	0.751685	0.592514	0.658483	0.962715	0.983131
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.834585	1.359415	1.140444	0.682160	0.743819	0.788616	0.661258	0.825381	0.670947
(3,-1)	0.834585	1.359415	1.140444	0.682160	0.743819	0.788616	0.661258	0.825381	0.670947
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.834585	0.926742	0.833234	0.703015	0.736874	0.757672	0.744466	0.747453	0.651695
(3,-1)	0.834585	0.926742	0.833234	0.703015	0.736874	0.757672	0.744466	0.747453	0.651695
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.834585	1.330170	0.695131	0.896361	0.754141	0.820362	0.806024		
(3,-1)	0.834585	1.330170	0.695131	0.896361	0.754141	0.820362	0.806023		

Table S273: Laplacian of the density value (a.u.) at the considered critical points for the BF<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	1.242942	1.053621	1.072438	1.102448	1.179517	1.142648	1.128201	1.186855	1.541789
(3,-1)	1.242942	1.053621	1.072438	1.102448	1.179517	1.142648	1.128201	1.186855	1.541789
(3,-1)	1.242942	1.053621	1.072438	1.102448	1.179517	1.142648	1.128201	1.186855	1.541789
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	1.242942	0.172349	1.465478	1.114779	1.155836	1.145277	1.082310	1.223693	1.222852
(3,-1)	1.242942	0.172349	1.465478	1.114779	1.155836	1.145277	1.082310	1.223693	1.222852
(3,-1)	1.242942	0.172349	1.465478	1.114779	1.155836	1.145277	1.082310	1.223693	1.222852
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	1.242942	1.128225	1.195398	1.154282	1.231719	1.131546	1.132638	1.140190	1.156833
(3,-1)	1.242942	1.128225	1.195398	1.154282	1.231719	1.131546	1.132638	1.140190	1.156833
(3,-1)	1.242942	1.128225	1.195398	1.154282	1.231719	1.131546	1.132638	1.140190	1.156833
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	1.242942	0.099646	1.131229	1.319070	1.168456	1.223279	1.216062		
(3,-1)	1.242942	0.099646	1.131229	1.319070	1.168456	1.223280	1.216165		
(3,-1)	1.242942	0.099646	1.131229	1.319070	1.168456	1.223280	1.216165		

Table S274: Laplacian of the density value (a.u.) at the considered critical points for the BCl<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.014863	-0.121055	-0.128819	-0.079794	-0.030113	-0.095323	-0.022720	0.028303	0.235563
(3,-1)	-0.014863	-0.121055	-0.128819	-0.079794	-0.030113	-0.095323	-0.022720	0.028303	0.235563
(3,-1)	-0.014863	-0.121055	-0.128819	-0.079794	-0.030113	-0.095323	-0.022720	0.028303	0.235563
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.014863	1.019658	0.207509	-0.102920	-0.048535	-0.001753	-0.097718	0.013235	-0.020455
(3,-1)	-0.014863	1.019658	0.207509	-0.102920	-0.048535	-0.001753	-0.097718	0.013235	-0.020455
(3,-1)	-0.014863	1.019658	0.207509	-0.102920	-0.048535	-0.001753	-0.097718	0.013235	-0.020455
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.014863	0.007584	-0.032172	-0.098319	-0.041468	-0.026431	-0.048848	-0.049428	-0.028114
(3,-1)	-0.014863	0.007584	-0.032172	-0.098319	-0.041468	-0.026431	-0.048848	-0.049428	-0.028114
(3,-1)	-0.014863	0.007584	-0.032172	-0.098319	-0.041468	-0.026431	-0.048848	-0.049428	-0.028114
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.014863	1.011258	-0.059841	0.040369	-0.067950	-0.011770	-0.024934		
(3,-1)	-0.014863	1.011258	-0.059841	0.040369	-0.067951	-0.011770	-0.024750		
(3,-1)	-0.014863	1.011258	-0.059841	0.040369	-0.067951	-0.011770	-0.024750		

Table S275: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{AlF}_3$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	1.031245	0.936206	0.949148	0.955763	0.988102	0.935784	0.941075	1.012312	1.099366
(3,-1)	1.031245	0.936206	0.949148	0.955763	0.988102	0.935784	0.941075	1.012312	1.099366
(3,-1)	1.031245	0.936206	0.949148	0.955763	0.988102	0.935784	0.941075	1.012312	1.099366
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	1.031245	0.387168	1.061266	0.969681	0.982080	0.995743	0.988772	1.007152	0.969706
(3,-1)	1.031245	0.387168	1.061266	0.969681	0.982080	0.995743	0.988772	1.007152	0.969706
(3,-1)	1.031245	0.387168	1.061266	0.969681	0.982080	0.995743	0.988772	1.007152	0.969706
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	1.031245	0.970288	0.994864	0.982320	0.964265	0.972698	0.976124	0.979036	0.955685
(3,-1)	1.031245	0.970288	0.994864	0.982320	0.964265	0.972698	0.976124	0.979036	0.955685
(3,-1)	1.031245	0.970288	0.994864	0.982320	0.964265	0.972698	0.976124	0.979036	0.955685
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	1.031245	0.371553	0.990905	1.057316	0.993215	1.013970	1.002603		
(3,-1)	1.031245	0.371553	0.990905	1.057316	0.993215	1.013971	1.002611		
(3,-1)	1.031245	0.371553	0.990905	1.057316	0.993215	1.013971	1.002612		

Table S276: Laplacian of the density value (a.u.) at the considered critical points for the AlCl<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.378431	0.307833	0.320091	0.327219	0.349592	0.331566	0.314123	0.353794	0.425529
(3,-1)	0.378431	0.307833	0.320091	0.327219	0.349592	0.331566	0.314123	0.353794	0.425529
(3,-1)	0.378431	0.307833	0.320091	0.327219	0.349592	0.331566	0.314123	0.353794	0.425529
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.378431	-0.370113	0.412090	0.332451	0.343259	0.329839	0.319165	0.356846	0.342996
(3,-1)	0.378431	-0.370113	0.412090	0.332451	0.343259	0.329839	0.319165	0.356846	0.342996
(3,-1)	0.378431	-0.370113	0.412090	0.332451	0.343259	0.329839	0.319165	0.356846	0.342996
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.378431	0.319978	0.351157	0.344392	0.370411	0.336314	0.334843	0.332755	0.332279
(3,-1)	0.378431	0.319978	0.351157	0.344392	0.370411	0.336314	0.334843	0.332755	0.332279
(3,-1)	0.378431	0.319978	0.351157	0.344392	0.370411	0.336314	0.334843	0.332755	0.332279
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.378431	-0.436136	0.355333	0.390510	0.350554	0.365908	0.359243		
(3,-1)	0.378431	-0.436136	0.355333	0.390510	0.350554	0.365908	0.359266		
(3,-1)	0.378431	-0.436136	0.355333	0.390510	0.350554	0.365908	0.359266		

Table S277: Laplacian of the density value (a.u.) at the considered critical points for the CF<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.644833	-0.737191	-0.796943	-0.725754	-0.650161	-0.780753	-0.708703	-0.504383	-0.228455
(3,-1)	-0.644833	-0.737191	-0.796943	-0.725754	-0.650161	-0.780753	-0.708703	-0.504383	-0.228455
(3,-1)	-0.644833	-0.737191	-0.796943	-0.725754	-0.650161	-0.780753	-0.708703	-0.504383	-0.228455
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.644833	-0.336189	-0.180581	-0.763613	-0.669124	-0.494744	-0.648400	-0.540430	-0.677109
(3,-1)	-0.644833	-0.336189	-0.180581	-0.763613	-0.669124	-0.494744	-0.648400	-0.540430	-0.677109
(3,-1)	-0.644833	-0.336189	-0.180581	-0.763613	-0.669124	-0.494744	-0.648400	-0.540430	-0.677109
(3,-1)	-0.644833	-0.336189	-0.180581	-0.763613	-0.669124	-0.494744	-0.648400	-0.540430	-0.677109
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.644833	-0.536873	-0.573611	-0.691244	-0.691524	-0.619656	-0.661410	-0.668935	-0.730814
(3,-1)	-0.644833	-0.536873	-0.573611	-0.691244	-0.691524	-0.619656	-0.661410	-0.668935	-0.730814
(3,-1)	-0.644833	-0.536873	-0.573611	-0.691244	-0.691524	-0.619656	-0.661410	-0.668935	-0.730814
(3,-1)	-0.644833	-0.536873	-0.573611	-0.691244	-0.691524	-0.619656	-0.661410	-0.668935	-0.730814
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.644833	-0.321777	-0.654538	-0.394300	-0.719827	-0.601891	-0.617842		
(3,-1)	-0.644833	-0.321777	-0.654538	-0.394300	-0.719827	-0.601891	-0.617842		
(3,-1)	-0.644833	-0.321777	-0.654538	-0.394300	-0.719827	-0.601891	-0.617844		
(3,-1)	-0.644833	-0.321777	-0.654538	-0.394300	-0.719827	-0.601891	-0.617842		



Table S278: Laplacian of the density value (a.u.) at the considered critical points for the CCl<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.333776	-0.249771	-0.268003	-0.262825	-0.308248	-0.232669	-0.235868	-0.247790	-0.328841
(3,-1)	-0.333776	-0.249771	-0.268003	-0.262825	-0.308248	-0.232669	-0.235868	-0.247790	-0.328841
(3,-1)	-0.333776	-0.249771	-0.268003	-0.262825	-0.308248	-0.232669	-0.235868	-0.247790	-0.328841
(3,-1)	-0.333776	-0.249771	-0.268003	-0.262825	-0.308248	-0.232669	-0.235868	-0.247790	-0.328841
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.333776	0.491007	-0.361558	-0.299123	-0.300963	-0.188518	-0.227486	-0.332900	-0.304131
(3,-1)	-0.333776	0.625705	-0.361558	-0.299123	-0.300963	-0.188518	-0.227486	-0.332900	-0.304131
(3,-1)	-0.333776		-0.361558	-0.299123	-0.300963	-0.188518	-0.227486	-0.332900	-0.304131
(3,-1)	-0.333776		-0.361558	-0.299123	-0.300963	-0.188518	-0.227486	-0.332900	-0.304131
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.333776	-0.210476	-0.283908	-0.323209	-0.332729	-0.329257	-0.317820	-0.292346	-0.283440
(3,-1)	-0.333776	-0.210476	-0.283908	-0.323209	-0.332729	-0.329257	-0.317820	-0.292346	-0.283440
(3,-1)	-0.333776	-0.210476	-0.283908	-0.323209	-0.332729	-0.329257	-0.317820	-0.292346	-0.283440
(3,-1)	-0.333776	-0.210476	-0.283908	-0.323209	-0.332729	-0.329257	-0.317820	-0.292346	-0.283440
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.333776	0.449036	-0.261061	-0.423752	-0.307250	-0.321649	-0.330195		
(3,-1)	-0.333776	0.478719	-0.261061	-0.423752	-0.307250	-0.321649	-0.330195		
(3,-1)	-0.333776		-0.261061	-0.423752	-0.307250	-0.321649	-0.330196		
(3,-1)	-0.333776		-0.261061	-0.423752	-0.307250	-0.321649	-0.330195		

Table S279: Laplacian of the density value (a.u.) at the considered critical points for the O=C=S system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.483546	0.087801	0.198838	0.213158	0.361374	0.075352	0.135713	0.466694	0.526127
(3,-1)	0.147404	-0.082754	-0.056106	0.048403	0.098352	-0.256978	0.027848	0.511807	0.772850
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.483546	0.357617	0.669103	0.293298	0.332614	0.261907	0.228513	0.446746	0.312845
(3,-1)	0.147404	0.357617	0.890311	-0.048036	0.060539	0.155059	0.010410	0.241861	0.078734
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.483546	0.382360	0.413076	0.368097	0.365066	0.412840	0.359143	0.284869	0.258492
(3,-1)	0.147404	0.387130	0.139258	-0.154406	-0.131504	0.071480	0.017566	0.033109	-0.160752
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.483546	0.314935	0.367366	0.669525	0.344627	0.417339	0.391107		
(3,-1)	0.147404	0.314935	-0.161892	0.063489	0.085455	0.172908	0.158347		

Table S280: Laplacian of the density value (a.u.) at the considered critical points for the CS<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.350892	-0.052044	0.058558	0.083180	0.232890	-0.054027	-0.010522	0.334305	0.390031
(3,-1)	0.350892	-0.052044	0.058558	0.083180	0.232890	-0.054027	-0.010522	0.334305	0.390031
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.350892	0.311456	0.577128	0.153384	0.202390	0.094109	0.062882	0.319395	0.170060
(3,-1)	0.350892	-0.153413	0.577128	0.153384	0.202390	0.094109	0.062882	0.319395	0.170060
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.350892	0.245587	0.273588	0.226265	0.219986	0.296785	0.236515	0.150967	0.117906
(3,-1)	0.350892	0.245587	0.273588	0.226265	0.219986	0.296785	0.236515	0.150967	0.117906
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.350892	0.162577	0.225311	0.547694	0.203159	0.282655	0.256764		
(3,-1)	0.350892	-0.223124	0.225311	0.547694	0.203159	0.282655	0.256764		

Table S281: Laplacian of the density value (a.u.) at the considered critical points for the COF<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.142225	-0.416430	-0.411594	-0.288218	-0.216141	-0.550585	-0.332135	0.155759	0.435753
(3,-1)	-0.428877	-0.538267	-0.582588	-0.514215	-0.437817	-0.549739	-0.488927	-0.295453	-0.025769
(3,-1)	-0.428877	-0.538267	-0.582588	-0.514215	-0.437817	-0.549739	-0.488927	-0.295453	-0.025769
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.142225	1.138561	0.595596	-0.380627	-0.248858	-0.176542	-0.329816	-0.048315	-0.255324
(3,-1)	-0.428877	1.138561	0.022049	-0.546131	-0.458540	-0.306499	-0.461176	-0.343181	-0.442275
(3,-1)	-0.428877	1.138561	0.022049	-0.546131	-0.458540	-0.306499	-0.461176	-0.343181	-0.442275
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.142225	0.102097	-0.146935	-0.438333	-0.361268	-0.196677	-0.267795	-0.276324	-0.492550
(3,-1)	-0.428877	-0.328568	-0.365599	-0.475707	-0.475209	-0.425283	-0.459687	-0.463854	-0.506673
(3,-1)	-0.428877	-0.328568	-0.365599	-0.475707	-0.475209	-0.425283	-0.459687	-0.463854	-0.506673
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.142225	1.127510	-0.442537	-0.145037	-0.272915	-0.154137	-0.182318		
(3,-1)	-0.428877	1.127510	-0.463863	-0.231294	-0.498108	-0.392761	-0.399785		
(3,-1)	-0.428877	1.127510	-0.463863	-0.231294	-0.498108	-0.392761	-0.399785		

Table S282: Laplacian of the density value (a.u.) at the considered critical points for the SiF<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	1.152353	1.021992	1.041066	1.054635	1.098205	1.048577	1.027252	1.130720	1.269807
(3,-1)	1.152353	1.021992	1.041066	1.054635	1.098205	1.048577	1.027252	1.130720	1.269807
(3,-1)	1.152353	1.021992	1.041066	1.054635	1.098205	1.048577	1.027252	1.130720	1.269807
(3,-1)	1.152353	1.021992	1.041066	1.054635	1.098205	1.048577	1.027252	1.130720	1.269807
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	1.152353	0.320524	1.216922	1.068321	1.089584	1.087852	1.065863	1.121366	1.072289
(3,-1)	1.152353	0.320524	1.216922	1.068321	1.089584	1.087852	1.065863	1.121366	1.072289
(3,-1)	1.152353	0.320524	1.216922	1.068321	1.089584	1.087852	1.065863	1.121366	1.072289
(3,-1)	1.152353	0.320524	1.216922	1.068321	1.089584	1.087852	1.065863	1.121366	1.072289
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	1.152353	1.063488	1.103456	1.081520	1.078675	1.066541	1.072380	1.076254	1.047521
(3,-1)	1.152353	1.063488	1.103456	1.081520	1.078675	1.066541	1.072380	1.076254	1.047521
(3,-1)	1.152353	1.063488	1.103456	1.081520	1.078675	1.066541	1.072380	1.076254	1.047521
(3,-1)	1.152353	1.063488	1.103456	1.081520	1.078675	1.066541	1.072380	1.076254	1.047521
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	1.152353	0.290482	1.089818	1.191994	1.101234	1.132195	1.119959		
(3,-1)	1.152353	0.290482	1.089818	1.191994	1.101234	1.132195	1.119959		
(3,-1)	1.152353	0.290482	1.089818	1.191994	1.101234	1.132195	1.119959		
(3,-1)	1.152353	0.290482	1.089818	1.191994	1.101234	1.132195	1.119959		

Table S283: Laplacian of the density value (a.u.) at the considered critical points for the SiCl<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.283758	0.187453	0.199313	0.218399	0.248075	0.199150	0.219035	0.280400	0.348082
(3,-1)	0.283758	0.187453	0.199313	0.218399	0.248075	0.199150	0.219035	0.280400	0.348082
(3,-1)	0.283758	0.187453	0.199313	0.218399	0.248075	0.199150	0.219035	0.280400	0.348082
(3,-1)	0.283758	0.187453	0.199313	0.218399	0.248075	0.199150	0.219035	0.280400	0.348082
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.283758	-1.328572	0.367207	0.218037	0.241947	0.243514	0.205582	0.273540	0.240817
(3,-1)	0.283758	-1.290442	0.367207	0.218037	0.241947	0.243514	0.205582	0.273540	0.240817
(3,-1)	0.283758		0.367207	0.218037	0.241947	0.243514	0.205582	0.273540	0.240817
(3,-1)	0.283758		0.367207	0.218037	0.241947	0.243514	0.205582	0.273540	0.240817
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.283758	0.258920	0.262215	0.226663	0.264325	0.238671	0.237023	0.238799	0.239532
(3,-1)	0.283758	0.258920	0.262215	0.226663	0.264325	0.238671	0.237023	0.238799	0.239532
(3,-1)	0.283758	0.258920	0.262215	0.226663	0.264325	0.238671	0.237023	0.238799	0.239532
(3,-1)	0.283758	0.258920	0.262215	0.226663	0.264325	0.238671	0.237023	0.238799	0.239532
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.283758	-1.397858	0.247973	0.310649	0.243669	0.271916	0.265905		
(3,-1)	0.283758	-1.292027	0.247973	0.310649	0.243669	0.271916	0.265906		
(3,-1)	0.283758		0.247973	0.310649	0.243669	0.271916	0.265906		
(3,-1)	0.283758		0.247973	0.310649	0.243669	0.271916	0.265907		

Table S284: Laplacian of the density value (a.u.) at the considered critical points for the N<sub>2</sub>O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.458947	-1.372729	-1.411487	-1.375834	-1.418339	-1.363996	-1.349062	-1.101058	-1.510961
(3,-1)	-1.298648	-1.240046	-1.265794	-1.248354	-1.311523	-1.133344	-1.158956	-1.031906	-1.221224
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.458947	0.092073	-1.403844	-1.436184	-1.412112	-1.088977	-1.102645	-1.447075	-1.277546
(3,-1)	-1.298648	-2.207768	-1.288230	-1.304459	-1.297813	-0.872351	-0.957105	-1.343340	-1.148240
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.458947	-1.234433	-1.478419	-1.710186	-2.040239	-1.304242	-1.366641	-1.408779	-1.345412
(3,-1)	-1.298648	-1.000994	-1.337524	-1.495909	-1.856366	-1.249936	-1.262793	-1.240132	-1.195578
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.458947	0.092026	-1.452374	-1.567556	-1.437422	-1.430052	-1.474895		
(3,-1)	-1.298648	-2.206550	-1.314962	-1.441462	-1.302254	-1.312185	-1.353845		

Table S285: Laplacian of the density value (a.u.) at the considered critical points for the ClNO system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.080210	0.123469	0.127195	0.122387	0.101223	0.116124	0.122619	0.123028	0.105463
(3,-1)	-2.282068	-2.035914	-2.103334	-2.076424	-2.215385	-1.914163	-2.023894	-1.859307	-2.261457
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.080210	-0.479123	0.100436	0.105695	0.096441	0.093906	0.094163	0.078941	0.103557
(3,-1)	-2.282068	-0.479123	-2.262711	-2.193796	-2.194888	-1.665840	-1.731850	-2.325720	-1.953242
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.080210	0.094813	0.093311	0.095648	0.103872	0.078260	0.082358	0.089545	0.091818
(3,-1)	-2.282068	-1.969093	-2.249774	-2.500191	-2.855946	-2.134267	-2.161188	-2.152266	-2.041407
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.080210	-0.438413	0.089656	0.023768	0.114208	0.096286	0.096953		
(3,-1)	-2.282068	-0.438413	-2.232514	-2.595449	-2.194914	-2.236349	-2.281325		



Table S286: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{NF}_3$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.412531	-0.217203	-0.221337	-0.229454	-0.347469	-0.194171	-0.221586	-0.321314	-0.444127
(3,-1)	-0.412531	-0.217203	-0.221337	-0.229454	-0.347469	-0.194171	-0.221586	-0.321314	-0.444127
(3,-1)	-0.412531	-0.217203	-0.221337	-0.229454	-0.347469	-0.194171	-0.221586	-0.321314	-0.444127
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.412531	0.823074	-0.443772	-0.321953	-0.352208	-0.282161	-0.337218	-0.442200	-0.343915
(3,-1)	-0.412531	0.823074	-0.443772	-0.321953	-0.352208	-0.282161	-0.337218	-0.442200	-0.343915
(3,-1)	-0.412531	0.823074	-0.443772	-0.321953	-0.352208	-0.282161	-0.337218	-0.442200	-0.343915
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.412531	-0.285962	-0.344594	-0.320709	-0.360712	-0.384313	-0.374773	-0.349362	-0.321498
(3,-1)	-0.412531	-0.285962	-0.344594	-0.320709	-0.360712	-0.384313	-0.374773	-0.349362	-0.321498
(3,-1)	-0.412531	-0.285962	-0.344594	-0.320709	-0.360712	-0.384313	-0.374773	-0.349362	-0.321498
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.412531	0.801215	-0.262183	-0.679015	-0.334281	-0.401364	-0.393657		
(3,-1)	-0.412531	0.801215	-0.262183	-0.679015	-0.334281	-0.401364	-0.393657		
(3,-1)	-0.412531	0.801215	-0.262183	-0.679015	-0.334281	-0.401364	-0.393657		

Table S287: Laplacian of the density value (a.u.) at the considered critical points for the PF<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.795680	0.640253	0.657288	0.679615	0.731615	0.663866	0.661512	0.788263	0.883285
(3,-1)	0.795680	0.640253	0.657288	0.679615	0.731615	0.663866	0.661512	0.788263	0.883285
(3,-1)	0.795680	0.640253	0.657288	0.679615	0.731615	0.663866	0.661512	0.788263	0.883285
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.795680	-0.323233	0.909613	0.693456	0.725658	0.727305	0.676810	0.772479	0.730247
(3,-1)	0.795680	-0.323233	0.909613	0.693456	0.725658	0.727305	0.676810	0.772479	0.730247
(3,-1)	0.795680		0.909613	0.693456	0.725658	0.727305	0.676810	0.772479	0.730247
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.795680	0.753367	0.773029	0.723653	0.764518	0.710162	0.712744	0.716504	0.706550
(3,-1)	0.795680	0.753367	0.773029	0.723653	0.764518	0.710162	0.712744	0.716504	0.706550
(3,-1)	0.795680	0.753367	0.773029	0.723653	0.764518	0.710162	0.712744	0.716504	0.706550
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.795680	-0.284164	0.720278	0.859769	0.731858	0.775633	0.769108		
(3,-1)	0.795680	-0.284164	0.720278	0.859769	0.731858	0.775632	0.768979		
(3,-1)	0.795680		0.720278	0.859769	0.731858	0.775632	0.768979		

Table S288: Laplacian of the density value (a.u.) at the considered critical points for the O<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.257655	-0.148647	-0.145743	-0.155538	-0.245462	-0.042407	-0.129115	-0.213164	-0.277593
(3,-1)	-0.257655	-0.148647	-0.145743	-0.155538	-0.245462	-0.042407	-0.129115	-0.213164	-0.277593
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.257655	0.210725	-0.299007	-0.224598	-0.250288	-0.096702	-0.163478	-0.323230	-0.188274
(3,-1)	-0.257655	0.210725	-0.299007	-0.224598	-0.250288	-0.096702	-0.163478	-0.323230	-0.188274
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.257655	-0.149527	-0.226762	-0.223868	-0.355640	-0.287717	-0.266383	-0.230948	-0.182923
(3,-1)	-0.257655	-0.149527	-0.226762	-0.223868	-0.355640	-0.287717	-0.266383	-0.230948	-0.182923
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.257655	0.200200	-0.166923	-0.439197	-0.203854	-0.257946	-0.263916		
(3,-1)	-0.257655	0.200200	-0.166923	-0.439197	-0.203854	-0.257946	-0.263916		

Table S289: Laplacian of the density value (a.u.) at the considered critical points for the F<sub>2</sub>O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.236555	0.332796	0.342425	0.327778	0.240405	0.330185	0.329468	0.244213	0.160805
(3,-1)	0.236555	0.332796	0.342425	0.327778	0.240405	0.330185	0.329468	0.244213	0.160805
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.236555	-0.320685	0.191343	0.259727	0.226727	0.196835	0.187365	0.157874	0.243293
(3,-1)	0.236555	-0.003216	0.191343	0.259727	0.226727	0.196835	0.187365	0.157874	0.243293
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.236555	0.228399	0.227816	0.253020	0.309650	0.198603	0.203755	0.216710	0.241942
(3,-1)	0.236555	0.228399	0.227816	0.253020	0.309650	0.198603	0.203755	0.216710	0.241942
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.236555	-0.302393	0.256143	-0.025542	0.272924	0.212222	0.211727		
(3,-1)	0.236555	0.004006	0.256143	-0.025542	0.272924	0.212222	0.211727		

Table S290: Laplacian of the density value (a.u.) at the considered critical points for the ClF<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.326868	-0.143228	-0.150367	-0.162062	-0.247178	-0.152809	-0.128361	-0.236859	-0.309471
(3,-1)	-0.024462	0.091647	0.091940	0.081080	0.031906	0.079763	0.106100	0.050748	-0.002792
(3,-1)	-0.024462	0.091647	0.091940	0.081080	0.031906	0.079763	0.106100	0.050748	-0.002792
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.326868	-1.126185	-0.342206	-0.224918	-0.254241	-0.244406	-0.262034	-0.321880	-0.256302
(3,-1)	-0.024462	0.197440	-0.008882	0.047168	0.025714	0.015874	0.017744	-0.013200	0.033132
(3,-1)	-0.024462	0.197440	-0.008882	0.047168	0.025714	0.015874	0.017744	-0.013200	0.033132
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.326868	-0.209322	-0.274000	-0.249747	-0.244259	-0.278150	-0.272192	-0.252946	-0.236767
(3,-1)	-0.024462	0.044569	0.019018	0.023208	0.057809	0.002364	0.011427	0.028030	0.031549
(3,-1)	-0.024462	0.044569	0.019018	0.023208	0.057809	0.002364	0.011427	0.028030	0.031549
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.326868	-1.106466	-0.212112	-0.508659	-0.242988	-0.299362	-0.291027		
(3,-1)	-0.024462	0.116373	0.029274	-0.108982	0.039479	0.002284	0.005415		
(3,-1)	-0.024462	0.116373	0.029274	-0.108982	0.039479	0.002284	0.005416		

Table S291: Laplacian of the density value (a.u.) at the considered critical points for the  $F_2C=CF_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.162646	-1.048682	-1.102257	-1.067090	-1.120230	-1.039631	-1.078672	-1.133209	-1.136623
(3,-1)	-0.111320	-0.280481	-0.295495	-0.230604	-0.116637	-0.269146	-0.161494	0.031433	0.392255
(3,-1)	-0.111320	-0.280481	-0.295495	-0.230604	-0.116637	-0.269146	-0.161494	0.031433	0.392255
(3,-1)	-0.111320	-0.280481	-0.295495	-0.230604	-0.116637	-0.269146	-0.161494	0.031433	0.392255
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.162646	-1.015098	-1.115010	-1.133906	-1.110639	-1.143309	-1.156130	-1.149047	-1.071286
(3,-1)	-0.111320	-0.414592	0.376401	-0.237193	-0.153093	0.047575	-0.153884	-0.022772	-0.136359
(3,-1)	-0.111320	-0.414592	0.376401	-0.237193	-0.153093	0.047575	-0.153884	-0.022772	-0.136359
(3,-1)	-0.111320	-0.414592	0.376401	-0.237193	-0.153093	0.047575	-0.153884	-0.022772	-0.136359
(3,-1)	-0.111320	-0.414592	0.376401	-0.237193	-0.153093	0.047575	-0.153884	-0.022772	-0.136359
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.162646	-1.064466	-1.162862	-1.195036	-1.143539	-1.069934	-1.099926	-1.122150	-1.075957
(3,-1)	-0.111320	-0.055774	-0.080038	-0.174640	-0.209289	-0.113848	-0.152813	-0.159724	-0.186489
(3,-1)	-0.111320	-0.055774	-0.080038	-0.174640	-0.209289	-0.113848	-0.152813	-0.159724	-0.186489
(3,-1)	-0.111320	-0.055774	-0.080038	-0.174640	-0.209289	-0.113848	-0.152813	-0.159724	-0.186489
(3,-1)	-0.111320	-0.055774	-0.080038	-0.174640	-0.209289	-0.113848	-0.152813	-0.159724	-0.186489
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.162646	-1.013175	-1.138674	-1.255623	-1.144645	-1.141659	-1.153127		
(3,-1)	-0.111320	-0.402374	-0.160755	0.112756	-0.185416	-0.080999	-0.091024		
(3,-1)	-0.111320	-0.402374	-0.160755	0.112756	-0.185416	-0.080999	-0.091024		
(3,-1)	-0.111320	-0.402374	-0.160755	0.112756	-0.185416	-0.080999	-0.091025		
(3,-1)	-0.111320	-0.402374	-0.160755	0.112756	-0.185416	-0.080999	-0.091025		

Table S292: Laplacian of the density value (a.u.) at the considered critical points for the Cl<sub>2</sub>C=CCl<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.066921	-0.957893	-1.006322	-0.975688	-1.026068	-0.961693	-0.973300	-1.016466	-1.091713
(3,-1)	-0.412236	-0.325518	-0.348291	-0.338623	-0.385109	-0.309541	-0.307562	-0.303647	-0.411172
(3,-1)	-0.412236	-0.325518	-0.348291	-0.338623	-0.385109	-0.309541	-0.307562	-0.303647	-0.411172
(3,-1)	-0.412236	-0.325518	-0.348291	-0.338623	-0.385109	-0.309541	-0.307562	-0.303647	-0.411172
(3,-1)	-0.412236	-0.325518	-0.348291	-0.338623	-0.385109	-0.309541	-0.307562	-0.303647	-0.411172
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.066921	-0.759305	-1.011754	-1.035711	-1.015812	-0.977816	-1.010595	-1.049194	-0.979368
(3,-1)	-0.412236	-0.316652	-0.437388	-0.378427	-0.376204	-0.239040	-0.288914	-0.408142	-0.380472
(3,-1)	-0.412236	-0.316652	-0.437388	-0.378427	-0.376204	-0.239040	-0.288914	-0.408142	-0.380472
(3,-1)	-0.412236	-0.316652	-0.437388	-0.378427	-0.376204	-0.239040	-0.288914	-0.408142	-0.380472
(3,-1)	-0.412236	0.208624	-0.437388	-0.378427	-0.376204	-0.239040	-0.288914	-0.408142	-0.380472
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.066921	-0.931135	-1.042555	-1.106302	-1.062809	-0.981881	-1.007557	-1.022610	-0.980885
(3,-1)	-0.412236	-0.255613	-0.361677	-0.411486	-0.437778	-0.394968	-0.389827	-0.368171	-0.357091
(3,-1)	-0.412236	-0.255613	-0.361677	-0.411486	-0.437778	-0.394968	-0.389827	-0.368171	-0.357091
(3,-1)	-0.412236	-0.255613	-0.361677	-0.411486	-0.437778	-0.394968	-0.389827	-0.368171	-0.357091
(3,-1)	-0.412236	-0.255613	-0.361677	-0.411486	-0.437778	-0.394968	-0.389827	-0.368171	-0.357091
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.066921	-0.783981	-1.052019	-1.156960	-1.045316	-1.044166	-1.061612		
(3,-1)	-0.412236	-0.381545	-0.339591	-0.505075	-0.385386	-0.396768	-0.410014		
(3,-1)	-0.412236	-0.381545	-0.339591	-0.505075	-0.385386	-0.396768	-0.410014		
(3,-1)	-0.412236	-0.381545	-0.339591	-0.505075	-0.385386	-0.396768	-0.410013		
(3,-1)	-0.412236	0.112236	-0.339591	-0.505075	-0.385386	-0.396768	-0.410013		

Table S293: Laplacian of the density value (a.u.) at the considered critical points for the CF<sub>3</sub>CN system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.903293	-0.765967	-0.818369	-0.789578	-0.860928	-0.736923	-0.782104	-0.885602	-0.770764
(3,-1)	-0.585996	-0.677475	-0.727706	-0.667599	-0.591551	-0.724233	-0.639561	-0.450396	-0.168523
(3,-1)	-0.585996	-0.677475	-0.727706	-0.667599	-0.591551	-0.724233	-0.639561	-0.450396	-0.168523
(3,-1)	-0.585996	-0.677475	-0.727706	-0.667599	-0.591551	-0.724233	-0.639561	-0.450396	-0.168523
(3,-1)	-0.174401	-0.649603	-0.556494	-0.477160	-0.309756	-0.886943	-0.583263	-0.060734	0.347541
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.903293	-1.214238	-0.812609	-0.862100	-0.846094	-0.899798	-0.878746	-0.893278	-0.812795
(3,-1)	-0.585996	-0.707712	-0.139489	-0.695488	-0.613375	-0.432058	-0.582630	-0.490291	-0.609716
(3,-1)	-0.585996	-1.132181	-0.139489	-0.695488	-0.613375	-0.432058	-0.582630	-0.490291	-0.609716
(3,-1)	-0.585996	-0.992146	-0.139489	-0.695488	-0.613375	-0.432058	-0.582630	-0.490291	-0.609716
(3,-1)	-0.174401	-0.992146	0.437346	-0.465776	-0.361332	-0.525844	-0.599510	-0.110685	-0.338658
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.903293	-0.749973	-0.913867	-0.934586	-0.936302	-0.861724	-0.862770	-0.848777	-0.819368
(3,-1)	-0.585996	-0.494581	-0.521321	-0.621794	-0.638154	-0.566470	-0.607337	-0.616570	-0.664015
(3,-1)	-0.585996	-0.494581	-0.521321	-0.621794	-0.638154	-0.566470	-0.607337	-0.616570	-0.664015
(3,-1)	-0.585996	-0.494581	-0.521321	-0.621794	-0.638154	-0.566470	-0.607337	-0.616570	-0.664015
(3,-1)	-0.174401	-0.078568	-0.230193	-0.417195	-0.196847	-0.248681	-0.367401	-0.459808	-0.629228
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.903293	-1.221352	-0.901495	-1.038988	-0.875231	-0.883236	-0.897491		
(3,-1)	-0.585996	-0.728755	-0.593348	-0.335242	-0.655396	-0.548477	-0.560506		
(3,-1)	-0.585996	-1.107285	-0.593348	-0.335242	-0.655396	-0.548477	-0.560427		
(3,-1)	-0.585996	-0.964287	-0.593348	-0.335242	-0.655396	-0.548477	-0.560428		
(3,-1)	-0.174401	-0.964287	-0.407074	-0.013021	-0.379297	-0.255792	-0.313171		



Table S294: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{CH}\equiv\text{C}-\text{CH}_3$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.227596	-1.184136	-1.218053	-1.182339	-1.182748	-1.259780	-1.226101	-1.077595	-0.877049
(3,-1)	-0.797566	-0.685154	-0.737401	-0.708071	-0.761269	-0.678056	-0.691357	-0.764159	-0.752205
(3,-1)	-1.258913	-1.178516	-1.216325	-1.178712	-1.229553	-1.080289	-1.193770	-1.062475	-1.038312
(3,-1)	-1.122870	-1.032774	-1.081410	-1.044378	-1.090304	-0.953784	-1.054635	-0.973342	-0.877049
(3,-1)	-1.122870	-1.032774	-1.081410	-1.044378	-1.090304	-0.953784	-1.054635	-0.973342	-0.877049
(3,-1)	-1.122870	-1.032774	-1.081410	-1.044378	-1.090304	-0.953784	-1.054635	-0.973342	-0.877049
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.227596	-1.143870	-1.001480	-1.222098	-1.193678	-1.159461	-1.120089	-1.201277	-1.127758
(3,-1)	-0.797566	-1.143870	-0.747116	-0.766369	-0.747112	-0.715983	-0.739343	-0.782192	-0.722958
(3,-1)	-1.258913	-1.021111	-1.187270	-1.243410	-1.214488	-1.168245	-1.042181	-1.244466	-1.206797
(3,-1)	-1.122870	-1.021111	-1.047481	-1.102097	-1.072465	-1.035887	-0.943541	-1.098338	-1.061346
(3,-1)	-1.122870	-1.021111	-1.047481	-1.102097	-1.072465	-1.035887	-0.943541	-1.098338	-1.061346
(3,-1)	-1.122870	-1.021111	-1.047481	-1.102097	-1.072465	-1.035887	-0.943541	-1.098338	-1.061346
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.227596	-1.351576	-1.245415	-1.369788	-1.413305	-1.065854	-1.136539	-1.219720	-1.167910
(3,-1)	-0.797566	-0.644531	-0.778906	-0.809409	-0.790124	-0.748524	-0.754640	-0.746019	-0.720236
(3,-1)	-1.258913	-1.146420	-1.327670	-1.423481	-1.652725	-1.225155	-1.226106	-1.215798	-1.187102
(3,-1)	-1.122870	-1.033401	-1.159947	-1.249800	-1.436262	-1.085927	-1.084572	-1.072452	-1.047708
(3,-1)	-1.122870	-1.033401	-1.159947	-1.249800	-1.436262	-1.085927	-1.084572	-1.072452	-1.047708
(3,-1)	-1.122870	-1.033401	-1.159947	-1.249800	-1.436262	-1.085927	-1.084572	-1.072452	-1.047708
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.227596	-1.154455	-1.199659	-1.261872	-1.225851	-1.207328	-1.205450		
(3,-1)	-0.797566	-1.154455	-0.770538	-0.909181	-0.777503	-0.777531	-0.795161		
(3,-1)	-1.258913	-0.997327	-1.352722	-1.341896	-1.254330	-1.247237	-1.253911		
(3,-1)	-1.122870	-0.997327	-1.147940	-1.184790	-1.117099	-1.105846	-1.114827		
(3,-1)	-1.122870	-0.997327	-1.147940	-1.184790	-1.117099	-1.105846	-1.114755		
(3,-1)	-1.122870	-0.997327	-1.147940	-1.184790	-1.117099	-1.105846	-1.114756		

Table S295: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{CH}_2=\text{C}=\text{CH}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.200975	-1.066811	-1.127793	-1.087968	-1.141313	-1.096084	-1.097248	-1.072174	-1.322011
(3,-1)	-1.200975	-1.066811	-1.127793	-1.087968	-1.141313	-1.096084	-1.097248	-1.072174	-1.322011
(3,-1)	-1.157256	-1.065518	-1.110213	-1.073195	-1.121794	-0.970468	-1.084679	-0.997400	-0.920323
(3,-1)	-1.157256	-1.065518	-1.110213	-1.073195	-1.121794	-0.970468	-1.084679	-0.997400	-0.920323
(3,-1)	-1.157256	-1.065518	-1.110213	-1.073195	-1.121794	-0.970468	-1.084679	-0.997400	-0.920323
(3,-1)	-1.157256	-1.065518	-1.110213	-1.073195	-1.121794	-0.970468	-1.084679	-0.997400	-0.920323
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.200975	0.127254	-1.162881	-1.158470	-1.132489	-1.047774	-1.061458	-1.176548	-1.082291
(3,-1)	-1.200975	-0.407855	-1.162881	-1.158470	-1.132489	-1.047774	-1.061458	-1.176548	-1.082291
(3,-1)	-1.157256	-0.407855	-1.074415	-1.134014	-1.104871	-1.069259	-0.970141	-1.133945	-1.095301
(3,-1)	-1.157256	-0.988750	-1.074415	-1.134014	-1.104871	-1.069259	-0.970141	-1.133945	-1.095301
(3,-1)	-1.157256	-1.016661	-1.074415	-1.134014	-1.104871	-1.069259	-0.970141	-1.133945	-1.095301
(3,-1)	-1.157256	-1.016661	-1.074415	-1.134014	-1.104871	-1.069259	-0.970141	-1.133945	-1.095301
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.200975	-1.099033	-1.185661	-1.266864	-1.271653	-1.076240	-1.114103	-1.143918	-1.096018
(3,-1)	-1.200975	-1.099033	-1.185661	-1.266864	-1.271653	-1.076240	-1.114103	-1.143918	-1.096018
(3,-1)	-1.157256	-1.058080	-1.199876	-1.292469	-1.486686	-1.120829	-1.119040	-1.106377	-1.077881
(3,-1)	-1.157256	-1.058080	-1.199876	-1.292469	-1.486686	-1.120829	-1.119040	-1.106377	-1.077881
(3,-1)	-1.157256	-1.058080	-1.199876	-1.292469	-1.486686	-1.120829	-1.119040	-1.106377	-1.077881
(3,-1)	-1.157256	-1.058080	-1.199876	-1.292469	-1.486686	-1.120829	-1.119040	-1.106377	-1.077881
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.200975	0.155068	-1.183639	-1.343883	-1.172951	-1.170945	-1.187764		
(3,-1)	-1.200975	-0.411224	-1.183639	-1.343883	-1.172951	-1.170945	-1.187764		
(3,-1)	-1.157256	-0.411224	-1.201782	-1.223857	-1.149194	-1.139625	-1.147687		
(3,-1)	-1.157256	-1.014634	-1.201782	-1.223857	-1.149194	-1.139625	-1.147687		
(3,-1)	-1.157256	-0.983936	-1.201782	-1.223857	-1.149194	-1.139625	-1.147687		
(3,-1)	-1.157256	-0.983936	-1.201782	-1.223857	-1.149194	-1.139625	-1.147687		

Table S296: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>3</sub>H<sub>4</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.151459	0.145805	0.165891	0.145238	0.126333	0.170438	0.213710	0.121411	0.092747
(3,-1)	-0.406466	-0.329172	-0.363047	-0.346097	-0.384515	-0.316359	-0.332079	-0.312761	-0.424977
(3,-1)	-0.406466	-0.329172	-0.363047	-0.346097	-0.384515	-0.316359	-0.332079	-0.312761	-0.424977
(3,-1)	-1.027779	-0.939693	-0.988144	-0.953535	-0.977662	-0.986764	-1.002181	-0.869785	-1.097074
(3,-1)	-1.149673	-1.059668	-1.102941	-1.068312	-1.115698	-0.969863	-1.077945	-0.997241	-0.883222
(3,-1)	-1.149673	-1.059668	-1.102941	-1.068312	-1.115698	-0.969863	-1.077945	-0.997241	-0.883222
(3,-1)	-1.199666	-1.118361	-1.155120	-1.120684	-1.169346	-1.021568	-1.134752	-1.022665	-0.962799
(3,-1)	-1.199666	-1.118361	-1.155120	-1.120684	-1.169346	-1.021568	-1.134752	-1.022665	-0.962799
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.151459	-1.082484	0.095745	0.160273	0.140228	0.132583	0.080997	0.131141	0.161515
(3,-1)	-0.406466	-1.032325	-0.423523	-0.385259	-0.375254	-0.228861	-0.264653	-0.405948	-0.376524
(3,-1)	-0.406466	-1.044884	-0.423523	-0.385259	-0.375254	-0.228861	-0.264653	-0.405948	-0.376524
(3,-1)	-1.027779	-0.661704	-0.977604	-1.006262	-0.980609	-0.852964	-0.824531	-1.004645	-0.936628
(3,-1)	-1.149673	-1.041580	-1.068840	-1.125821	-1.098696	-1.067809	-0.972149	-1.127037	-1.087267
(3,-1)	-1.149673	-0.987437	-1.068840	-1.125821	-1.098696	-1.067809	-0.972149	-1.127037	-1.087267
(3,-1)	-1.199666	-0.967333	-1.125100	-1.181133	-1.154651	-1.114278	-0.999828	-1.182774	-1.144248
(3,-1)	-1.199666	-0.967333	-1.125100	-1.181133	-1.154651	-1.114278	-0.999828	-1.182774	-1.144248
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.151459	0.469999	0.133398	0.157104	0.208562	0.151526	0.145260	0.165230	0.157521
(3,-1)	-0.406466	-0.348216	-0.363629	-0.419343	-0.461470	-0.381898	-0.382422	-0.373934	-0.359451
(3,-1)	-0.406466	-0.348216	-0.363629	-0.419343	-0.461470	-0.381898	-0.382422	-0.373934	-0.359451
(3,-1)	-1.027779	-1.036380	-1.005360	-1.106979	-1.177111	-0.926107	-0.965987	-1.018958	-0.958106
(3,-1)	-1.149673	-1.058138	-1.184689	-1.279678	-1.463013	-1.113084	-1.110727	-1.097998	-1.072473
(3,-1)	-1.149673	-1.058138	-1.184689	-1.279678	-1.463013	-1.113084	-1.110727	-1.097998	-1.072473
(3,-1)	-1.199666	-1.098293	-1.253875	-1.353285	-1.555540	-1.167158	-1.166621	-1.155615	-1.129532
(3,-1)	-1.199666	-1.098293	-1.253875	-1.353285	-1.555540	-1.167158	-1.166621	-1.155615	-1.129532
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.151459	-1.097061	0.170160	0.146897	0.152307	0.136473	0.102453		
(3,-1)	-0.406466	-1.002066	-0.343206	-0.485672	-0.390389	-0.393733	-0.404930		
(3,-1)	-0.406466	-1.013397	-0.343206	-0.485672	-0.390389	-0.393733	-0.404930		
(3,-1)	-1.027779	-0.673154	-1.009033	-1.095854	-1.011783	-1.002390	-1.003440		
(3,-1)	-1.149673	-1.004972	-1.173222	-1.213072	-1.141963	-1.133421	-1.141882		
(3,-1)	-1.149673	-0.957865	-1.173222	-1.213072	-1.141963	-1.133421	-1.141882		
(3,-1)	-1.199666	-0.941544	-1.272827	-1.274186	-1.194536	-1.188185	-1.194450		
(3,-1)	-1.199666	-0.941544	-1.272827	-1.274186	-1.194536	-1.188185	-1.194451		

Table S297: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>2</sub>=CHCH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.152266	-1.029865	-1.091570	-1.050534	-1.100294	-1.028720	-1.052430	-1.071577	-1.176114
(3,-1)	-1.162277	-1.072715	-1.117987	-1.081583	-1.129603	-0.982736	-1.093786	-1.001214	-0.908181
(3,-1)	-1.174435	-1.085083	-1.130018	-1.093204	-1.141263	-0.993290	-1.105117	-1.008755	-0.917779
(3,-1)	-0.733411	-0.625946	-0.678012	-0.649296	-0.702214	-0.601891	-0.631324	-0.715826	-0.693635
(3,-1)	-1.166355	-1.080711	-1.122433	-1.087302	-1.135801	-0.982908	-1.099344	-1.004655	-0.902046
(3,-1)	-1.112812	-1.025732	-1.073901	-1.037775	-1.082585	-0.951677	-1.047318	-0.969968	-0.865353
(3,-1)	-1.095175	-1.006191	-1.053075	-1.017316	-1.062027	-0.928897	-1.025704	-0.957047	-0.857050
(3,-1)	-1.095175	-1.006191	-1.053075	-1.017316	-1.062027	-0.928897	-1.025704	-0.957047	-0.857050
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.152266	0.044607	-1.080044	-1.119045	-1.089783	-1.031972	-1.061639	-1.127531	-1.052334
(3,-1)	-1.162277	-0.493686	-1.085872	-1.140989	-1.112455	-1.074069	-0.974658	-1.139467	-1.105778
(3,-1)	-1.174435	-0.493686	-1.099308	-1.153191	-1.124277	-1.083972	-0.983034	-1.151928	-1.118327
(3,-1)	-0.733411	-0.493686	-0.701984	-0.706584	-0.687379	-0.669655	-0.695751	-0.727035	-0.672487
(3,-1)	-1.166355	-1.031751	-1.096321	-1.146777	-1.119422	-1.079064	-0.979583	-1.147355	-1.113729
(3,-1)	-1.112812	-1.031751	-1.039637	-1.093604	-1.064704	-1.030267	-0.941371	-1.089129	-1.053914
(3,-1)	-1.095175	-1.031751	-1.016256	-1.073150	-1.044564	-1.012895	-0.928670	-1.069519	-1.032980
(3,-1)	-1.095175	-1.031751	-1.016256	-1.073150	-1.044564	-1.012895	-0.928670	-1.069519	-1.032980
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.152266	-1.042254	-1.142725	-1.213077	-1.198750	-1.040256	-1.074856	-1.099119	-1.054485
(3,-1)	-1.162277	-1.069706	-1.205002	-1.298367	-1.488848	-1.125556	-1.123665	-1.112189	-1.085696
(3,-1)	-1.174435	-1.081187	-1.218112	-1.311971	-1.503155	-1.137266	-1.135716	-1.124089	-1.097508
(3,-1)	-0.733411	-0.596757	-0.717043	-0.744096	-0.715018	-0.693504	-0.697033	-0.685795	-0.661514
(3,-1)	-1.166355	-1.076651	-1.207799	-1.301822	-1.485386	-1.135306	-1.132925	-1.120345	-1.093478
(3,-1)	-1.112812	-1.027198	-1.149461	-1.237849	-1.421092	-1.075681	-1.074193	-1.063055	-1.039873
(3,-1)	-1.095175	-1.007835	-1.129629	-1.216024	-1.402066	-1.057374	-1.055741	-1.043817	-1.019851
(3,-1)	-1.095175	-1.007835	-1.129629	-1.216024	-1.402066	-1.057374	-1.055741	-1.043817	-1.019851
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.152266	0.079710	-1.147740	-1.249356	-1.132118	-1.123927	-1.144382		
(3,-1)	-1.162277	-0.497470	-1.200242	-1.228485	-1.156057	-1.146649	-1.155033		
(3,-1)	-1.174435	-0.497470	-1.216369	-1.241054	-1.168348	-1.158737	-1.167629		
(3,-1)	-0.733411	-0.497470	-0.698509	-0.838496	-0.717884	-0.716977	-0.734934		
(3,-1)	-1.166355	-1.000726	-1.206830	-1.237336	-1.160789	-1.152609	-1.160558		
(3,-1)	-1.112812	-1.000726	-1.128907	-1.173793	-1.107686	-1.096565	-1.105228		
(3,-1)	-1.095175	-1.000726	-1.107066	-1.153445	-1.088422	-1.077641	-1.086572		
(3,-1)	-1.095175	-1.000726	-1.107066	-1.153445	-1.088422	-1.077641	-1.086572		

Table S298: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>3</sub>H<sub>6</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.082975	0.106880	0.116604	0.102318	0.073700	0.131444	0.151632	0.097059	0.049008
(3,-1)	-0.503321	-0.423210	-0.463560	-0.442546	-0.481720	-0.400634	-0.427075	-0.438327	-0.534899
(3,-1)	-0.503321	-0.423210	-0.463560	-0.442546	-0.481720	-0.400634	-0.427075	-0.438327	-0.534899
(3,-1)	-0.503321	-0.423210	-0.463560	-0.442546	-0.481720	-0.400634	-0.427075	-0.438327	-0.534899
(3,-1)	-1.162950	-1.075745	-1.118574	-1.083072	-1.129424	-0.979303	-1.092822	-1.008353	-0.907004
(3,-1)	-1.162950	-1.075745	-1.118574	-1.083072	-1.129424	-0.979303	-1.092822	-1.008353	-0.907004
(3,-1)	-1.162950	-1.075745	-1.118574	-1.083072	-1.129424	-0.979303	-1.092822	-1.008353	-0.907004
(3,-1)	-1.162950	-1.075745	-1.118574	-1.083072	-1.129424	-0.979303	-1.092822	-1.008353	-0.907004
(3,-1)	-1.162950	-1.075745	-1.118574	-1.083072	-1.129424	-0.979303	-1.092822	-1.008353	-0.907004
(3,-1)	-1.162950	-1.075745	-1.118574	-1.083072	-1.129424	-0.979303	-1.092822	-1.008353	-0.907004
(3,-1)	-1.162950	-1.075745	-1.118574	-1.083072	-1.129424	-0.979303	-1.092822	-1.008353	-0.907004
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.082975	-0.604178	0.033967	0.102640	0.086625	0.110106	0.063754	0.067335	0.097010
(3,-1)	-0.503321	-0.604178	-0.515426	-0.484320	-0.470393	-0.352517	-0.394563	-0.502440	-0.468893
(3,-1)	-0.503321	-0.981555	-0.515426	-0.484320	-0.470393	-0.352517	-0.394563	-0.502440	-0.468893
(3,-1)	-0.503321	-0.981555	-0.515426	-0.484320	-0.470393	-0.352517	-0.394563	-0.502440	-0.468893
(3,-1)	-1.162950	-0.979754	-1.083415	-1.140483	-1.112353	-1.075865	-0.981291	-1.138705	-1.101805
(3,-1)	-1.162950	-0.979754	-1.083415	-1.140483	-1.112353	-1.075865	-0.981291	-1.138705	-1.101805
(3,-1)	-1.162950	-0.972078	-1.083415	-1.140483	-1.112353	-1.075865	-0.981291	-1.138705	-1.101805
(3,-1)	-1.162950	-0.972078	-1.083415	-1.140483	-1.112353	-1.075865	-0.981291	-1.138705	-1.101805
(3,-1)	-1.162950	-0.972078	-1.083415	-1.140483	-1.112353	-1.075865	-0.981291	-1.138705	-1.101805
(3,-1)	-1.162950	-0.972078	-1.083415	-1.140483	-1.112353	-1.075865	-0.981291	-1.138705	-1.101805
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.082975	0.368705	0.073001	0.087342	0.074773	0.082696	0.078239	0.095544	0.097787
(3,-1)	-0.503321	-0.420753	-0.455694	-0.509798	-0.520330	-0.474948	-0.475530	-0.467401	-0.448567
(3,-1)	-0.503321	-0.420753	-0.455694	-0.509798	-0.520330	-0.474948	-0.475530	-0.467401	-0.448567
(3,-1)	-0.503321	-0.420753	-0.455694	-0.509798	-0.520330	-0.474948	-0.475530	-0.467401	-0.448567
(3,-1)	-1.162950	-1.068705	-1.204107	-1.296121	-1.486140	-1.125294	-1.123684	-1.111906	-1.085663
(3,-1)	-1.162950	-1.068705	-1.204107	-1.296121	-1.486140	-1.125294	-1.123684	-1.111906	-1.085663
(3,-1)	-1.162950	-1.068705	-1.204107	-1.296121	-1.486140	-1.125294	-1.123684	-1.111906	-1.085663
(3,-1)	-1.162950	-1.068705	-1.204107	-1.296121	-1.486140	-1.125294	-1.123684	-1.111906	-1.085663
(3,-1)	-1.162950	-1.068705	-1.204107	-1.296121	-1.486140	-1.125294	-1.123684	-1.111906	-1.085663
(3,-1)	-1.162950	-1.068705	-1.204107	-1.296121	-1.486140	-1.125294	-1.123684	-1.111906	-1.085663
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.082975	-0.609279	0.136942	0.053011	0.091669	0.074757	0.043250		
(3,-1)	-0.503321	-0.609279	-0.445176	-0.580833	-0.490677	-0.490427	-0.500138		
(3,-1)	-0.503321	-0.949830	-0.445176	-0.580833	-0.490677	-0.490427	-0.500136		
(3,-1)	-0.503321	-0.949830	-0.445176	-0.580833	-0.490677	-0.490427	-0.500208		
(3,-1)	-1.162950	-0.950759	-1.196318	-1.223217	-1.156444	-1.146741	-1.155456		
(3,-1)	-1.162950	-0.950759	-1.196318	-1.223217	-1.156444	-1.146741	-1.155456		
(3,-1)	-1.162950	-0.944026	-1.196318	-1.223217	-1.156444	-1.146741	-1.155532		
(3,-1)	-1.162950	-0.944026	-1.196318	-1.223217	-1.156444	-1.146741	-1.155532		
(3,-1)	-1.162950	-0.944026	-1.196318	-1.223217	-1.156444	-1.146741	-1.155534		
(3,-1)	-1.162950	-0.944026	-1.196318	-1.223217	-1.156444	-1.146741	-1.155535		

Table S299: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>3</sub>H<sub>8</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.658259	-0.560906	-0.611156	-0.584864	-0.633988	-0.540856	-0.565072	-0.646303	-0.628746
(3,-1)	-0.658259	-0.560906	-0.611156	-0.584864	-0.633988	-0.540856	-0.565072	-0.646303	-0.628746
(3,-1)	-1.105785	-1.019618	-1.063117	-1.029089	-1.073560	-0.938202	-1.038111	-0.966734	-0.850667
(3,-1)	-1.105785	-1.019618	-1.063117	-1.029089	-1.073560	-0.938202	-1.038111	-0.966734	-0.850667
(3,-1)	-1.103183	-1.015820	-1.062357	-1.026922	-1.071288	-0.938944	-1.035820	-0.964802	-0.858557
(3,-1)	-1.103183	-1.015820	-1.062357	-1.026922	-1.071288	-0.938944	-1.035820	-0.964802	-0.858557
(3,-1)	-1.097985	-1.010313	-1.056999	-1.021831	-1.066082	-0.937127	-1.030595	-0.960437	-0.854201
(3,-1)	-1.097985	-1.010313	-1.056999	-1.021831	-1.066082	-0.937127	-1.030595	-0.960437	-0.854201
(3,-1)	-1.097985	-1.010313	-1.056999	-1.021831	-1.066082	-0.937127	-1.030595	-0.960437	-0.854201
(3,-1)	-1.097985	-1.010313	-1.056999	-1.021831	-1.066082	-0.937127	-1.030595	-0.960437	-0.854201
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.658259	-0.766705	-0.643763	-0.636779	-0.618999	-0.590860	-0.622513	-0.655534	-0.605272
(3,-1)	-0.658259	-1.069762	-0.643763	-0.636779	-0.618999	-0.590860	-0.622513	-0.655534	-0.605272
(3,-1)	-1.105785	-1.053440	-1.027807	-1.083644	-1.056660	-1.022967	-0.940903	-1.081768	-1.044817
(3,-1)	-1.105785	-1.069762	-1.027807	-1.083644	-1.056660	-1.022967	-0.940903	-1.081768	-1.044817
(3,-1)	-1.103183	-1.053440	-1.026655	-1.082043	-1.053801	-1.020338	-0.937574	-1.078173	-1.042794
(3,-1)	-1.103183	-1.038170	-1.026655	-1.082043	-1.053801	-1.020338	-0.937574	-1.078173	-1.042794
(3,-1)	-1.097985	-1.045310	-1.020424	-1.076556	-1.048512	-1.016768	-0.932771	-1.072664	-1.037204
(3,-1)	-1.097985	-1.045310	-1.020424	-1.076556	-1.048512	-1.016768	-0.932771	-1.072664	-1.037204
(3,-1)	-1.097985	-1.038170	-1.020424	-1.076556	-1.048512	-1.016768	-0.932771	-1.072664	-1.037204
(3,-1)	-1.097985	-1.020424	-1.076556	-1.048512	-1.016768	-0.932771	-1.072664	-1.037204	-1.037204
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.658259	-0.528025	-0.634176	-0.662044	-0.627556	-0.626224	-0.627541	-0.614541	-0.595542
(3,-1)	-0.658259	-0.528025	-0.634176	-0.662044	-0.627556	-0.626224	-0.627541	-0.614541	-0.595542
(3,-1)	-1.105785	-1.021497	-1.137847	-1.225676	-1.410033	-1.068594	-1.067208	-1.056352	-1.032109
(3,-1)	-1.105785	-1.021497	-1.137847	-1.225676	-1.410033	-1.068594	-1.067208	-1.056352	-1.032109
(3,-1)	-1.103183	-1.017805	-1.138952	-1.225644	-1.411254	-1.064636	-1.063441	-1.052920	-1.028829
(3,-1)	-1.103183	-1.017805	-1.138952	-1.225644	-1.411254	-1.064636	-1.063441	-1.052920	-1.028829
(3,-1)	-1.097985	-1.012885	-1.132898	-1.219088	-1.404318	-1.059611	-1.058106	-1.047252	-1.023394
(3,-1)	-1.097985	-1.012885	-1.132898	-1.219088	-1.404318	-1.059611	-1.058106	-1.047252	-1.023394
(3,-1)	-1.097985	-1.012885	-1.132898	-1.219088	-1.404318	-1.059611	-1.058106	-1.047252	-1.023394
(3,-1)	-1.097985	-1.012885	-1.132898	-1.219088	-1.404318	-1.059611	-1.058106	-1.047252	-1.023394
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.658259	-0.784910	-0.612776	-0.757107	-0.646305	-0.644962	-0.661519		
(3,-1)	-0.658259	-1.087165	-0.612776	-0.757107	-0.646305	-0.644962	-0.661519		
(3,-1)	-1.105785	-1.021561	-1.115927	-1.163179	-1.098727	-1.089206	-1.097558		
(3,-1)	-1.105785	-1.087165	-1.115927	-1.163179	-1.098727	-1.089206	-1.097558		
(3,-1)	-1.103183	-1.021561	-1.116218	-1.161006	-1.096927	-1.086317	-1.095160		
(3,-1)	-1.103183	-1.007602	-1.116218	-1.161006	-1.096927	-1.086317	-1.095160		
(3,-1)	-1.097985	-1.007977	-1.106123	-1.155061	-1.091610	-1.081045	-1.089698		
(3,-1)	-1.097985	-1.007977	-1.106123	-1.155061	-1.091610	-1.081045	-1.089698		
(3,-1)	-1.097985	-1.007602	-1.106123	-1.155061	-1.091610	-1.081045	-1.089699		
(3,-1)	-1.097985	-1.007602	-1.106123	-1.155061	-1.091610	-1.081045	-1.089698		

Table S300: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>6</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.861420	-0.739812	-0.791691	-0.760529	-0.819709	-0.718524	-0.744164	-0.830473	-0.809718
(3,-1)	-1.140703	-1.023652	-1.086504	-1.044989	-1.093697	-1.022887	-1.045434	-1.070873	-1.164297
(3,-1)	-1.181843	-1.093716	-1.137639	-1.101009	-1.149568	-0.996950	-1.113514	-1.014068	-0.924091
(3,-1)	-1.140703	-1.023652	-1.086504	-1.044989	-1.093697	-1.022887	-1.045434	-1.070873	-1.164297
(3,-1)	-1.181843	-1.093716	-1.137639	-1.101009	-1.149568	-0.996950	-1.113514	-1.014068	-0.924091
(3,-1)	-1.167197	-1.079637	-1.123851	-1.087667	-1.135761	-0.986272	-1.099976	-1.004793	-0.912231
(3,-1)	-1.168407	-1.083293	-1.126455	-1.090939	-1.139486	-0.986627	-1.103748	-1.004779	-0.902860
(3,-1)	-1.168407	-1.083293	-1.126455	-1.090939	-1.139486	-0.986627	-1.103748	-1.004779	-0.902860
(3,-1)	-1.167197	-1.079637	-1.123851	-1.087667	-1.135761	-0.986272	-1.099976	-1.004793	-0.912231
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.861420	-1.166977	-0.803007	-0.826188	-0.806139	-0.789631	-0.817145	-0.846834	-0.788489
(3,-1)	-1.140703	-0.700230	-1.071772	-1.112289	-1.082261	-1.026076	-1.056096	-1.118841	-1.043364
(3,-1)	-1.181843	-0.700230	-1.109054	-1.161400	-1.132717	-1.091496	-0.988383	-1.161207	-1.127307
(3,-1)	-1.140703	-0.987915	-1.071772	-1.112289	-1.082261	-1.026076	-1.056096	-1.118841	-1.043364
(3,-1)	-1.181843	-0.987915	-1.109054	-1.161400	-1.132717	-1.091496	-0.988383	-1.161207	-1.127307
(3,-1)	-1.167197	-0.987915	-1.092812	-1.147079	-1.118731	-1.079530	-0.978066	-1.145991	-1.112166
(3,-1)	-1.168407	-0.987915	-1.101835	-1.150321	-1.122561	-1.080534	-0.979360	-1.150599	-1.117060
(3,-1)	-1.168407	-0.987915	-1.101835	-1.150321	-1.122561	-1.080534	-0.979360	-1.150599	-1.117060
(3,-1)	-1.167197	-0.987915	-1.092812	-1.147079	-1.118731	-1.079530	-0.978066	-1.145991	-1.112166
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.861420	-0.710462	-0.854535	-0.884817	-0.868404	-0.811465	-0.818698	-0.809611	-0.775449
(3,-1)	-1.140703	-1.028098	-1.135276	-1.203969	-1.187513	-1.029406	-1.063710	-1.087710	-1.047567
(3,-1)	-1.181843	-1.088368	-1.227268	-1.321827	-1.512057	-1.146746	-1.145027	-1.133302	-1.105915
(3,-1)	-1.140703	-1.028098	-1.135276	-1.203969	-1.187513	-1.029406	-1.063710	-1.087710	-1.047567
(3,-1)	-1.181843	-1.088368	-1.227268	-1.321827	-1.512057	-1.146746	-1.145027	-1.133302	-1.105915
(3,-1)	-1.167197	-1.074611	-1.211778	-1.305886	-1.495767	-1.131955	-1.130020	-1.118541	-1.092007
(3,-1)	-1.168407	-1.077806	-1.209907	-1.303875	-1.485092	-1.137488	-1.135252	-1.123291	-1.096636
(3,-1)	-1.168407	-1.077806	-1.209907	-1.303875	-1.485092	-1.137488	-1.135252	-1.123291	-1.096636
(3,-1)	-1.167197	-1.074611	-1.211778	-1.305886	-1.495767	-1.131955	-1.130020	-1.118541	-1.092007
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.861420	-1.184471	-0.845479	-0.977862	-0.838336	-0.839508	-0.859986		
(3,-1)	-1.140703	-0.723132	-1.139870	-1.237396	-1.123749	-1.114238	-1.134589		
(3,-1)	-1.181843	-0.723132	-1.229748	-1.251014	-1.176061	-1.166895	-1.175529		
(3,-1)	-1.140703	-0.960064	-1.139870	-1.237396	-1.123749	-1.114238	-1.134589		
(3,-1)	-1.181843	-0.960064	-1.229748	-1.251014	-1.176061	-1.166895	-1.175530		
(3,-1)	-1.167197	-0.960064	-1.210785	-1.235175	-1.161587	-1.152440	-1.160623		
(3,-1)	-1.168407	-0.960064	-1.212299	-1.240120	-1.163389	-1.154661	-1.161949		
(3,-1)	-1.168407	-0.960064	-1.212299	-1.240120	-1.163389	-1.154661	-1.161948		
(3,-1)	-1.167197	-0.960064	-1.210785	-1.235175	-1.161587	-1.152440	-1.160625		

Table S301: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>6</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.181019	-1.141784	-1.174662	-1.141155	-1.139037	-1.212075	-1.189646	-1.037544	-1.382196
(3,-1)	-0.790558	-0.679826	-0.731882	-0.702604	-0.755200	-0.675530	-0.685493	-0.752793	-0.747274
(3,-1)	-0.790558	-0.679826	-0.731882	-0.702604	-0.755200	-0.675530	-0.685493	-0.752793	-0.747274
(3,-1)	-1.118055	-1.027538	-1.075980	-1.039282	-1.085216	-0.949545	-1.049236	-0.970539	-0.872263
(3,-1)	-1.118055	-1.027538	-1.075980	-1.039282	-1.085216	-0.949545	-1.049236	-0.970539	-0.872263
(3,-1)	-1.118055	-1.027538	-1.075980	-1.039282	-1.085216	-0.949545	-1.049236	-0.970539	-0.872263
(3,-1)	-1.118055	-1.027538	-1.075980	-1.039282	-1.085216	-0.949545	-1.049236	-0.970539	-0.872263
(3,-1)	-1.118055	-1.027538	-1.075980	-1.039282	-1.085216	-0.949545	-1.049236	-0.970539	-0.872263
(3,-1)	-1.118055	-1.027538	-1.075980	-1.039282	-1.085216	-0.949545	-1.049236	-0.970539	-0.872263
(3,-1)	-1.118055	-1.027538	-1.075980	-1.039282	-1.085216	-0.949545	-1.049236	-0.970539	-0.872263
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.181019	-0.586797	-1.131579	-1.177735	-1.150731	-1.121202	-1.085724	-1.161306	-1.095446
(3,-1)	-0.790558	-0.586797	-0.739385	-0.760520	-0.741178	-0.703462	-0.729148	-0.774926	-0.716870
(3,-1)	-0.790558	0.089944	-0.739385	-0.760520	-0.741178	-0.703462	-0.729148	-0.774926	-0.716870
(3,-1)	-1.118055	-0.406852	-1.041742	-1.096761	-1.067454	-1.031916	-0.941015	-1.093328	-1.055962
(3,-1)	-1.118055	-1.074945	-1.041742	-1.096761	-1.067454	-1.031916	-0.941015	-1.093328	-1.055962
(3,-1)	-1.118055	-1.016619	-1.041742	-1.096761	-1.067454	-1.031916	-0.941015	-1.093328	-1.055962
(3,-1)	-1.118055	-1.016619	-1.041742	-1.096761	-1.067454	-1.031916	-0.941015	-1.093328	-1.055962
(3,-1)	-1.118055	-1.016619	-1.041742	-1.096761	-1.067454	-1.031916	-0.941015	-1.093328	-1.055962
(3,-1)	-1.118055	-1.016619	-1.041742	-1.096761	-1.067454	-1.031916	-0.941015	-1.093328	-1.055962
(3,-1)	-1.118055	-1.016619	-1.041742	-1.096761	-1.067454	-1.031916	-0.941015	-1.093328	-1.055962
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.181019	-1.334855	-1.195595	-1.309380	-1.372464	-1.028312	-1.096341	-1.180467	-1.128660
(3,-1)	-0.790558	-0.636257	-0.772192	-0.804397	-0.791031	-0.742274	-0.748635	-0.739990	-0.714718
(3,-1)	-0.790558	-0.636257	-0.772192	-0.804397	-0.791031	-0.742274	-0.748635	-0.739990	-0.714718
(3,-1)	-1.118055	-1.029521	-1.154227	-1.243921	-1.429885	-1.080961	-1.079509	-1.067401	-1.042691
(3,-1)	-1.118055	-1.029521	-1.154227	-1.243921	-1.429885	-1.080961	-1.079509	-1.067401	-1.042691
(3,-1)	-1.118055	-1.029521	-1.154227	-1.243921	-1.429885	-1.080961	-1.079509	-1.067401	-1.042691
(3,-1)	-1.118055	-1.029521	-1.154227	-1.243921	-1.429885	-1.080961	-1.079509	-1.067401	-1.042691
(3,-1)	-1.118055	-1.029521	-1.154227	-1.243921	-1.429885	-1.080961	-1.079509	-1.067401	-1.042691
(3,-1)	-1.118055	-1.029521	-1.154227	-1.243921	-1.429885	-1.080961	-1.079509	-1.067401	-1.042691
(3,-1)	-1.118055	-1.029521	-1.154227	-1.243921	-1.429885	-1.080961	-1.079509	-1.067401	-1.042691
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.181019	-0.598156	-1.148918	-1.202120	-1.181566	-1.163548	-1.158386		
(3,-1)	-0.790558	-0.598156	-0.766074	-0.900211	-0.770879	-0.770556	-0.788410		
(3,-1)	-0.790558	0.122062	-0.766074	-0.900211	-0.770879	-0.770556	-0.788409		
(3,-1)	-1.118055	-0.407633	-1.139902	-1.179598	-1.111905	-1.100893	-1.109778		
(3,-1)	-1.118055	-1.090027	-1.139902	-1.179598	-1.111905	-1.100893	-1.109702		
(3,-1)	-1.118055	-0.989244	-1.139902	-1.179598	-1.111905	-1.100893	-1.109702		
(3,-1)	-1.118055	-0.989244	-1.139902	-1.179598	-1.111905	-1.100893	-1.109777		
(3,-1)	-1.118055	-0.989244	-1.139902	-1.179598	-1.111905	-1.100893	-1.109701		
(3,-1)	-1.118055	-0.989244	-1.139902	-1.179598	-1.111905	-1.100893	-1.109702		



Table S302: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>6</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.619644	-0.529944	-0.572209	-0.548405	-0.590464	-0.523137	-0.540986	-0.544887	-0.632217
(3,-1)	-0.619644	-0.529944	-0.572209	-0.548405	-0.590464	-0.523137	-0.540986	-0.544887	-0.632217
(3,+1)	0.125154	0.141451	0.155134	0.137726	0.110932	0.168865	0.197482	0.125380	0.083369
(3,-1)	-0.410994	-0.332122	-0.368717	-0.350985	-0.390948	-0.310437	-0.333567	-0.346360	-0.438277
(3,-1)	-1.142170	-1.024733	-1.081957	-1.042459	-1.088229	-1.039185	-1.051507	-1.029413	-1.184426
(3,-1)	-1.148417	-1.060961	-1.103415	-1.068091	-1.114762	-0.961750	-1.077897	-0.997576	-0.901770
(3,-1)	-1.148417	-1.060961	-1.103415	-1.068091	-1.114762	-0.961750	-1.077897	-0.997576	-0.901770
(3,-1)	-1.148417	-1.060961	-1.103415	-1.068091	-1.114762	-0.961750	-1.077897	-0.997576	-0.901770
(3,-1)	-1.148417	-1.060961	-1.103415	-1.068091	-1.114762	-0.961750	-1.077897	-0.997576	-0.901770
(3,-1)	-1.167114	-1.076837	-1.120790	-1.084533	-1.132954	-0.978970	-1.096358	-1.004600	-0.915696
(3,-1)	-1.167114	-1.076837	-1.120790	-1.084533	-1.132954	-0.978970	-1.096358	-1.004600	-0.915696
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.619644	-0.610487	-0.610114	-0.597522	-0.582046	-0.462816	-0.498493	-0.614974	-0.570259
(3,-1)	-0.619644	-0.602877	-0.610114	-0.597522	-0.582046	-0.462816	-0.498493	-0.614974	-0.570259
(3,+1)	0.125154	-0.979301	0.075985	0.142860	0.124387	0.137130	0.087362	0.107328	0.137506
(3,-1)	-0.410994	-0.602877	-0.427229	-0.390417	-0.379553	-0.261959	-0.304382	-0.411049	-0.381117
(3,-1)	-1.142170	-0.979301	-1.072507	-1.109229	-1.081473	-1.000173	-1.023820	-1.116256	-1.038305
(3,-1)	-1.148417	-0.972359	-1.066942	-1.125742	-1.097785	-1.063342	-0.970274	-1.124866	-1.085510
(3,-1)	-1.148417	-0.972359	-1.066942	-1.125742	-1.097785	-1.063342	-0.970274	-1.124866	-1.085510
(3,-1)	-1.148417	-0.972359	-1.066942	-1.125742	-1.097785	-1.063342	-0.970274	-1.124866	-1.085510
(3,-1)	-1.148417	-0.972359	-1.066942	-1.125742	-1.097785	-1.063342	-0.970274	-1.124866	-1.085510
(3,-1)	-1.167114	-0.972082	-1.088354	-1.144429	-1.116091	-1.079648	-0.978935	-1.145107	-1.108878
(3,-1)	-1.167114	-0.972082	-1.088354	-1.144429	-1.116091	-1.079648	-0.978935	-1.145107	-1.108878
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.619644	-0.540588	-0.572977	-0.632742	-0.639544	-0.582157	-0.587696	-0.585735	-0.560652
(3,-1)	-0.619644	-0.540588	-0.572977	-0.632742	-0.639544	-0.582157	-0.587696	-0.585735	-0.560652
(3,+1)	0.125154	0.409341	0.113889	0.132489	0.144620	0.120790	0.120027	0.143860	0.137491
(3,-1)	-0.410994	-0.332568	-0.363451	-0.413253	-0.426468	-0.390556	-0.388373	-0.375744	-0.361166
(3,-1)	-1.142170	-1.056340	-1.126534	-1.206769	-1.199511	-1.026653	-1.064252	-1.094114	-1.049978
(3,-1)	-1.148417	-1.052466	-1.188741	-1.281018	-1.469932	-1.111902	-1.110177	-1.098027	-1.071731
(3,-1)	-1.148417	-1.052466	-1.188741	-1.281018	-1.469932	-1.111902	-1.110177	-1.098027	-1.071731
(3,-1)	-1.148417	-1.052466	-1.188741	-1.281018	-1.469932	-1.111902	-1.110177	-1.098027	-1.071731
(3,-1)	-1.148417	-1.052466	-1.188741	-1.281018	-1.469932	-1.111902	-1.110177	-1.098027	-1.071731
(3,-1)	-1.167114	-1.072942	-1.210893	-1.304359	-1.495973	-1.130809	-1.128699	-1.116579	-1.089456
(3,-1)	-1.167114	-1.072942	-1.210893	-1.304359	-1.495973	-1.130809	-1.128699	-1.116579	-1.089456
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.619644	-0.613072	-0.567683	-0.712218	-0.603808	-0.604329	-0.613343		
(3,-1)	-0.619644	-0.608246	-0.567683	-0.712218	-0.603808	-0.604329	-0.613343		
(3,+1)	0.125154	-0.950477	0.167683	0.101248	0.132946	0.115093	0.084162		
(3,-1)	-0.410994	-0.608246	-0.346784	-0.489202	-0.397039	-0.399454	-0.410491		
(3,-1)	-1.142170	-0.950477	-1.133873	-1.243415	-1.120968	-1.114118	-1.130763		
(3,-1)	-1.148417	-0.944384	-1.184431	-1.209880	-1.141497	-1.132071	-1.140370		
(3,-1)	-1.148417	-0.944384	-1.184431	-1.209880	-1.141497	-1.132071	-1.140369		
(3,-1)	-1.148417	-0.944384	-1.184431	-1.209880	-1.141497	-1.132071	-1.140369		
(3,-1)	-1.148417	-0.944384	-1.184431	-1.209880	-1.141497	-1.132071	-1.140370		
(3,-1)	-1.167114	-0.941446	-1.210689	-1.232780	-1.160179	-1.151239	-1.159794		
(3,-1)	-1.167114	-0.941446	-1.210689	-1.232780	-1.160179	-1.151239	-1.159794		

Table S303: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>10</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.683071	-0.566899	-0.615593	-0.590046	-0.639631	-0.549663	-0.569460	-0.653055	-0.632417
(3,-1)	-0.676203	-0.559774	-0.610149	-0.583783	-0.632840	-0.541789	-0.564072	-0.645041	-0.627317
(3,-1)	-1.112007	-1.015612	-1.061939	-1.026575	-1.070904	-0.938944	-1.035088	-0.964594	-0.858604
(3,-1)	-0.676203	-0.559774	-0.610149	-0.583783	-0.632840	-0.541789	-0.564072	-0.645041	-0.627317
(3,-1)	-1.112007	-1.015612	-1.061939	-1.026575	-1.070904	-0.938944	-1.035088	-0.964594	-0.858604
(3,-1)	-1.107283	-1.010639	-1.057326	-1.022138	-1.066341	-0.937782	-1.030515	-0.960711	-0.854601
(3,-1)	-1.107283	-1.010639	-1.057326	-1.022138	-1.066341	-0.937782	-1.030515	-0.960711	-0.854601
(3,-1)	-1.107283	-1.010639	-1.057326	-1.022138	-1.066341	-0.937782	-1.030515	-0.960711	-0.854601
(3,-1)	-1.105272	-1.010400	-1.053649	-1.020146	-1.064331	-0.932499	-1.028618	-0.959762	-0.843652
(3,-1)	-1.105272	-1.010400	-1.053649	-1.020146	-1.064331	-0.932499	-1.028618	-0.959762	-0.843652
(3,-1)	-1.105272	-1.010400	-1.053649	-1.020146	-1.064331	-0.932499	-1.028618	-0.959762	-0.843652
(3,-1)	-1.105272	-1.010400	-1.053649	-1.020146	-1.064331	-0.932499	-1.028618	-0.959762	-0.843652
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.683071	-0.980299	-0.649035	-0.641990	-0.624969	-0.594501	-0.628348	-0.659949	-0.610524
(3,-1)	-0.676203	-0.609568	-0.641981	-0.635745	-0.617911	-0.589538	-0.621678	-0.653764	-0.604000
(3,-1)	-1.112007	-0.963175	-1.026153	-1.081643	-1.053458	-1.020025	-0.937350	-1.077663	-1.042368
(3,-1)	-0.676203	-0.974518	-0.641981	-0.635745	-0.617911	-0.589538	-0.621678	-0.653764	-0.604000
(3,-1)	-1.112007	-0.974518	-1.026153	-1.081643	-1.053458	-1.020025	-0.937350	-1.077663	-1.042368
(3,-1)	-1.107283	-0.609568	-1.020816	-1.076853	-1.048780	-1.017021	-0.932911	-1.072865	-1.037446
(3,-1)	-1.107283	-0.963175	-1.020816	-1.076853	-1.048780	-1.017021	-0.932911	-1.072865	-1.037446
(3,-1)	-1.107283	-0.974518	-1.020816	-1.076853	-1.048780	-1.017021	-0.932911	-1.072865	-1.037446
(3,-1)	-1.107283	-0.974518	-1.020816	-1.076853	-1.048780	-1.017021	-0.932911	-1.072865	-1.037446
(3,-1)	-1.105272	-0.609568	-1.016982	-1.073948	-1.047404	-1.015066	-0.934351	-1.071736	-1.034475
(3,-1)	-1.105272	-0.963175	-1.016982	-1.073948	-1.047404	-1.015066	-0.934351	-1.071736	-1.034475
(3,-1)	-1.105272	-0.974518	-1.016982	-1.073948	-1.047404	-1.015066	-0.934351	-1.071736	-1.034475
(3,-1)	-1.105272	-0.974518	-1.016982	-1.073948	-1.047404	-1.015066	-0.934351	-1.071736	-1.034475
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.683071	-0.530066	-0.637982	-0.666395	-0.629481	-0.631850	-0.633209	-0.619924	-0.600734
(3,-1)	-0.676203	-0.526270	-0.633019	-0.661220	-0.627679	-0.624366	-0.625944	-0.613206	-0.594671
(3,-1)	-1.112007	-1.017384	-1.138672	-1.225432	-1.411135	-1.064051	-1.062890	-1.052285	-1.028465
(3,-1)	-0.676203	-0.526270	-0.633019	-0.661220	-0.627679	-0.624366	-0.625944	-0.613206	-0.594671
(3,-1)	-1.112007	-1.017384	-1.138672	-1.225432	-1.411135	-1.064051	-1.062890	-1.052285	-1.028465
(3,-1)	-1.107283	-1.013253	-1.133075	-1.219535	-1.404943	-1.059677	-1.058133	-1.047133	-1.023644
(3,-1)	-1.107283	-1.013253	-1.133075	-1.219535	-1.404943	-1.059677	-1.058133	-1.047133	-1.023644
(3,-1)	-1.107283	-1.013253	-1.133075	-1.219535	-1.404943	-1.059677	-1.058133	-1.047133	-1.023644
(3,-1)	-1.105272	-1.011649	-1.127365	-1.214919	-1.399433	-1.058370	-1.056979	-1.046379	-1.022939
(3,-1)	-1.105272	-1.011649	-1.127365	-1.214919	-1.399433	-1.058370	-1.056979	-1.046379	-1.022939
(3,-1)	-1.105272	-1.011649	-1.127365	-1.214919	-1.399433	-1.058370	-1.056979	-1.046379	-1.022939
(3,-1)	-1.105272	-1.011649	-1.127365	-1.214919	-1.399433	-1.058370	-1.056979	-1.046379	-1.022939
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.683071	-0.945731	-0.618194	-0.763789	-0.650507	-0.649868	-0.665948		
(3,-1)	-0.676203	-0.611709	-0.612498	-0.756045	-0.644749	-0.643321	-0.659813		
(3,-1)	-1.112007	-0.936345	-1.115936	-1.160570	-1.096428	-1.085860	-1.094654		
(3,-1)	-0.676203	-0.946174	-0.612498	-0.756045	-0.644749	-0.643321	-0.659814		
(3,-1)	-1.112007	-0.946174	-1.115936	-1.160570	-1.096428	-1.085860	-1.094656		
(3,-1)	-1.107283	-0.611709	-1.106660	-1.155325	-1.091945	-1.081341	-1.089958		
(3,-1)	-1.107283	-0.936345	-1.106660	-1.155325	-1.091945	-1.081341	-1.089958		
(3,-1)	-1.107283	-0.946174	-1.106660	-1.155325	-1.091945	-1.081341	-1.089958		
(3,-1)	-1.105272	-0.611709	-1.104217	-1.152689	-1.088497	-1.079147	-1.086871		
(3,-1)	-1.105272	-0.936345	-1.104217	-1.152689	-1.088497	-1.079147	-1.086871		
(3,-1)	-1.105272	-0.946174	-1.104217	-1.152689	-1.088497	-1.079147	-1.086873		
(3,-1)	-1.105272	-0.946174	-1.104217	-1.152689	-1.088497	-1.079147	-1.086871		

Table S304: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>10</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.112580	-1.018832	-1.058852	-1.026710	-1.071138	-0.935697	-1.035721	-0.965005	-0.839763
(3,-1)	-0.680911	-0.565496	-0.613579	-0.588311	-0.637717	-0.545684	-0.567551	-0.650546	-0.631409
(3,-1)	-1.097205	-1.002003	-1.048508	-1.013882	-1.057816	-0.932202	-1.022466	-0.953739	-0.847440
(3,-1)	-1.107027	-1.011649	-1.058158	-1.023072	-1.067129	-0.939533	-1.031667	-0.960879	-0.853745
(3,-1)	-1.107027	-1.011649	-1.058158	-1.023072	-1.067129	-0.939533	-1.031667	-0.960879	-0.853745
(3,-1)	-0.680911	-0.565496	-0.613579	-0.588311	-0.637717	-0.545684	-0.567551	-0.650546	-0.631409
(3,-1)	-1.097205	-1.002003	-1.048508	-1.013882	-1.057816	-0.932202	-1.022466	-0.953739	-0.847440
(3,-1)	-1.107029	-1.011649	-1.058158	-1.023072	-1.067129	-0.939533	-1.031667	-0.960879	-0.853745
(3,-1)	-1.107025	-1.011649	-1.058158	-1.023072	-1.067129	-0.939533	-1.031667	-0.960879	-0.853745
(3,-1)	-0.680911	-0.565496	-0.613579	-0.588311	-0.637717	-0.545684	-0.567551	-0.650546	-0.631409
(3,-1)	-1.097205	-1.002003	-1.048508	-1.013882	-1.057816	-0.932202	-1.022466	-0.953739	-0.847440
(3,-1)	-1.107025	-1.011649	-1.058158	-1.023072	-1.067129	-0.939533	-1.031667	-0.960879	-0.853745
(3,-1)	-1.107029	-1.011649	-1.058158	-1.023072	-1.067129	-0.939533	-1.031667	-0.960879	-0.853745
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.112580	-0.552820	-1.021953	-1.079991	-1.054759	-1.019430	-0.940892	-1.078955	-1.040559
(3,-1)	-0.680911	-0.552820	-0.647664	-0.639907	-0.623111	-0.591251	-0.626100	-0.657912	-0.609111
(3,-1)	-1.097205	0.073170	-1.010166	-1.067799	-1.040216	-1.009667	-0.926428	-1.063396	-1.027516
(3,-1)	-1.107027	-0.438516	-1.020793	-1.077577	-1.049623	-1.016689	-0.934029	-1.072926	-1.037534
(3,-1)	-1.107027	-0.552820	-1.020793	-1.077577	-1.049623	-1.016689	-0.934029	-1.072926	-1.037534
(3,-1)	-0.680911	-0.552820	-0.647664	-0.639907	-0.623111	-0.591251	-0.626100	-0.657912	-0.609111
(3,-1)	-1.097205	0.073170	-1.010166	-1.067799	-1.040216	-1.009667	-0.926428	-1.063396	-1.027516
(3,-1)	-1.107029	-0.438516	-1.020793	-1.077577	-1.049623	-1.016689	-0.934029	-1.072926	-1.037534
(3,-1)	-1.107025	-1.024603	-1.020793	-1.077577	-1.049623	-1.016689	-0.934029	-1.072926	-1.037534
(3,-1)	-0.680911	-1.024603	-0.647664	-0.639907	-0.623111	-0.591251	-0.626100	-0.657912	-0.609111
(3,-1)	-1.097205	-1.024603	-1.010166	-1.067799	-1.040216	-1.009667	-0.926428	-1.063396	-1.027516
(3,-1)	-1.107025	-1.024603	-1.020793	-1.077577	-1.049623	-1.016689	-0.934029	-1.072926	-1.037534
(3,-1)	-1.107029	-1.024603	-1.020793	-1.077577	-1.049623	-1.016689	-0.934029	-1.072926	-1.037534
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.112580	-1.017352	-1.130819	-1.220853	-1.404925	-1.065126	-1.064136	-1.054290	-1.030639
(3,-1)	-0.680911	-0.527909	-0.635498	-0.664592	-0.628831	-0.629678	-0.631127	-0.617941	-0.599100
(3,-1)	-1.097205	-1.003519	-1.123413	-1.209485	-1.394865	-1.050151	-1.048760	-1.038358	-1.015241
(3,-1)	-1.107027	-1.012625	-1.133545	-1.220689	-1.406866	-1.059016	-1.058011	-1.047902	-1.024673
(3,-1)	-1.107027	-1.012625	-1.133545	-1.220689	-1.406866	-1.059016	-1.058011	-1.047902	-1.024673
(3,-1)	-0.680911	-0.527909	-0.635498	-0.664592	-0.628831	-0.629678	-0.631127	-0.617941	-0.599100
(3,-1)	-1.097205	-1.003519	-1.123413	-1.209485	-1.394865	-1.050151	-1.048760	-1.038358	-1.015241
(3,-1)	-1.107029	-1.012625	-1.133545	-1.220689	-1.406866	-1.059016	-1.058011	-1.047902	-1.024673
(3,-1)	-1.107025	-1.012625	-1.133545	-1.220689	-1.406866	-1.059016	-1.058011	-1.047902	-1.024673
(3,-1)	-0.680911	-0.527909	-0.635498	-0.664592	-0.628831	-0.629678	-0.631127	-0.617941	-0.599100
(3,-1)	-1.097205	-1.003519	-1.123413	-1.209485	-1.394865	-1.050151	-1.048760	-1.038358	-1.015241
(3,-1)	-1.107025	-1.012625	-1.133545	-1.220689	-1.406866	-1.059016	-1.058011	-1.047902	-1.024673
(3,-1)	-1.107029	-1.012625	-1.133545	-1.220689	-1.406866	-1.059016	-1.058011	-1.047902	-1.024673
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.112580	-0.556598	-1.115191	-1.159075	-1.094218	-1.086131	-1.092875		
(3,-1)	-0.680911	-0.556598	-0.616123	-0.761148	-0.648327	-0.647862	-0.663743		
(3,-1)	-1.097205	0.105373	-1.095814	-1.145452	-1.082253	-1.071849	-1.079990		
(3,-1)	-1.107027	-0.439853	-1.110505	-1.155831	-1.091928	-1.081349	-1.089783		
(3,-1)	-1.107027	-0.556598	-1.110505	-1.155831	-1.091928	-1.081349	-1.089783		
(3,-1)	-0.680911	-0.556598	-0.616123	-0.761148	-0.648327	-0.647862	-0.663743		
(3,-1)	-1.097205	0.105373	-1.095814	-1.145452	-1.082253	-1.071849	-1.080007		
(3,-1)	-1.107029	-0.439853	-1.110505	-1.155831	-1.091928	-1.081349	-1.089788		
(3,-1)	-1.107025	-0.994808	-1.110505	-1.155831	-1.091928	-1.081349	-1.089835		
(3,-1)	-0.680911	-0.994808	-0.616123	-0.761148	-0.648327	-0.647862	-0.663787		
(3,-1)	-1.097205	-0.994808	-1.095814	-1.145452	-1.082253	-1.071849	-1.080008		
(3,-1)	-1.107025	-0.994808	-1.110505	-1.155831	-1.091928	-1.081349	-1.089834		
(3,-1)	-1.107029	-0.994808	-1.110505	-1.155831	-1.091928	-1.081349	-1.089788		







Table S307: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>2</sub>CF<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.230160	-0.414945	-0.452647	-0.399428	-0.267192	-0.429483	-0.321637	-0.182399	0.197578
(3,-1)	-0.230160	-0.414945	-0.452647	-0.399428	-0.267192	-0.429483	-0.321637	-0.182399	0.197578
(3,-1)	-1.333596	-1.215804	-1.273195	-1.230071	-1.290975	-1.134247	-1.260417	-1.077838	-0.931400
(3,-1)	-1.333596	-1.215804	-1.273195	-1.230071	-1.290975	-1.134247	-1.260417	-1.077838	-0.931400
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.230160	-1.269712	0.155964	-0.374644	-0.294230	-0.122950	-0.291019	-0.158843	-0.279208
(3,-1)	-0.230160	-0.160349	0.155964	-0.374644	-0.294230	-0.122950	-0.291019	-0.158843	-0.279208
(3,-1)	-1.333596	-0.160349	-1.298578	-1.304926	-1.271865	-1.212447	-1.067153	-1.312338	-1.294057
(3,-1)	-1.333596	-0.160349	-1.298578	-1.304926	-1.271865	-1.212447	-1.067153	-1.312338	-1.294057
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.230160	-0.211944	-0.205595	-0.270759	-0.242110	-0.243773	-0.281223	-0.297448	-0.305483
(3,-1)	-0.230160	-0.211944	-0.205595	-0.270759	-0.242110	-0.243773	-0.281223	-0.297448	-0.305483
(3,-1)	-1.333596	-1.233295	-1.366438	-1.457645	-1.607630	-1.295014	-1.292327	-1.276840	-1.253301
(3,-1)	-1.333596	-1.233295	-1.366438	-1.457645	-1.607630	-1.295014	-1.292327	-1.276840	-1.253301
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.230160	-1.194990	-0.249348	0.078109	-0.324359	-0.206099	-0.224841		
(3,-1)	-0.230160	-0.222058	-0.249348	0.078109	-0.324359	-0.206099	-0.224841		
(3,-1)	-1.333596	-0.222058	-1.373011	-1.421952	-1.325861	-1.317045	-1.327193		
(3,-1)	-1.333596	-0.222058	-1.373011	-1.421952	-1.325861	-1.317045	-1.327194		

Table S308: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{HCF}_3$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.423299	-1.291234	-1.348588	-1.303574	-1.373644	-1.195035	-1.341706	-1.123039	-0.969997
(3,-1)	-0.431663	-0.583121	-0.631712	-0.567162	-0.458096	-0.615020	-0.517943	-0.337389	0.001948
(3,-1)	-0.431663	-0.583121	-0.631712	-0.567162	-0.458096	-0.615020	-0.517943	-0.337389	0.001948
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.423299	-0.347261	-1.407920	-1.387994	-1.354650	-1.290117	-1.122213	-1.403806	-1.391158
(3,-1)	-0.431663	-0.347261	-0.005908	-0.571564	-0.481259	-0.309083	-0.469125	-0.344386	-0.476609
(3,-1)	-0.431663	-1.125525	-0.005908	-0.571564	-0.481259	-0.309083	-0.469125	-0.344386	-0.476609
(3,-1)	-0.431663	-1.125525	-0.005908	-0.571564	-0.481259	-0.309083	-0.469125	-0.344386	-0.476609
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.423299	-1.312164	-1.465439	-1.541690	-1.688597	-1.379199	-1.378252	-1.362920	-1.338955
(3,-1)	-0.431663	-0.366926	-0.383365	-0.481538	-0.465452	-0.431777	-0.471093	-0.481705	-0.520948
(3,-1)	-0.431663	-0.366926	-0.383365	-0.481538	-0.465452	-0.431777	-0.471093	-0.481705	-0.520948
(3,-1)	-0.431663	-0.366926	-0.383365	-0.481538	-0.465452	-0.431777	-0.471093	-0.481705	-0.520948
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.423299	-0.329772	-1.473982	-1.527154	-1.411180	-1.405602	-1.413083		
(3,-1)	-0.431663	-0.329772	-0.454296	-0.148835	-0.521656	-0.400340	-0.420338		
(3,-1)	-0.431663	-1.078612	-0.454296	-0.148835	-0.521656	-0.400340	-0.420299		
(3,-1)	-0.431663	-1.078612	-0.454296	-0.148835	-0.521656	-0.400340	-0.420298		



Table S309: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>2</sub>CCl<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.337168	-0.255888	-0.278230	-0.270205	-0.312385	-0.239135	-0.247204	-0.250199	-0.333134
(3,-1)	-0.337168	-0.255888	-0.278230	-0.270205	-0.312385	-0.239135	-0.247204	-0.250199	-0.333134
(3,-1)	-1.267260	-1.167425	-1.217137	-1.178304	-1.234251	-1.060582	-1.199946	-1.067748	-0.946908
(3,-1)	-1.267260	-1.167425	-1.217137	-1.178304	-1.234251	-1.060582	-1.199946	-1.067748	-0.946908
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.337168	-1.177581	-0.368810	-0.305261	-0.303854	-0.192853	-0.231501	-0.334736	-0.308642
(3,-1)	-0.337168	-0.347017	-0.368810	-0.305261	-0.303854	-0.192853	-0.231501	-0.334736	-0.308642
(3,-1)	-1.267260	-0.347017	-1.212859	-1.244681	-1.214738	-1.171738	-1.044430	-1.251339	-1.218888
(3,-1)	-1.267260	-0.347017	-1.212859	-1.244681	-1.214738	-1.171738	-1.044430	-1.251339	-1.218888
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.337168	-0.214519	-0.283566	-0.322834	-0.336259	-0.327681	-0.317916	-0.295040	-0.289021
(3,-1)	-0.337168	-0.214519	-0.283566	-0.322834	-0.336259	-0.327681	-0.317916	-0.295040	-0.289021
(3,-1)	-1.267260	-1.165239	-1.309528	-1.405524	-1.581371	-1.239739	-1.235496	-1.219897	-1.190099
(3,-1)	-1.267260	-1.165239	-1.309528	-1.405524	-1.581371	-1.239739	-1.235496	-1.219897	-1.190099
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.337168	-1.122901	-0.255972	-0.419763	-0.315211	-0.326071	-0.335449		
(3,-1)	-0.337168	-0.331668	-0.255972	-0.419763	-0.315211	-0.326071	-0.335449		
(3,-1)	-1.267260	-0.331668	-1.319624	-1.348908	-1.261877	-1.253549	-1.262749		
(3,-1)	-1.267260	-0.331668	-1.319624	-1.348908	-1.261877	-1.253549	-1.262749		

Table S310: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{HCCl}_3$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.326363	-1.221476	-1.268820	-1.230180	-1.292007	-1.101054	-1.255043	-1.106489	-0.974315
(3,-1)	-0.341714	-0.257603	-0.278269	-0.271410	-0.316069	-0.240557	-0.246074	-0.252807	-0.336818
(3,-1)	-0.341714	-0.257603	-0.278269	-0.271410	-0.316069	-0.240557	-0.246074	-0.252807	-0.336818
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.326363	-0.790744	-1.278880	-1.301183	-1.272325	-1.228204	-1.085943	-1.314348	-1.281405
(3,-1)	-0.341714	-0.976055	-0.370919	-0.307953	-0.308063	-0.194134	-0.233918	-0.340128	-0.312073
(3,-1)	-0.341714	-1.566512	-0.370919	-0.307953	-0.308063	-0.194134	-0.233918	-0.340128	-0.312073
(3,-1)	-0.341714	-1.566512	-0.370919	-0.307953	-0.308063	-0.194134	-0.233918	-0.340128	-0.312073
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.326363	-1.216423	-1.370602	-1.467707	-1.645123	-1.303276	-1.297984	-1.280489	-1.247075
(3,-1)	-0.341714	-0.216451	-0.289703	-0.329841	-0.341682	-0.334369	-0.323831	-0.299437	-0.291732
(3,-1)	-0.341714	-0.216451	-0.289703	-0.329841	-0.341682	-0.334369	-0.323831	-0.299437	-0.291732
(3,-1)	-0.341714	-0.216451	-0.289703	-0.329841	-0.341682	-0.334369	-0.323831	-0.299437	-0.291732
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.326363	-0.757798	-1.393277	-1.418735	-1.318880	-1.313485	-1.321392		
(3,-1)	-0.341714	-0.945382	-0.265133	-0.429389	-0.317195	-0.329957	-0.339228		
(3,-1)	-0.341714	-1.577959	-0.265133	-0.429389	-0.317195	-0.329957	-0.339311		
(3,-1)	-0.341714	-1.577959	-0.265133	-0.429389	-0.317195	-0.329957	-0.339311		

Table S311: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>3</sub>C–NH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.787542	-0.637937	-0.687717	-0.670632	-0.739274	-0.609706	-0.659739	-0.703644	-0.832866
(3,-1)	-1.108615	-1.013862	-1.061787	-1.026087	-1.072941	-0.943552	-1.035417	-0.960334	-0.841825
(3,-1)	-1.822290	-1.764994	-1.742945	-1.726039	-1.789155	-1.558191	-1.729991	-1.726361	-1.723437
(3,-1)	-1.822290	-1.764994	-1.742945	-1.726039	-1.789155	-1.558191	-1.729991	-1.726361	-1.723437
(3,-1)	-1.155067	-1.060195	-1.111426	-1.073272	-1.120558	-0.982561	-1.085512	-0.992706	-0.876387
(3,-1)	-1.155067	-1.060195	-1.111426	-1.073272	-1.120558	-0.982561	-1.085512	-0.992706	-0.876387
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.787542	-0.711975	-0.822558	-0.728537	-0.724212	-0.586497	-0.634046	-0.784308	-0.697023
(3,-1)	-1.108615	0.072183	-1.029304	-1.083805	-1.055627	-1.026823	-0.936025	-1.082930	-1.047524
(3,-1)	-1.822290	-1.006657	-1.636429	-1.788259	-1.780507	-1.776720	-1.627120	-1.822886	-1.588701
(3,-1)	-1.822290	-1.006657	-1.636429	-1.788259	-1.780507	-1.776720	-1.627120	-1.822886	-1.588701
(3,-1)	-1.155067	-1.006657	-1.084379	-1.132625	-1.102217	-1.063719	-0.967129	-1.129761	-1.097494
(3,-1)	-1.155067	-1.006657	-1.084379	-1.132625	-1.102217	-1.063719	-0.967129	-1.129761	-1.097494
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.787542	-0.644518	-0.680574	-0.734151	-0.707412	-0.744996	-0.736885	-0.718475	-0.689455
(3,-1)	-1.108615	-1.023019	-1.138474	-1.228831	-1.407486	-1.071105	-1.068414	-1.055086	-1.031544
(3,-1)	-1.822290	-1.672179	-1.850581	-1.978940	-2.209224	-1.803063	-1.791102	-1.760097	-1.724771
(3,-1)	-1.822290	-1.672179	-1.850581	-1.978940	-2.209224	-1.803063	-1.791102	-1.760097	-1.724771
(3,-1)	-1.155067	-1.068264	-1.187938	-1.279257	-1.457624	-1.116614	-1.114829	-1.102597	-1.078145
(3,-1)	-1.155067	-1.068264	-1.187938	-1.279257	-1.457624	-1.116614	-1.114829	-1.102597	-1.078145
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.787542	-0.726462	-0.656801	-0.932816	-0.749861	-0.767739	-0.772906		
(3,-1)	-1.108615	-0.030710	-1.113843	-1.170472	-1.100896	-1.091180	-1.101163		
(3,-1)	-1.822290	-0.978880	-1.908507	-1.935977	-1.817693	-1.836317	-1.818741		
(3,-1)	-1.822290	-0.978880	-1.908507	-1.935977	-1.817693	-1.836317	-1.818742		
(3,-1)	-1.155067	-0.978880	-1.171260	-1.218211	-1.149129	-1.137688	-1.148140		
(3,-1)	-1.155067	-0.978880	-1.171260	-1.218211	-1.149129	-1.137688	-1.148140		

Table S312: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>-CN system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.796210	-0.678115	-0.730963	-0.702086	-0.756140	-0.668047	-0.685706	-0.769708	-0.749874
(3,-1)	-0.310612	-0.757835	-0.680663	-0.591843	-0.446920	-1.009102	-0.715534	-0.175640	0.219307
(3,-1)	-1.140166	-1.049946	-1.098955	-1.060805	-1.107409	-0.966860	-1.072624	-0.981848	-0.890239
(3,-1)	-1.140166	-1.049946	-1.098955	-1.060805	-1.107409	-0.966860	-1.072624	-0.981848	-0.890239
(3,-1)	-1.140166	-1.049946	-1.098955	-1.060805	-1.107409	-0.966860	-1.072624	-0.981848	-0.890239
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.796210	-0.701460	-0.749695	-0.760068	-0.741506	-0.721728	-0.744709	-0.779502	-0.718514
(3,-1)	-0.310612	-1.044107	0.308124	-0.606690	-0.496540	-0.632373	-0.714845	-0.253576	-0.483723
(3,-1)	-1.140166	-1.081242	-1.065961	-1.120136	-1.089527	-1.049359	-0.952016	-1.115932	-1.080157
(3,-1)	-1.140166	-1.081242	-1.065961	-1.120136	-1.089527	-1.049359	-0.952016	-1.115932	-1.080157
(3,-1)	-1.140166	-1.174154	-1.065961	-1.120136	-1.089527	-1.049359	-0.952016	-1.115932	-1.080157
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.796210	-0.640664	-0.768853	-0.794389	-0.755689	-0.741544	-0.747399	-0.739550	-0.714524
(3,-1)	-0.310612	-0.203262	-0.364575	-0.572311	-0.356833	-0.393058	-0.510117	-0.594381	-0.777729
(3,-1)	-1.140166	-1.047651	-1.179742	-1.270730	-1.459153	-1.103809	-1.102490	-1.090008	-1.065411
(3,-1)	-1.140166	-1.047651	-1.179742	-1.270730	-1.459153	-1.103809	-1.102490	-1.090008	-1.065411
(3,-1)	-1.140166	-1.047651	-1.179742	-1.270730	-1.459153	-1.103809	-1.102490	-1.090008	-1.065411
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.796210	-0.691928	-0.746816	-0.910444	-0.772986	-0.774245	-0.789218		
(3,-1)	-0.310612	-1.011388	-0.565129	-0.207453	-0.508416	-0.386649	-0.439575		
(3,-1)	-1.140166	-1.042438	-1.176360	-1.203895	-1.134955	-1.123270	-1.132440		
(3,-1)	-1.140166	-1.042438	-1.176360	-1.203895	-1.134955	-1.123270	-1.132375		
(3,-1)	-1.140166	-1.146498	-1.176360	-1.203895	-1.134955	-1.123270	-1.132375		

Table S313: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>-NO<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.762730	-0.600519	-0.645428	-0.633001	-0.699870	-0.576909	-0.626097	-0.683940	-0.794345
(3,-1)	-1.180408	-1.081438	-1.133162	-1.092747	-1.143237	-0.993547	-1.109215	-1.000917	-0.905643
(3,-1)	-1.216638	-1.118686	-1.171425	-1.130475	-1.182218	-1.031213	-1.148278	-1.024672	-0.923368
(3,-1)	-1.216649	-1.118686	-1.171425	-1.130475	-1.182218	-1.031213	-1.148278	-1.024672	-0.923368
(3,-1)	-1.156837	-1.020991	-1.050538	-1.037555	-1.134149	-0.887809	-0.963739	-0.935219	-1.101170
(3,-1)	-1.157105	-1.020991	-1.050538	-1.037555	-1.134149	-0.887809	-0.963739	-0.935219	-1.101170
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.762730	-0.323755	-0.725551	-0.690035	-0.690008	-0.585378	-0.623475	-0.733993	-0.663577
(3,-1)	-1.180408	-1.087999	-1.108851	-1.157089	-1.124898	-1.080212	-0.975194	-1.155935	-1.124967
(3,-1)	-1.216638	-1.059269	-1.154288	-1.196035	-1.163563	-1.113092	-1.000433	-1.195084	-1.165774
(3,-1)	-1.216649	-1.059269	-1.154288	-1.196035	-1.163563	-1.113092	-1.000433	-1.195084	-1.165774
(3,-1)	-1.156837	-0.501743	-1.164002	-1.119809	-1.123603	-0.754073	-0.856136	-1.202892	-1.009044
(3,-1)	-1.157105	-1.580342	-1.164002	-1.119809	-1.123603	-0.754073	-0.856136	-1.202892	-1.009044
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.762730	-0.636686	-0.634998	-0.680487	-0.586209	-0.704011	-0.701836	-0.690340	-0.662386
(3,-1)	-1.180408	-1.083032	-1.218990	-1.310013	-1.496388	-1.143878	-1.141791	-1.127893	-1.102700
(3,-1)	-1.216638	-1.119426	-1.259076	-1.351659	-1.535640	-1.180670	-1.179051	-1.165834	-1.140843
(3,-1)	-1.216649	-1.119426	-1.259076	-1.351659	-1.535640	-1.180670	-1.179051	-1.165834	-1.140843
(3,-1)	-1.156837	-0.898593	-1.131678	-1.258808	-1.510727	-1.114845	-1.113169	-1.077720	-1.020252
(3,-1)	-1.157105	-0.898593	-1.131678	-1.258808	-1.510727	-1.114845	-1.113169	-1.077720	-1.020252
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.762730	-0.400524	-0.595001	-0.634659	-0.712740	-0.730896	-0.728280		
(3,-1)	-1.180408	-1.045055	-1.221324	-1.250339	-1.173407	-1.161754	-1.171476		
(3,-1)	-1.216638	-1.020268	-1.263725	-1.292621	-1.210685	-1.199205	-1.208775		
(3,-1)	-1.216649	-1.020268	-1.263725	-1.292621	-1.210685	-1.199205	-1.208776		
(3,-1)	-1.156837	-0.459122	-1.091269	-1.380652	-1.114277	-1.145841	-1.171478		
(3,-1)	-1.157105	-1.554271	-1.091269	-1.380652	-1.114277	-1.145841	-1.171478		

Table S314: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>-O-N=O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.573918	-0.531498	-0.573249	-0.557044	-0.538433	-0.548074	-0.534436	-0.491467	-0.311213
(3,-1)	-1.220464	-1.122187	-1.175373	-1.134148	-1.185739	-1.030371	-1.153837	-1.030492	-0.915623
(3,-1)	-1.198915	-1.097561	-1.149917	-1.110383	-1.163034	-1.020567	-1.128226	-1.010873	-0.896964
(3,-1)	-1.194936	-1.097561	-1.149917	-1.110383	-1.163034	-1.020567	-1.128226	-1.010873	-0.896964
(3,-1)	-0.477126	-0.262604	-0.272748	-0.275478	-0.379342	-0.203605	-0.264621	-0.320566	-0.409333
(3,-1)	-1.609120	-1.395561	-1.439394	-1.420977	-1.535734	-1.271841	-1.361371	-1.282491	-1.524927
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.573918	0.244634	-0.275846	-0.575128	-0.545116	-0.422565	-0.490946	-0.477445	-0.553347
(3,-1)	-1.220464	-0.934324	-1.158127	-1.199449	-1.166736	-1.118291	-1.007237	-1.197748	-1.170584
(3,-1)	-1.198915	-0.934324	-1.130511	-1.175345	-1.144351	-1.100242	-0.988391	-1.173867	-1.145552
(3,-1)	-1.194936	-0.934324	-1.130511	-1.175345	-1.144351	-1.100242	-0.988391	-1.173867	-1.145552
(3,-1)	-0.477126	0.199018	-0.459178	-0.360115	-0.381756	-0.232498	-0.297282	-0.465085	-0.367124
(3,-1)	-1.609120	0.199018	-1.571893	-1.518996	-1.521966	-1.088273	-1.185383	-1.620689	-1.370601
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.573918	-0.503288	-0.478834	-0.515682	-0.472298	-0.509406	-0.534706	-0.548468	-0.533991
(3,-1)	-1.220464	-1.127842	-1.259776	-1.353466	-1.528195	-1.184318	-1.182615	-1.169965	-1.145468
(3,-1)	-1.198915	-1.103675	-1.235804	-1.331789	-1.507005	-1.161659	-1.159331	-1.145597	-1.122252
(3,-1)	-1.194936	-1.103675	-1.235804	-1.331789	-1.507005	-1.161659	-1.159331	-1.145597	-1.122252
(3,-1)	-0.477126	-0.300102	-0.376066	-0.377954	-0.518780	-0.433213	-0.413376	-0.377837	-0.342729
(3,-1)	-1.609120	-1.295378	-1.542120	-1.707931	-1.992380	-1.497549	-1.506507	-1.481741	-1.405424
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.573918	0.224519	-0.447106	-0.256705	-0.571734	-0.515696	-0.521063		
(3,-1)	-1.220464	-0.917223	-1.261036	-1.293571	-1.215344	-1.203604	-1.214152		
(3,-1)	-1.198915	-0.917223	-1.232674	-1.273818	-1.190694	-1.180525	-1.189828		
(3,-1)	-1.194936	-0.917223	-1.232674	-1.273818	-1.190694	-1.180525	-1.189828		
(3,-1)	-0.477126	0.199471	-0.308183	-0.691646	-0.347673	-0.405022	-0.395571		
(3,-1)	-1.609120	0.199471	-1.511706	-1.846433	-1.512841	-1.550021	-1.580776		

Table S315: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>-SiH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.219152	0.104747	0.124039	0.143501	0.174932	0.129494	0.150218	0.206139	0.307709
(3,-1)	-1.063492	-0.987139	-1.028042	-0.994907	-1.035518	-0.906609	-1.001232	-0.945120	-0.857693
(3,-1)	-1.063492	-0.987139	-1.028042	-0.994907	-1.035518	-0.906609	-1.001232	-0.945120	-0.857693
(3,-1)	-1.063492	-0.987139	-1.028042	-0.994907	-1.035518	-0.906609	-1.001232	-0.945120	-0.857693
(3,-1)	0.185265	0.062785	0.101731	0.112325	0.142177	0.116070	0.119099	0.172788	0.219097
(3,-1)	0.185265	0.062785	0.101731	0.112325	0.142177	0.116070	0.119099	0.172788	0.219097
(3,-1)	0.185265	0.062785	0.101731	0.112325	0.142177	0.116070	0.119099	0.172788	0.219097
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.219152	-0.414945	0.304488	0.143433	0.168032	0.152857	0.121074	0.201418	0.161074
(3,-1)	-1.063492	0.121239	-0.980532	-1.045401	-1.018653	-0.992206	-0.913552	-1.038589	-1.001778
(3,-1)	-1.063492	-2.596366	-0.980532	-1.045401	-1.018653	-0.992206	-0.913552	-1.038589	-1.001778
(3,-1)	-1.063492	-1.142247	-0.980532	-1.045401	-1.018653	-0.992206	-0.913552	-1.038589	-1.001778
(3,-1)	0.185265		0.215172	0.116875	0.133187	0.138856	0.114592	0.164177	0.127915
(3,-1)	0.185265		0.215172	0.116875	0.133187	0.138856	0.114592	0.164177	0.127915
(3,-1)	0.185265		0.215172	0.116875	0.133187	0.138856	0.114592	0.164177	0.127915
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.219152	0.207062	0.188983	0.148714	0.187636	0.161433	0.161846	0.168069	0.162654
(3,-1)	-1.063492	-0.975773	-1.105745	-1.189400	-1.383030	-1.026266	-1.025019	-1.014502	-0.991300
(3,-1)	-1.063492	-0.975773	-1.105745	-1.189400	-1.383030	-1.026266	-1.025019	-1.014502	-0.991300
(3,-1)	-1.063492	-0.975773	-1.105745	-1.189400	-1.383030	-1.026266	-1.025019	-1.014502	-0.991300
(3,-1)	0.185265	0.181804	0.179476	0.141686	0.252007	0.121582	0.126239	0.135633	0.133503
(3,-1)	0.185265	0.181804	0.179476	0.141686	0.252007	0.121582	0.126239	0.135633	0.133503
(3,-1)	0.185265	0.181804	0.179476	0.141686	0.252007	0.121582	0.126239	0.135633	0.133503
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.219152	-0.515682	0.173621	0.244588	0.173871	0.203227	0.195047		
(3,-1)	-1.063492	-0.008691	-1.076566	-1.113737	-1.058414	-1.047718	-1.054793		
(3,-1)	-1.063492	-2.634144	-1.076566	-1.113737	-1.058414	-1.047718	-1.054744		
(3,-1)	-1.063492	-1.086402	-1.076566	-1.113737	-1.058414	-1.047718	-1.054743		
(3,-1)	0.185265		0.094386	0.204424	0.144533	0.166507	0.163424		
(3,-1)	0.185265		0.094386	0.204424	0.144533	0.166507	0.163457		
(3,-1)	0.185265		0.094386	0.204424	0.144533	0.166507	0.163457		

Table S316: Laplacian of the density value (a.u.) at the considered critical points for the HCOOH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.744231	-0.784443	-0.832339	-0.767451	-0.724145	-0.824429	-0.758144	-0.535012	-0.337698
(3,-1)	-0.311579	-0.567116	-0.567524	-0.457560	-0.377736	-0.713927	-0.473305	-0.016792	0.256003
(3,-1)	-2.667000	-2.599843	-2.568245	-2.559714	-2.637418	-2.403078	-2.639531	-2.636110	-2.731379
(3,-1)	-1.275239	-1.160642	-1.209461	-1.169962	-1.233585	-1.061280	-1.196088	-1.041166	-0.914234
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.744231	0.122088	-0.261463	-0.824871	-0.742999	-0.580470	-0.704160	-0.630343	-0.761865
(3,-1)	-0.311579	-0.391988	0.366441	-0.528509	-0.407601	-0.289206	-0.441008	-0.214643	-0.407342
(3,-1)	-2.667000	-1.127891	-2.506716	-2.643722	-2.647198	-2.626563	-2.540791	-2.760425	-2.369705
(3,-1)	-1.275239	-0.264580	-1.237285	-1.245627	-1.216488	-1.166466	-1.028750	-1.260431	-1.235414
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.744231	-0.616483	-0.665892	-0.806925	-0.768479	-0.695010	-0.740979	-0.750629	-0.804612
(3,-1)	-0.311579	-0.090271	-0.299297	-0.573521	-0.504289	-0.352826	-0.418162	-0.423946	-0.613711
(3,-1)	-2.667000	-2.626257	-2.544402	-2.651026	-2.679422	-2.719642	-2.714791	-2.699936	-2.644058
(3,-1)	-1.275239	-1.174595	-1.310395	-1.405066	-1.549945	-1.244463	-1.240080	-1.223085	-1.197517
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.744231	-0.008341	-0.726405	-0.591468	-0.785493	-0.693665	-0.704770		
(3,-1)	-0.311579	-0.493523	-0.553792	-0.274658	-0.431930	-0.317974	-0.343008		
(3,-1)	-2.667000	-1.074170	-2.922869	-2.885520	-2.661809	-2.698144	-2.664147		
(3,-1)	-1.275239	-0.348845	-1.329627	-1.375836	-1.261389	-1.257605	-1.263431		



Table S317: Laplacian of the density value (a.u.) at the considered critical points for the HCOOCH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.314615	-0.558577	-0.559538	-0.450351	-0.371425	-0.706699	-0.464704	-0.011457	0.260991
(3,-1)	-0.663870	-0.776758	-0.825029	-0.756509	-0.712379	-0.808553	-0.749093	-0.516104	-0.303048
(3,-1)	-1.280720	-1.145812	-1.194139	-1.155022	-1.219007	-1.036877	-1.180095	-1.032498	-0.905277
(3,-1)	-0.429532	-0.522522	-0.563102	-0.541146	-0.500295	-0.536848	-0.511594	-0.440057	-0.197235
(3,-1)	-1.239826	-1.127457	-1.181675	-1.140810	-1.191945	-1.037644	-1.160071	-1.034568	-0.915515
(3,-1)	-1.223135	-1.110214	-1.163037	-1.123462	-1.175488	-1.029839	-1.141214	-1.020587	-0.903933
(3,-1)	-1.223135	-1.110214	-1.163037	-1.123462	-1.175488	-1.029839	-1.141214	-1.020587	-0.903933
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.314615	-0.067087	0.370368	-0.521763	-0.401829	-0.278594	-0.435095	-0.210158	-0.402149
(3,-1)	-0.663870	-0.991203	-0.239851	-0.817212	-0.731620	-0.570432	-0.696848	-0.618209	-0.755355
(3,-1)	-1.280720	-0.644224	-1.217762	-1.230857	-1.202159	-1.153887	-1.020116	-1.246203	-1.219642
(3,-1)	-0.429532	-1.737101	-0.194410	-0.553017	-0.512709	-0.375716	-0.461691	-0.430675	-0.527901
(3,-1)	-1.239826	-1.023960	-1.167771	-1.205095	-1.172690	-1.123882	-1.011484	-1.203879	-1.176084
(3,-1)	-1.223135	-0.972123	-1.145603	-1.187620	-1.156499	-1.112065	-0.997759	-1.186697	-1.157585
(3,-1)	-1.223135	-0.959307	-1.145603	-1.187620	-1.156499	-1.112065	-0.997759	-1.186697	-1.157585
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.314615	-0.089479	-0.297129	-0.567165	-0.502600	-0.345823	-0.411894	-0.418358	-0.605826
(3,-1)	-0.663870	-0.606919	-0.657208	-0.802860	-0.770225	-0.685317	-0.732422	-0.742087	-0.799633
(3,-1)	-1.280720	-1.161809	-1.295745	-1.391318	-1.537587	-1.230903	-1.226249	-1.208905	-1.183139
(3,-1)	-0.429532	-0.480865	-0.450307	-0.491476	-0.461622	-0.469138	-0.499688	-0.516667	-0.508027
(3,-1)	-1.239826	-1.134937	-1.263566	-1.358165	-1.529345	-1.189520	-1.187795	-1.175401	-1.150482
(3,-1)	-1.223135	-1.115847	-1.247246	-1.343542	-1.516059	-1.173735	-1.171403	-1.157980	-1.133609
(3,-1)	-1.223135	-1.115847	-1.247246	-1.343542	-1.516059	-1.173735	-1.171403	-1.157980	-1.133609
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.314615	-0.189911	-0.545277	-0.269875	-0.425464	-0.312471	-0.336735		
(3,-1)	-0.663870	-1.049630	-0.722464	-0.594893	-0.774583	-0.681137	-0.690488		
(3,-1)	-1.280720	-0.656346	-1.312905	-1.362396	-1.246020	-1.242660	-1.248169		
(3,-1)	-0.429532	-1.759985	-0.427782	-0.220275	-0.541437	-0.470599	-0.478145		
(3,-1)	-1.239826	-0.992866	-1.262359	-1.297858	-1.221661	-1.209881	-1.220616		
(3,-1)	-1.223135	-0.947762	-1.244639	-1.283907	-1.203931	-1.193432	-1.203256		
(3,-1)	-1.223135	-0.937007	-1.244639	-1.283907	-1.203931	-1.193432	-1.203256		

Table S318: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>CONH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.471506	-0.699334	-0.706240	-0.601164	-0.528942	-0.832844	-0.617301	-0.186292	0.055962
(3,-1)	-1.168781	-1.002426	-1.060961	-1.035553	-1.122263	-0.977083	-1.032833	-1.003276	-0.943183
(3,-1)	-0.754468	-0.613010	-0.664465	-0.638073	-0.697603	-0.585907	-0.621401	-0.717860	-0.674117
(3,-1)	-2.057599	-1.934865	-1.904316	-1.888699	-1.961157	-1.712950	-1.899115	-1.879023	-1.941988
(3,-1)	-1.163799	-1.064413	-1.113699	-1.075328	-1.121932	-0.977294	-1.087735	-0.995452	-0.896592
(3,-1)	-1.112831	-1.013926	-1.061265	-1.024633	-1.070073	-0.936525	-1.034548	-0.961008	-0.864125
(3,-1)	-1.099089	-1.001572	-1.048362	-1.012065	-1.056673	-0.923421	-1.020997	-0.952451	-0.858468
(3,-1)	-2.084496	-1.959339	-1.929645	-1.913280	-1.986030	-1.732653	-1.926468	-1.909381	-1.969530
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.471506	0.143872	0.176035	-0.674450	-0.559321	-0.416764	-0.579067	-0.378475	-0.563442
(3,-1)	-1.168781	-0.563908	-0.852514	-1.127190	-1.113910	-0.937271	-0.993911	-1.128599	-1.083864
(3,-1)	-0.754468	-0.582292	-0.692197	-0.698760	-0.682777	-0.692508	-0.701053	-0.726914	-0.663962
(3,-1)	-2.057599	-0.563908	-1.804473	-1.959544	-1.954515	-1.950542	-1.773616	-2.015396	-1.734109
(3,-1)	-1.163799	-1.586567	-1.082570	-1.134494	-1.103687	-1.062650	-0.967060	-1.130618	-1.095637
(3,-1)	-1.112831	-1.073091	-1.022114	-1.081904	-1.052566	-1.018731	-0.932394	-1.076820	-1.041886
(3,-1)	-1.099089	-1.073091	-1.007908	-1.068441	-1.039271	-1.007068	-0.923213	-1.063361	-1.027474
(3,-1)	-2.084496	-1.044565	-1.835705	-1.985432	-1.979789	-1.983882	-1.803177	-2.047413	-1.756335
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.471506	-0.262084	-0.458602	-0.714120	-0.655311	-0.502350	-0.570546	-0.580066	-0.753671
(3,-1)	-1.168781	-0.999543	-1.066559	-1.174985	-1.121775	-1.110300	-1.125140	-1.111513	-1.089105
(3,-1)	-0.754468	-0.599616	-0.718338	-0.740476	-0.695395	-0.694736	-0.695058	-0.680486	-0.657576
(3,-1)	-2.057599	-1.838280	-2.011890	-2.155018	-2.383337	-1.977586	-1.967797	-1.936835	-1.895132
(3,-1)	-1.163799	-1.062132	-1.193843	-1.285130	-1.470265	-1.116457	-1.115220	-1.103822	-1.079324
(3,-1)	-1.112831	-1.014468	-1.141411	-1.228631	-1.419771	-1.064650	-1.063296	-1.051682	-1.028154
(3,-1)	-1.099089	-1.001505	-1.127445	-1.213011	-1.404282	-1.051581	-1.050102	-1.038284	-1.014815
(3,-1)	-2.084496	-1.870443	-2.026857	-2.174208	-2.377898	-2.007821	-1.997379	-1.965765	-1.921854
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.471506	0.168126	-0.680703	-0.444876	-0.584007	-0.475513	-0.495817		
(3,-1)	-1.168781	-0.531046	-1.073392	-1.235175	-1.153101	-1.159096	-1.166300		
(3,-1)	-0.754468	-0.579497	-0.694711	-0.849621	-0.711071	-0.715011	-0.729515		
(3,-1)	-2.057599	-0.531046	-2.126645	-2.137041	-1.994674	-2.019586	-1.995403		
(3,-1)	-1.163799	-1.599766	-1.188530	-1.218080	-1.148315	-1.136374	-1.145323		
(3,-1)	-1.112831	-1.034403	-1.121986	-1.163631	-1.096508	-1.085390	-1.093956		
(3,-1)	-1.099089	-1.034403	-1.106228	-1.147969	-1.083200	-1.071956	-1.080615		
(3,-1)	-2.084496	-1.010038	-2.158618	-2.170208	-2.020685	-2.045509	-2.020535		

Table S319: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>2</sub>-NH-CH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.161124	0.185543	0.200272	0.180918	0.151350	0.214711	0.225567	0.143285	0.102279
(3,-1)	-0.516531	-0.411739	-0.443217	-0.434823	-0.487742	-0.387250	-0.421593	-0.426110	-0.567374
(3,-1)	-0.583606	-0.497201	-0.544952	-0.518488	-0.559180	-0.473453	-0.509916	-0.520968	-0.609015
(3,-1)	-0.516931	-0.411739	-0.443217	-0.434823	-0.487742	-0.387250	-0.421593	-0.426110	-0.567374
(3,-1)	-1.847675	-1.789970	-1.761377	-1.745920	-1.811359	-1.581896	-1.753564	-1.745892	-1.725485
(3,-1)	-1.202183	-1.114507	-1.160486	-1.122835	-1.172265	-1.016222	-1.136960	-1.030415	-0.918228
(3,-1)	-1.202615	-1.114507	-1.160486	-1.122835	-1.172265	-1.016222	-1.136960	-1.030415	-0.918228
(3,-1)	-1.174487	-1.087726	-1.132819	-1.096038	-1.145095	-0.993488	-1.108620	-1.012958	-0.903053
(3,-1)	-1.174023	-1.087726	-1.132819	-1.096038	-1.145095	-0.993488	-1.108620	-1.012958	-0.903053
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.161124	-0.893280	0.118450	0.183165	0.161880	0.147001	0.112877	0.140374	0.181054
(3,-1)	-0.516531	0.110081	-0.575197	-0.476846	-0.478032	-0.331234	-0.365490	-0.524341	-0.469408
(3,-1)	-0.583606	0.110081	-0.595872	-0.565730	-0.547004	-0.427397	-0.472501	-0.580720	-0.546727
(3,-1)	-0.516931		-0.575197	-0.476846	-0.478032	-0.331234	-0.365490	-0.524341	-0.469408
(3,-1)	-1.847675		-1.647574	-1.811273	-1.805450	-1.803441	-1.652363	-1.849380	-1.610654
(3,-1)	-1.202183		-1.135714	-1.184570	-1.154856	-1.111706	-1.006588	-1.184812	-1.151162
(3,-1)	-1.202615		-1.135714	-1.184570	-1.154856	-1.111706	-1.006588	-1.184812	-1.151162
(3,-1)	-1.174487		-1.102620	-1.156754	-1.127794	-1.089250	-0.988339	-1.156215	-1.121850
(3,-1)	-1.174023		-1.102620	-1.156754	-1.127794	-1.089250	-0.988339	-1.156215	-1.121850
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.161124	0.422226	0.161855	0.178080	0.237349	0.149699	0.153673	0.174906	0.177968
(3,-1)	-0.516531	-0.438801	-0.445807	-0.490662	-0.537343	-0.496502	-0.485976	-0.468772	-0.448600
(3,-1)	-0.583606	-0.497159	-0.536456	-0.586550	-0.598686	-0.548758	-0.552867	-0.549120	-0.526346
(3,-1)	-0.516931	-0.438801	-0.445807	-0.490662	-0.537343	-0.496502	-0.485976	-0.468772	-0.448600
(3,-1)	-1.847675	-1.700505	-1.870114	-2.004349	-2.228733	-1.828343	-1.817392	-1.785577	-1.755776
(3,-1)	-1.202183	-1.112662	-1.245550	-1.341448	-1.520206	-1.171508	-1.169580	-1.156793	-1.130414
(3,-1)	-1.202615	-1.112662	-1.245550	-1.341448	-1.520206	-1.171508	-1.169580	-1.156793	-1.130414
(3,-1)	-1.174487	-1.085982	-1.219384	-1.313754	-1.497375	-1.143466	-1.141320	-1.128641	-1.102514
(3,-1)	-1.174023	-1.085982	-1.219384	-1.313754	-1.497375	-1.143466	-1.141320	-1.128641	-1.102514
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.161124	-0.953298	0.192038	0.124007	0.171899	0.150007	0.127650		
(3,-1)	-0.516531	0.023865	-0.408912	-0.633626	-0.486169	-0.503493	-0.502820		
(3,-1)	-0.583606	0.023865	-0.512593	-0.665270	-0.573174	-0.569702	-0.582318		
(3,-1)	-0.516931		-0.408912	-0.633626	-0.486169	-0.503493	-0.502820		
(3,-1)	-1.847675		-1.947670	-1.970975	-1.840974	-1.862986	-1.844523		
(3,-1)	-1.202183		-1.247303	-1.275147	-1.201268	-1.191421	-1.201238		
(3,-1)	-1.202615		-1.247303	-1.275147	-1.201268	-1.191421	-1.201238		
(3,-1)	-1.174487		-1.214703	-1.247039	-1.173046	-1.163640	-1.172911		
(3,-1)	-1.174023		-1.214703	-1.247039	-1.173046	-1.163640	-1.172911		

Table S320: Laplacian of the density value (a.u.) at the considered critical points for the NCCN system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.034911	-0.900575	-0.949812	-0.917006	-0.983664	-0.862031	-0.913875	-0.993679	-0.989377
(3,-1)	-0.261850	-0.724594	-0.640581	-0.556020	-0.385629	-0.982839	-0.676252	-0.148919	0.255961
(3,-1)	-0.261850	-0.724594	-0.640581	-0.556020	-0.385629	-0.982839	-0.676252	-0.148919	0.255961
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.034911	-0.825808	-0.914640	-0.991637	-0.972087	-0.986364	-0.990954	-1.014291	-0.933187
(3,-1)	-0.261850	-0.825808	0.345009	-0.546590	-0.436423	-0.593536	-0.674425	-0.185250	-0.438753
(3,-1)	-0.261850	-0.957561	0.345009	-0.546590	-0.436423	-0.593536	-0.674425	-0.185250	-0.438753
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.034911	-0.866064	-1.051677	-1.081157	-1.100598	-0.982196	-0.990846	-0.987870	-0.937720
(3,-1)	-0.261850	-0.191575	-0.299619	-0.482143	-0.215917	-0.312401	-0.433245	-0.530492	-0.708672
(3,-1)	-0.261850	-0.191575	-0.299619	-0.482143	-0.215917	-0.312401	-0.433245	-0.530492	-0.708672
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.034911	-0.792318	-1.093933	-1.164474	-0.996807	-1.003151	-1.022550		
(3,-1)	-0.261850	-0.792318	-0.441060	-0.076055	-0.468477	-0.338989	-0.394921		
(3,-1)	-0.261850	-0.928353	-0.441060	-0.076055	-0.468477	-0.338989	-0.394922		

Table S321: Laplacian of the density value (a.u.) at the considered critical points for the  $(\text{CH}_3)_2\text{CH}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.839102	-0.670177	-0.719971	-0.702990	-0.774239	-0.642328	-0.691096	-0.736514	-0.871452
(3,-1)	-0.839102	-0.670177	-0.719971	-0.702990	-0.774239	-0.642328	-0.691096	-0.736514	-0.871452
(3,-1)	-1.097133	-0.994137	-1.040902	-1.006393	-1.052818	-0.927623	-1.015508	-0.946419	-0.828173
(3,-1)	-1.161686	-1.057117	-1.107566	-1.069724	-1.116924	-0.976119	-1.082107	-0.990346	-0.875258
(3,-1)	-1.155222	-1.050830	-1.101511	-1.064136	-1.111196	-0.975114	-1.076243	-0.985639	-0.868968
(3,-1)	-1.870625	-1.772607	-1.743957	-1.730664	-1.792506	-1.562497	-1.733880	-1.725475	-1.714505
(3,-1)	-1.097133	-0.994137	-1.040902	-1.006393	-1.052818	-0.927623	-1.015508	-0.946419	-0.828173
(3,-1)	-1.161686	-1.057117	-1.107566	-1.069724	-1.116924	-0.976119	-1.082107	-0.990346	-0.875258
(3,-1)	-1.155222	-1.050830	-1.101511	-1.064136	-1.111196	-0.975114	-1.076243	-0.985639	-0.868968
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.839102	-0.608807	-0.857241	-0.762845	-0.759170	-0.612470	-0.664290	-0.820858	-0.728662
(3,-1)	-0.839102	-0.801863	-0.857241	-0.762845	-0.759170	-0.612470	-0.664290	-0.820858	-0.728662
(3,-1)	-1.097133	-0.972110	-1.007508	-1.062681	-1.035566	-1.010508	-0.922961	-1.062288	-1.025427
(3,-1)	-1.161686	-0.968664	-1.081054	-1.128795	-1.098703	-1.059630	-0.965481	-1.126351	-1.093850
(3,-1)	-1.155222	-0.968664	-1.074014	-1.122566	-1.092870	-1.055575	-0.960740	-1.119924	-1.086738
(3,-1)	-1.870625	-1.025622	-1.633533	-1.789446	-1.784921	-1.782353	-1.630256	-1.823847	-1.589069
(3,-1)	-1.097133	-1.025622	-1.007508	-1.062681	-1.035566	-1.010508	-0.922961	-1.062288	-1.025427
(3,-1)	-1.161686	-1.542560	-1.081054	-1.128795	-1.098703	-1.059630	-0.965481	-1.126351	-1.093850
(3,-1)	-1.155222	-1.542560	-1.074014	-1.122566	-1.092870	-1.055575	-0.960740	-1.119924	-1.086738
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.839102	-0.675357	-0.715015	-0.771976	-0.744325	-0.778514	-0.770950	-0.752579	-0.722365
(3,-1)	-0.839102	-0.675357	-0.715015	-0.771976	-0.744325	-0.778514	-0.770950	-0.752579	-0.722365
(3,-1)	-1.097133	-1.002041	-1.116145	-1.205372	-1.381456	-1.050494	-1.047586	-1.034692	-1.012183
(3,-1)	-1.161686	-1.064261	-1.184938	-1.275833	-1.453956	-1.113053	-1.111348	-1.099623	-1.074750
(3,-1)	-1.155222	-1.057833	-1.176985	-1.268081	-1.444626	-1.106724	-1.104969	-1.093195	-1.068847
(3,-1)	-1.870625	-1.670872	-1.848833	-1.980888	-2.201967	-1.803776	-1.792865	-1.762719	-1.729476
(3,-1)	-1.097133	-1.002041	-1.116145	-1.205372	-1.381456	-1.050494	-1.047586	-1.034692	-1.012183
(3,-1)	-1.161686	-1.064261	-1.184938	-1.275833	-1.453956	-1.113053	-1.111348	-1.099623	-1.074750
(3,-1)	-1.155222	-1.057833	-1.176985	-1.268081	-1.444626	-1.106724	-1.104969	-1.093195	-1.068847
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.839102	-0.615565	-0.693040	-0.976096	-0.783624	-0.802924	-0.807466		
(3,-1)	-0.839102	-0.764743	-0.693040	-0.976096	-0.783624	-0.802924	-0.807466		
(3,-1)	-1.097133	-0.944438	-1.089594	-1.148286	-1.078585	-1.069545	-1.078519		
(3,-1)	-1.161686	-0.940999	-1.171709	-1.214286	-1.144697	-1.133478	-1.143678		
(3,-1)	-1.155222	-0.940999	-1.159631	-1.207532	-1.138479	-1.127414	-1.137264		
(3,-1)	-1.870625	-0.986275	-1.907930	-1.933157	-1.818069	-1.838942	-1.819738		
(3,-1)	-1.097133	-0.986275	-1.089594	-1.148286	-1.078585	-1.069545	-1.078520		
(3,-1)	-1.161686	-1.555357	-1.171709	-1.214286	-1.144697	-1.133478	-1.143678		
(3,-1)	-1.155222	-1.555357	-1.159631	-1.207532	-1.138479	-1.127414	-1.137264		

Table S322: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>-CH<sub>2</sub>-NH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.692663	-0.568464	-0.619266	-0.593108	-0.645012	-0.545231	-0.574026	-0.659818	-0.635971
(3,-1)	-0.809127	-0.643311	-0.690748	-0.674801	-0.744483	-0.620156	-0.663293	-0.708214	-0.844075
(3,-1)	-1.105149	-1.008174	-1.054454	-1.018964	-1.063585	-0.931508	-1.027730	-0.959276	-0.855530
(3,-1)	-1.103220	-1.007149	-1.053931	-1.018535	-1.062286	-0.934001	-1.027226	-0.958106	-0.852128
(3,-1)	-1.103220	-1.007149	-1.053931	-1.018535	-1.062286	-0.934001	-1.027226	-0.958106	-0.852128
(3,-1)	-1.164629	-1.060388	-1.108128	-1.071636	-1.119043	-0.976549	-1.084330	-0.992192	-0.866597
(3,-1)	-1.164629	-1.060388	-1.108128	-1.071636	-1.119043	-0.976549	-1.084330	-0.992192	-0.866597
(3,-1)	-1.844502	-1.743183	-1.721196	-1.704966	-1.766372	-1.534824	-1.708562	-1.702135	-1.700644
(3,-1)	-1.844502	-1.743183	-1.721196	-1.704966	-1.766372	-1.534824	-1.708562	-1.702135	-1.700644
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.692663	-0.676234	-0.651754	-0.647147	-0.629934	-0.614285	-0.638767	-0.669161	-0.614876
(3,-1)	-0.809127	-0.997084	-0.831083	-0.733078	-0.730034	-0.585285	-0.637078	-0.789426	-0.703413
(3,-1)	-1.105149	-0.997084	-1.018629	-1.074515	-1.046221	-1.014275	-0.931892	-1.070953	-1.035897
(3,-1)	-1.103220	0.578329	-1.016605	-1.073075	-1.044736	-1.013635	-0.930440	-1.068798	-1.033297
(3,-1)	-1.103220		-1.016605	-1.073075	-1.044736	-1.013635	-0.930440	-1.068798	-1.033297
(3,-1)	-1.164629		-1.081574	-1.130171	-1.101305	-1.061918	-0.968786	-1.129319	-1.095380
(3,-1)	-1.164629		-1.081574	-1.130171	-1.101305	-1.061918	-0.968786	-1.129319	-1.095380
(3,-1)	-1.844502		-1.612571	-1.765103	-1.757704	-1.753633	-1.603713	-1.796868	-1.566796
(3,-1)	-1.844502		-1.612571	-1.765103	-1.757704	-1.753633	-1.603713	-1.796868	-1.566796
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.692663	-0.542030	-0.649782	-0.676291	-0.633819	-0.640095	-0.640479	-0.626398	-0.606095
(3,-1)	-0.809127	-0.646570	-0.682760	-0.737577	-0.710977	-0.751491	-0.743188	-0.724301	-0.694546
(3,-1)	-1.105149	-1.010681	-1.132153	-1.217902	-1.402614	-1.058401	-1.056750	-1.045566	-1.021744
(3,-1)	-1.103220	-1.009001	-1.128917	-1.214544	-1.399677	-1.055769	-1.054333	-1.043530	-1.019630
(3,-1)	-1.103220	-1.009001	-1.128917	-1.214544	-1.399677	-1.055769	-1.054333	-1.043530	-1.019630
(3,-1)	-1.164629	-1.067168	-1.183664	-1.276021	-1.453521	-1.116120	-1.114468	-1.102740	-1.077770
(3,-1)	-1.164629	-1.067168	-1.183664	-1.276021	-1.453521	-1.116120	-1.114468	-1.102740	-1.077770
(3,-1)	-1.844502	-1.648444	-1.826192	-1.954197	-2.183856	-1.777938	-1.766131	-1.735739	-1.702383
(3,-1)	-1.844502	-1.648444	-1.826192	-1.954197	-2.183856	-1.777938	-1.766131	-1.735739	-1.702383
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.692663	-0.777763	-0.627056	-0.775123	-0.658144	-0.658177	-0.674879		
(3,-1)	-0.809127	-0.984320	-0.661349	-0.941317	-0.753676	-0.772972	-0.777383		
(3,-1)	-1.105149	-0.984320	-1.109144	-1.154187	-1.089246	-1.078681	-1.087348		
(3,-1)	-1.103220	0.452549	-1.101491	-1.150620	-1.088088	-1.077160	-1.085992		
(3,-1)	-1.103220		-1.101491	-1.150620	-1.088088	-1.077160	-1.085989		
(3,-1)	-1.164629		-1.170925	-1.216328	-1.146154	-1.136019	-1.145614		
(3,-1)	-1.164629		-1.170925	-1.216328	-1.146154	-1.136019	-1.145616		
(3,-1)	-1.844502		-1.879962	-1.908172	-1.793748	-1.812017	-1.794425		
(3,-1)	-1.844502		-1.879962	-1.908172	-1.793748	-1.812017	-1.794426		

Table S323: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>2</sub>C=C=O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.939118	-0.959522	-1.006830	-0.971469	-0.934671	-0.997815	-0.982950	-0.787491	-0.478050
(3,-1)	-1.139427	-1.050902	-1.092048	-1.055114	-1.102138	-0.959167	-1.065553	-0.987747	-0.939213
(3,-1)	-1.139427	-1.050902	-1.092048	-1.055114	-1.102138	-0.959167	-1.065553	-0.987747	-0.939213
(3,-1)	0.141807	-0.133355	-0.104275	-0.004961	0.058644	-0.320055	-0.022708	0.449015	0.692945
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.939118	0.247567	-0.526760	-1.007151	-0.963124	-0.891549	-0.921148	-0.828190	-0.955354
(3,-1)	-1.139427	-0.445477	-1.043390	-1.115195	-1.085708	-1.053464	-0.958180	-1.111180	-1.068875
(3,-1)	-1.139427	-0.659512	-1.043390	-1.115195	-1.085708	-1.053464	-0.958180	-1.111180	-1.068875
(3,-1)	0.141807	-0.445477	0.833312	-0.081609	0.024725	0.090571	-0.036736	0.214905	0.059157
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.939118	-0.934641	-0.924064	-0.999171	-0.968074	-0.836513	-0.923620	-0.992725	-0.976224
(3,-1)	-1.139427	-1.030870	-1.187838	-1.277287	-1.493629	-1.095940	-1.095911	-1.084679	-1.057982
(3,-1)	-1.139427	-1.030870	-1.187838	-1.277287	-1.493629	-1.095940	-1.095911	-1.084679	-1.057982
(3,-1)	0.141807	0.383886	0.124269	-0.170440	-0.077315	0.061686	0.004810	0.014392	-0.196003
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.939118	0.248603	-0.902207	-0.636946	-1.002381	-0.930529	-0.939425		
(3,-1)	-1.139427	-0.461253	-1.189197	-1.200470	-1.127938	-1.117795	-1.122846		
(3,-1)	-1.139427	-0.461253	-1.189197	-1.200470	-1.127938	-1.117795	-1.122846		
(3,-1)	0.141807	-0.461253	-0.153180	0.083412	0.034044	0.127834	0.105390		

Table S324: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>2</sub>-O-CH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.236579	0.258768	0.278733	0.256117	0.228410	0.282622	0.291102	0.228679	0.152588
(3,-1)	-0.489696	-0.382179	-0.406635	-0.404962	-0.442557	-0.384371	-0.395801	-0.413234	-0.387980
(3,-1)	-0.656496	-0.562959	-0.615572	-0.585571	-0.628899	-0.537118	-0.581857	-0.610054	-0.673257
(3,-1)	-0.489696	-0.382179	-0.406635	-0.404962	-0.442557	-0.384371	-0.395801	-0.413234	-0.387980
(3,-1)	-1.219320	-1.122407	-1.169750	-1.131299	-1.183225	-1.026444	-1.148478	-1.031507	-0.915275
(3,-1)	-1.219320	-1.122407	-1.169750	-1.131299	-1.183225	-1.026444	-1.148478	-1.031507	-0.915275
(3,-1)	-1.219320	-1.122407	-1.169750	-1.131299	-1.183225	-1.026444	-1.148478	-1.031507	-0.915275
(3,-1)	-1.219320	-1.122407	-1.169750	-1.131299	-1.183225	-1.026444	-1.148478	-1.031507	-0.915275
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.236579	0.204282	0.202508	0.259927	0.235214	0.199116	0.186305	0.212912	0.257548
(3,-1)	-0.489696	-0.668018	-0.339026	-0.440067	-0.442109	-0.342076	-0.382504	-0.450320	-0.455732
(3,-1)	-0.656496	-1.030718	-0.664200	-0.637273	-0.615547	-0.512576	-0.558059	-0.651082	-0.615182
(3,-1)	-0.489696	-1.013079	-0.339026	-0.440067	-0.442109	-0.342076	-0.382504	-0.450320	-0.455732
(3,-1)	-1.219320	-0.958331	-1.151264	-1.195786	-1.165645	-1.121503	-1.009591	-1.198021	-1.165992
(3,-1)	-1.219320	-0.958331	-1.151264	-1.195786	-1.165645	-1.121503	-1.009591	-1.198021	-1.165992
(3,-1)	-1.219320		-1.151264	-1.195786	-1.165645	-1.121503	-1.009591	-1.198021	-1.165992
(3,-1)	-1.219320		-1.151264	-1.195786	-1.165645	-1.121503	-1.009591	-1.198021	-1.165992
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.236579	0.470258	0.242790	0.244821	0.305775	0.219543	0.224556	0.241212	0.250673
(3,-1)	-0.489696	-0.441376	-0.405328	-0.397258	-0.434323	-0.446829	-0.445284	-0.437114	-0.427973
(3,-1)	-0.656496	-0.559679	-0.608876	-0.649894	-0.648429	-0.616262	-0.621380	-0.618286	-0.595424
(3,-1)	-0.489696	-0.441376	-0.405328	-0.397258	-0.434323	-0.446829	-0.445284	-0.437114	-0.427973
(3,-1)	-1.219320	-1.124536	-1.256317	-1.353801	-1.525491	-1.184652	-1.181945	-1.168089	-1.142639
(3,-1)	-1.219320	-1.124536	-1.256317	-1.353801	-1.525491	-1.184652	-1.181945	-1.168089	-1.142639
(3,-1)	-1.219320	-1.124536	-1.256317	-1.353801	-1.525491	-1.184652	-1.181945	-1.168089	-1.142639
(3,-1)	-1.219320	-1.124536	-1.256317	-1.353801	-1.525491	-1.184652	-1.181945	-1.168089	-1.142639
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.236579	0.093643	0.229789	0.198621	0.250554	0.225571	0.209393		
(3,-1)	-0.489696	-0.682387	-0.351485	-0.395529	-0.448118	-0.456287	-0.440479		
(3,-1)	-0.656496	-0.987543	-0.570961	-0.742744	-0.646525	-0.641531	-0.656108		
(3,-1)	-0.489696	-0.982808	-0.351485	-0.395529	-0.448118	-0.456287	-0.440479		
(3,-1)	-1.219320	-0.935798	-1.260270	-1.292773	-1.212414	-1.203134	-1.212677		
(3,-1)	-1.219320	-0.935798	-1.260270	-1.292773	-1.212414	-1.203134	-1.212677		
(3,-1)	-1.219320		-1.260270	-1.292773	-1.212414	-1.203134	-1.212677		
(3,-1)	-1.219320		-1.260270	-1.292773	-1.212414	-1.203134	-1.212678		



Table S325: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>CHO system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.185794	-0.498624	-0.487909	-0.389172	-0.283392	-0.638729	-0.384511	0.044877	0.323290
(3,-1)	-0.760192	-0.637737	-0.691574	-0.663269	-0.722746	-0.608598	-0.647636	-0.740106	-0.697685
(3,-1)	-1.159703	-1.061275	-1.104649	-1.070019	-1.126002	-0.969224	-1.088496	-0.979606	-0.843865
(3,-1)	-1.142173	-1.055646	-1.104726	-1.066637	-1.112432	-0.970996	-1.078898	-0.988012	-0.889920
(3,-1)	-1.087794	-0.999414	-1.046374	-1.009863	-1.054348	-0.922823	-1.019134	-0.950018	-0.859029
(3,-1)	-1.087794	-0.999414	-1.046374	-1.009863	-1.054348	-0.922823	-1.019134	-0.950018	-0.859029
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.185794	-0.671524	0.430843	-0.426843	-0.312084	-0.207985	-0.356150	-0.110071	-0.293376
(3,-1)	-0.760192	0.248299	-0.716986	-0.725370	-0.707645	-0.713590	-0.722454	-0.753014	-0.689301
(3,-1)	-1.159703	-1.060226	-1.100015	-1.135691	-1.109877	-1.079417	-0.963967	-1.147722	-1.112692
(3,-1)	-1.142173	0.248299	-1.072533	-1.124879	-1.094167	-1.055832	-0.959085	-1.120713	-1.085640
(3,-1)	-1.087794	-1.060226	-1.006941	-1.066354	-1.037002	-1.004813	-0.920384	-1.061053	-1.025488
(3,-1)	-1.087794		-1.006941	-1.066354	-1.037002	-1.004813	-0.920384	-1.061053	-1.025488
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.185794	0.006430	-0.181861	-0.448616	-0.339101	-0.245169	-0.310769	-0.321684	-0.502040
(3,-1)	-0.760192	-0.625086	-0.744987	-0.768839	-0.727714	-0.719048	-0.720386	-0.706718	-0.681569
(3,-1)	-1.159703	-1.074649	-1.189036	-1.291537	-1.436010	-1.136747	-1.130770	-1.113475	-1.090144
(3,-1)	-1.142173	-1.052414	-1.182569	-1.273712	-1.455102	-1.107147	-1.105623	-1.093821	-1.070242
(3,-1)	-1.087794	-0.997323	-1.124367	-1.209383	-1.397689	-1.049735	-1.048196	-1.036193	-1.013027
(3,-1)	-1.087794	-0.997323	-1.124367	-1.209383	-1.397689	-1.049735	-1.048196	-1.036193	-1.013027
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.185794	-0.692337	-0.418140	-0.103543	-0.338489	-0.219896	-0.245768		
(3,-1)	-0.760192	0.137437	-0.721520	-0.875037	-0.739651	-0.742227	-0.758992		
(3,-1)	-1.159703	-1.015583	-1.198079	-1.247125	-1.149748	-1.145694	-1.152070		
(3,-1)	-1.142173	0.137437	-1.174681	-1.206997	-1.138370	-1.126301	-1.135118		
(3,-1)	-1.087794	-1.015583	-1.104684	-1.145855	-1.080785	-1.069436	-1.078065		
(3,-1)	-1.087794		-1.104684	-1.145855	-1.080785	-1.069436	-1.078064		

Table S326: Laplacian of the density value (a.u.) at the considered critical points for the O=CH-CH=O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.792040	-0.658869	-0.705757	-0.681369	-0.750137	-0.621322	-0.668781	-0.773838	-0.707584
(3,-1)	-0.151456	-0.472721	-0.462058	-0.363267	-0.248287	-0.623222	-0.352960	0.079064	0.369458
(3,-1)	-1.190897	-1.095091	-1.138833	-1.102767	-1.159565	-0.993809	-1.123570	-0.995314	-0.870481
(3,-1)	-0.151456	-0.472721	-0.462058	-0.363267	-0.248287	-0.623222	-0.352960	0.079064	0.369458
(3,-1)	-1.190897	-1.095091	-1.138833	-1.102767	-1.159565	-0.993809	-1.123570	-0.995314	-0.870481
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.792040	-0.655595	-0.730890	-0.748769	-0.736162	-0.779606	-0.764424	-0.788006	-0.713248
(3,-1)	-0.151456	-0.473594	0.469869	-0.392814	-0.276465	-0.176790	-0.320708	-0.070333	-0.254708
(3,-1)	-1.190897	-2.540916	-1.142110	-1.170321	-1.143133	-1.105664	-0.979616	-1.182470	-1.149958
(3,-1)	-0.151456	-1.020187	0.469869	-0.392814	-0.276465	-0.176790	-0.320708	-0.070333	-0.254708
(3,-1)	-1.190897	-1.020187	-1.142110	-1.170321	-1.143133	-1.105664	-0.979616	-1.182470	-1.149958
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.792040	-0.660676	-0.787141	-0.808871	-0.762470	-0.758233	-0.754559	-0.735258	-0.709005
(3,-1)	-0.151456	0.039682	-0.145427	-0.410807	-0.308847	-0.205681	-0.271883	-0.284212	-0.462889
(3,-1)	-1.190897	-1.100623	-1.227830	-1.328859	-1.472049	-1.170132	-1.164720	-1.147451	-1.123933
(3,-1)	-0.151456	0.039682	-0.145427	-0.410807	-0.308847	-0.205681	-0.271883	-0.284212	-0.462889
(3,-1)	-1.190897	-1.100623	-1.227830	-1.328859	-1.472049	-1.170132	-1.164720	-1.147451	-1.123933
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.792040	-0.661115	-0.766589	-0.923568	-0.763645	-0.773983	-0.787577		
(3,-1)	-0.151456	-0.552479	-0.381749	-0.041530	-0.308656	-0.186384	-0.215940		
(3,-1)	-1.190897	-2.587216	-1.246812	-1.283751	-1.183360	-1.178640	-1.184724		
(3,-1)	-0.151456	-0.981893	-0.381749	-0.041530	-0.308656	-0.186384	-0.215940		
(3,-1)	-1.190897	-0.981893	-1.246812	-1.283751	-1.183360	-1.178640	-1.184724		

Table S327: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>CH<sub>2</sub>OH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.746569	-0.616890	-0.673140	-0.644109	-0.697376	-0.593966	-0.628031	-0.716185	-0.673672
(3,-1)	-0.609113	-0.625498	-0.664991	-0.647392	-0.650463	-0.644207	-0.635637	-0.560634	-0.414153
(3,-1)	-2.712985	-2.601332	-2.557557	-2.552978	-2.627447	-2.385383	-2.622197	-2.624345	-2.729914
(3,-1)	-1.167992	-1.057791	-1.105686	-1.069292	-1.118888	-0.977914	-1.083254	-0.987652	-0.853800
(3,-1)	-1.167992	-1.057791	-1.105686	-1.069292	-1.118888	-0.977914	-1.083254	-0.987652	-0.853800
(3,-1)	-1.108913	-1.012291	-1.059267	-1.023572	-1.067830	-0.935430	-1.032242	-0.961103	-0.858688
(3,-1)	-1.128277	-1.030117	-1.077676	-1.041062	-1.086128	-0.949488	-1.051285	-0.973333	-0.868757
(3,-1)	-1.128277	-1.030117	-1.077676	-1.041062	-1.086128	-0.949488	-1.051285	-0.973333	-0.868757
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.746569	-0.447807	-0.699660	-0.700906	-0.681326	-0.677922	-0.694795	-0.722218	-0.663515
(3,-1)	-0.609113	-0.447807	-0.370488	-0.682769	-0.657489	-0.499658	-0.577900	-0.605822	-0.670521
(3,-1)	-2.712985	-1.073389	-2.479269	-2.629648	-2.635519	-2.603320	-2.511043	-2.737075	-2.349353
(3,-1)	-1.167992	-1.008596	-1.080206	-1.129873	-1.101391	-1.066010	-0.967146	-1.131480	-1.097247
(3,-1)	-1.167992	-1.008596	-1.080206	-1.129873	-1.101391	-1.066010	-0.967146	-1.131480	-1.097247
(3,-1)	-1.108913	-1.073389	-1.024192	-1.078821	-1.050272	-1.016085	-0.933248	-1.074582	-1.039506
(3,-1)	-1.128277	-1.008596	-1.041153	-1.097656	-1.068297	-1.033463	-0.945572	-1.093596	-1.059097
(3,-1)	-1.128277	-1.008596	-1.041153	-1.097656	-1.068297	-1.033463	-0.945572	-1.093596	-1.059097
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.746569	-0.595924	-0.708397	-0.731765	-0.685223	-0.689111	-0.691278	-0.679262	-0.657807
(3,-1)	-0.609113	-0.601407	-0.592689	-0.641539	-0.642258	-0.625834	-0.652177	-0.661471	-0.657905
(3,-1)	-2.712985	-2.586662	-2.567984	-2.657397	-2.757489	-2.708233	-2.698788	-2.679570	-2.615846
(3,-1)	-1.167992	-1.068912	-1.182993	-1.278700	-1.447994	-1.119404	-1.116544	-1.103010	-1.078953
(3,-1)	-1.167992	-1.068912	-1.182993	-1.278700	-1.447994	-1.119404	-1.116544	-1.103010	-1.078953
(3,-1)	-1.108913	-1.014795	-1.135927	-1.221540	-1.406722	-1.060936	-1.059672	-1.049022	-1.025575
(3,-1)	-1.128277	-1.031715	-1.155391	-1.243113	-1.428451	-1.080955	-1.079411	-1.068065	-1.043750
(3,-1)	-1.128277	-1.031715	-1.155391	-1.243113	-1.428451	-1.080955	-1.079411	-1.068065	-1.043750
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.746569	-0.536580	-0.682207	-0.832252	-0.712595	-0.711117	-0.728818		
(3,-1)	-0.609113	-0.536580	-0.569618	-0.467034	-0.685664	-0.644932	-0.643888		
(3,-1)	-2.712985	-1.029669	-2.917017	-2.852242	-2.650345	-2.686144	-2.655930		
(3,-1)	-1.167992	-0.972784	-1.171434	-1.222395	-1.146886	-1.137834	-1.147695		
(3,-1)	-1.167992	-0.972784	-1.171434	-1.222395	-1.146886	-1.137834	-1.147695		
(3,-1)	-1.108913	-1.029669	-1.112880	-1.157198	-1.093585	-1.082658	-1.091197		
(3,-1)	-1.128277	-0.972784	-1.135842	-1.177314	-1.112819	-1.101521	-1.110725		
(3,-1)	-1.128277	-0.972784	-1.135842	-1.177314	-1.112819	-1.101521	-1.110724		

Table S328: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>-O-CH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.618383	-0.656278	-0.703069	-0.676692	-0.665613	-0.666081	-0.662100	-0.561168	-0.360023
(3,-1)	-0.618383	-0.656278	-0.703069	-0.676692	-0.665613	-0.666081	-0.662100	-0.561168	-0.360023
(3,-1)	-1.215229	-1.104759	-1.158154	-1.118226	-1.167907	-1.018461	-1.135409	-1.019261	-0.898254
(3,-1)	-1.153634	-1.044403	-1.094822	-1.057918	-1.107072	-0.974490	-1.071652	-0.978243	-0.854240
(3,-1)	-1.153634	-1.044403	-1.094822	-1.057918	-1.107072	-0.974490	-1.071652	-0.978243	-0.854240
(3,-1)	-1.215229	-1.104759	-1.158154	-1.118226	-1.167907	-1.018461	-1.135409	-1.019261	-0.898254
(3,-1)	-1.153634	-1.044403	-1.094822	-1.057918	-1.107072	-0.974490	-1.071652	-0.978243	-0.854240
(3,-1)	-1.153634	-1.044403	-1.094822	-1.057918	-1.107072	-0.974490	-1.071652	-0.978243	-0.854240
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.618383	0.074249	-0.339555	-0.714300	-0.675377	-0.505774	-0.597624	-0.608057	-0.695337
(3,-1)	-0.618383	-0.206584	-0.339555	-0.714300	-0.675377	-0.505774	-0.597624	-0.608057	-0.695337
(3,-1)	-1.215229	-0.638560	-1.142317	-1.180716	-1.148996	-1.103886	-0.996680	-1.179678	-1.150789
(3,-1)	-1.153634	-0.206584	-1.069832	-1.117982	-1.089005	-1.056102	-0.955911	-1.117640	-1.084348
(3,-1)	-1.153634	-1.065236	-1.069832	-1.117982	-1.089005	-1.056102	-0.955911	-1.117640	-1.084348
(3,-1)	-1.215229	-1.065236	-1.142317	-1.180716	-1.148996	-1.103886	-0.996680	-1.179678	-1.150789
(3,-1)	-1.153634	-1.065236	-1.069832	-1.117982	-1.089005	-1.056102	-0.955911	-1.117640	-1.084348
(3,-1)	-1.153634	-1.065236	-1.069832	-1.117982	-1.089005	-1.056102	-0.955911	-1.117640	-1.084348
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.618383	-0.624118	-0.615735	-0.675724	-0.682337	-0.640323	-0.672273	-0.684067	-0.684113
(3,-1)	-0.618383	-0.624118	-0.615735	-0.675724	-0.682337	-0.640323	-0.672273	-0.684067	-0.684113
(3,-1)	-1.215229	-1.113594	-1.236462	-1.330253	-1.498178	-1.166605	-1.164301	-1.151525	-1.126628
(3,-1)	-1.153634	-1.054697	-1.171992	-1.266373	-1.434448	-1.105512	-1.102591	-1.089238	-1.066352
(3,-1)	-1.153634	-1.054697	-1.171992	-1.266373	-1.434448	-1.105512	-1.102591	-1.089238	-1.066352
(3,-1)	-1.215229	-1.113594	-1.236462	-1.330253	-1.498178	-1.166605	-1.164301	-1.151525	-1.126628
(3,-1)	-1.153634	-1.054697	-1.171992	-1.266373	-1.434448	-1.105512	-1.102591	-1.089238	-1.066352
(3,-1)	-1.153634	-1.054697	-1.171992	-1.266373	-1.434448	-1.105512	-1.102591	-1.089238	-1.066352
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.618383	0.094878	-0.596264	-0.481617	-0.709470	-0.652048	-0.656612		
(3,-1)	-0.618383	-0.190563	-0.596264	-0.481617	-0.709470	-0.652048	-0.656612		
(3,-1)	-1.215229	-0.644666	-1.232079	-1.271020	-1.197382	-1.185677	-1.196838		
(3,-1)	-1.153634	-0.190563	-1.155708	-1.209194	-1.134393	-1.124691	-1.134347		
(3,-1)	-1.153634	-1.028949	-1.155708	-1.209194	-1.134393	-1.124691	-1.134346		
(3,-1)	-1.215229	-1.028949	-1.232079	-1.271020	-1.197382	-1.185677	-1.196837		
(3,-1)	-1.153634	-1.028949	-1.155708	-1.209194	-1.134393	-1.124691	-1.134346		
(3,-1)	-1.153634	-1.028949	-1.155708	-1.209194	-1.134393	-1.124691	-1.134346		

Table S329: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>2</sub>-S-CH<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.090173	0.111414	0.116918	0.105072	0.085588	0.131868	0.138757	0.077281	0.074923
(3,-1)	-0.186945	-0.133247	-0.151093	-0.145186	-0.171364	-0.121739	-0.124099	-0.134026	-0.172386
(3,-1)	-0.670092	-0.577674	-0.625736	-0.599175	-0.643331	-0.557236	-0.594982	-0.614346	-0.671033
(3,-1)	-0.186945	-0.133247	-0.151093	-0.145186	-0.171364	-0.121739	-0.124099	-0.134026	-0.172386
(3,-1)	-1.199746	-1.108858	-1.153461	-1.117262	-1.167397	-1.005214	-1.131702	-1.030357	-0.925898
(3,-1)	-1.199746	-1.108858	-1.153461	-1.117262	-1.167397	-1.005214	-1.131702	-1.030357	-0.925898
(3,-1)	-1.199746	-1.108858	-1.153461	-1.117262	-1.167397	-1.005214	-1.131702	-1.030357	-0.925898
(3,-1)	-1.199746	-1.108858	-1.153461	-1.117262	-1.167397	-1.005214	-1.131702	-1.030357	-0.925898
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.090173	0.506056	0.063871	0.105482	0.092232	0.085531	0.062525	0.078249	0.107126
(3,-1)	-0.186945	-0.389128	-0.225001	-0.167273	-0.165443	-0.084993	-0.115989	-0.185354	-0.175358
(3,-1)	-0.670092	-0.389127	-0.667277	-0.649650	-0.631571	-0.537597	-0.574494	-0.668115	-0.621819
(3,-1)	-0.186945	-0.987948	-0.225001	-0.167273	-0.165443	-0.084993	-0.115989	-0.185354	-0.175358
(3,-1)	-1.199746	-1.006330	-1.128144	-1.177790	-1.149526	-1.110276	-1.003812	-1.179520	-1.143627
(3,-1)	-1.199746	-0.981257	-1.128144	-1.177790	-1.149526	-1.110276	-1.003812	-1.179520	-1.143627
(3,-1)	-1.199746	-1.006330	-1.128144	-1.177790	-1.149526	-1.110276	-1.003812	-1.179520	-1.143627
(3,-1)	-1.199746	-0.981257	-1.128144	-1.177790	-1.149526	-1.110276	-1.003812	-1.179520	-1.143627
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.090173	0.246550	0.091415	0.099722	0.146915	0.079028	0.082907	0.100868	0.096888
(3,-1)	-0.186945	-0.109913	-0.158303	-0.175988	-0.213443	-0.181126	-0.176118	-0.161925	-0.156425
(3,-1)	-0.670092	-0.560106	-0.630892	-0.681365	-0.686955	-0.629406	-0.638217	-0.639077	-0.610155
(3,-1)	-0.186945	-0.109913	-0.158303	-0.175988	-0.213443	-0.181126	-0.176118	-0.161925	-0.156425
(3,-1)	-1.199746	-1.101828	-1.241923	-1.337676	-1.520773	-1.167348	-1.164439	-1.151019	-1.123774
(3,-1)	-1.199746	-1.101828	-1.241923	-1.337676	-1.520773	-1.167348	-1.164439	-1.151019	-1.123774
(3,-1)	-1.199746	-1.101828	-1.241923	-1.337676	-1.520773	-1.167348	-1.164439	-1.151019	-1.123774
(3,-1)	-1.199746	-1.101828	-1.241923	-1.337676	-1.520773	-1.167348	-1.164439	-1.151019	-1.123774
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.090173	0.447013	0.106911	0.063943	0.097929	0.084007	0.064808		
(3,-1)	-0.186945	-0.386920	-0.122898	-0.236361	-0.171422	-0.177206	-0.184577		
(3,-1)	-0.670092	-0.386919	-0.615258	-0.762717	-0.655709	-0.653925	-0.667633		
(3,-1)	-0.186945	-0.964094	-0.122898	-0.236361	-0.171422	-0.177206	-0.184578		
(3,-1)	-1.199746	-0.977907	-1.244569	-1.269631	-1.193537	-1.184815	-1.193597		
(3,-1)	-1.199746	-0.956039	-1.244569	-1.269631	-1.193537	-1.184815	-1.193597		
(3,-1)	-1.199746	-0.977907	-1.244569	-1.269631	-1.193537	-1.184815	-1.193598		
(3,-1)	-1.199746	-0.956039	-1.244569	-1.269631	-1.193537	-1.184815	-1.193597		

Table S330: Laplacian of the density value (a.u.) at the considered critical points for the  $(\text{CH}_3)_2\text{SO}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.340854	0.228030	0.260183	0.317044	0.357721	0.211964	0.266708	0.612317	0.575813
(3,-1)	-0.428929	-0.326768	-0.359422	-0.345630	-0.387298	-0.309482	-0.322589	-0.376945	-0.408919
(3,-1)	-0.428928	-0.326767	-0.359421	-0.345630	-0.387298	-0.309481	-0.322588	-0.376944	-0.408919
(3,-1)	-1.134094	-1.034330	-1.080544	-1.044420	-1.092273	-0.955185	-1.057157	-0.975350	-0.880325
(3,-1)	-1.147593	-1.049272	-1.095760	-1.058756	-1.105893	-0.960851	-1.072050	-0.984787	-0.887892
(3,-1)	-1.122078	-1.022800	-1.068888	-1.033174	-1.080435	-0.944729	-1.045102	-0.967219	-0.873624
(3,-1)	-1.147592	-1.049272	-1.095760	-1.058756	-1.105893	-0.960851	-1.072050	-0.984787	-0.887892
(3,-1)	-1.122079	-1.022800	-1.068888	-1.033174	-1.080435	-0.944730	-1.045103	-0.967220	-0.873624
(3,-1)	-1.134095	-1.034329	-1.080544	-1.044420	-1.092273	-0.955185	-1.057157	-0.975350	-0.880325
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.340854	-0.608262	0.757992	0.283756	0.348528	0.460013	0.307024	0.421514	0.274079
(3,-1)	-0.428929	-0.324261	-0.425105	-0.386023	-0.379196	-0.313694	-0.355709	-0.410695	-0.373650
(3,-1)	-0.428928	-0.616947	-0.425104	-0.386022	-0.379196	-0.313693	-0.355708	-0.410695	-0.373650
(3,-1)	-1.134094	-1.018992	-1.044822	-1.102697	-1.074109	-1.042270	-0.947771	-1.101033	-1.065420
(3,-1)	-1.147593	-1.018992	-1.063507	-1.117181	-1.087704	-1.051033	-0.957035	-1.114609	-1.080459
(3,-1)	-1.122078	-0.983738	-1.035486	-1.090668	-1.062428	-1.030688	-0.939003	-1.088418	-1.053980
(3,-1)	-1.147592	-0.990425	-1.063507	-1.117181	-1.087704	-1.051032	-0.957034	-1.114609	-1.080459
(3,-1)	-1.122079	-0.990425	-1.035486	-1.090669	-1.062428	-1.030689	-0.939004	-1.088418	-1.053980
(3,-1)	-1.134095	-1.044822	-1.102696	-1.1074108	-1.042270	-0.947770	-1.101033	-1.065420	-1.065420
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.340854	0.545536	0.410879	0.284970	0.220567	0.374426	0.344983	0.337663	0.257175
(3,-1)	-0.428929	-0.307394	-0.367930	-0.398241	-0.360692	-0.399856	-0.395601	-0.379377	-0.365130
(3,-1)	-0.428928	-0.307393	-0.367929	-0.398241	-0.360691	-0.399856	-0.395600	-0.379376	-0.365129
(3,-1)	-1.134094	-1.029488	-1.165761	-1.256564	-1.446253	-1.089990	-1.086919	-1.073887	-1.049709
(3,-1)	-1.147593	-1.043332	-1.179457	-1.270419	-1.459982	-1.101973	-1.099778	-1.087648	-1.063586
(3,-1)	-1.122078	-1.019550	-1.153988	-1.242307	-1.432304	-1.076625	-1.073807	-1.061299	-1.037885
(3,-1)	-1.147592	-1.043332	-1.179457	-1.270419	-1.459982	-1.101973	-1.099778	-1.087647	-1.063586
(3,-1)	-1.122079	-1.019550	-1.153989	-1.242307	-1.432305	-1.076625	-1.073808	-1.061300	-1.037886
(3,-1)	-1.134095	-1.029488	-1.165761	-1.256563	-1.446253	-1.089990	-1.086919	-1.073886	-1.049709
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.340854	-0.612557	0.302949	0.447095	0.350533	0.412211	0.393290		
(3,-1)	-0.428929	-0.317756	-0.355428	-0.497882	-0.396504	-0.403192	-0.414751		
(3,-1)	-0.428928	-0.608530	-0.355427	-0.497881	-0.396504	-0.403192	-0.414749		
(3,-1)	-1.134094	-0.985654	-1.153794	-1.188696	-1.116548	-1.106708	-1.114337		
(3,-1)	-1.147593	-0.985654	-1.171711	-1.200769	-1.131138	-1.120371	-1.128916		
(3,-1)	-1.122078	-0.954828	-1.136920	-1.175702	-1.104700	-1.094882	-1.102486		
(3,-1)	-1.147592	-0.960462	-1.171711	-1.200769	-1.131137	-1.120371	-1.128916		
(3,-1)	-1.122079	-0.960462	-1.136921	-1.175702	-1.104700	-1.094882	-1.102486		
(3,-1)	-1.134095	-1.153793	-1.153793	-1.188696	-1.116548	-1.106708	-1.114338		

Table S331: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>-CH<sub>2</sub>-SH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.681462	-0.562858	-0.613495	-0.587215	-0.636995	-0.541818	-0.568471	-0.649291	-0.632906
(3,-1)	-0.341601	-0.263366	-0.289777	-0.278091	-0.311704	-0.252754	-0.256263	-0.277877	-0.335384
(3,-1)	-0.684684	-0.626818	-0.649549	-0.629187	-0.658006	-0.608166	-0.623685	-0.641931	-0.561597
(3,-1)	-1.164675	-1.063847	-1.108200	-1.073413	-1.121107	-0.972225	-1.085812	-0.998755	-0.882975
(3,-1)	-1.164675	-1.063847	-1.108200	-1.073413	-1.121107	-0.972225	-1.085812	-0.998755	-0.882975
(3,-1)	-1.118597	-1.021052	-1.067856	-1.032167	-1.076943	-0.942762	-1.040929	-0.967771	-0.863769
(3,-1)	-1.128189	-1.030853	-1.077932	-1.042194	-1.087257	-0.952266	-1.052082	-0.973200	-0.868048
(3,-1)	-1.128189	-1.030853	-1.077932	-1.042194	-1.087257	-0.952266	-1.052082	-0.973200	-0.868048
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.681462	-0.349891	-0.647891	-0.639363	-0.621718	-0.592664	-0.624356	-0.658783	-0.609141
(3,-1)	-0.341601	-0.349891	-0.353442	-0.310194	-0.303875	-0.213411	-0.257522	-0.327898	-0.304638
(3,-1)	-0.684684	-1.003941	-0.644545	-0.666931	-0.651162	-0.641944	-0.625262	-0.664148	-0.643774
(3,-1)	-1.164675	-0.996911	-1.076223	-1.130607	-1.103299	-1.068629	-0.972432	-1.130665	-1.094624
(3,-1)	-1.164675	-0.996911	-1.076223	-1.130607	-1.103299	-1.068629	-0.972432	-1.130665	-1.094624
(3,-1)	-1.118597	-1.003941	-1.032740	-1.087873	-1.059429	-1.024894	-0.940263	-1.083756	-1.048769
(3,-1)	-1.128189	-0.996911	-1.043392	-1.097926	-1.069424	-1.034696	-0.944991	-1.093970	-1.059451
(3,-1)	-1.128189	-0.996911	-1.043392	-1.097926	-1.069424	-1.034696	-0.944991	-1.093970	-1.059451
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.681462	-0.530786	-0.636597	-0.664888	-0.628041	-0.629310	-0.630382	-0.617392	-0.598336
(3,-1)	-0.341601	-0.223290	-0.285556	-0.317881	-0.304987	-0.320461	-0.316696	-0.301549	-0.292200
(3,-1)	-0.684684	-0.627513	-0.691738	-0.731644	-0.816569	-0.653154	-0.656402	-0.650870	-0.638606
(3,-1)	-1.164675	-1.062367	-1.190503	-1.283970	-1.469112	-1.119239	-1.116415	-1.103658	-1.078018
(3,-1)	-1.164675	-1.062367	-1.190503	-1.283970	-1.469112	-1.119239	-1.116415	-1.103658	-1.078018
(3,-1)	-1.118597	-1.022448	-1.145964	-1.233228	-1.419825	-1.070817	-1.069558	-1.058600	-1.034512
(3,-1)	-1.128189	-1.031770	-1.156365	-1.244544	-1.430401	-1.080915	-1.079350	-1.068211	-1.044315
(3,-1)	-1.128189	-1.031770	-1.156365	-1.244544	-1.430401	-1.080915	-1.079350	-1.068211	-1.044315
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.681462	-0.344599	-0.614569	-0.761310	-0.648989	-0.647977	-0.664360		
(3,-1)	-0.341601	-0.344599	-0.268486	-0.399449	-0.317222	-0.321383	-0.331869		
(3,-1)	-0.684684	-0.974210	-0.663963	-0.734076	-0.677576	-0.673998	-0.678778		
(3,-1)	-1.164675	-0.968501	-1.179665	-1.216453	-1.146067	-1.137111	-1.145608		
(3,-1)	-1.164675	-0.968501	-1.179665	-1.216453	-1.146067	-1.137111	-1.145607		
(3,-1)	-1.118597	-0.974210	-1.125717	-1.167795	-1.102833	-1.092184	-1.101113		
(3,-1)	-1.128189	-0.968501	-1.136702	-1.177905	-1.112768	-1.102038	-1.110768		
(3,-1)	-1.128189	-0.968501	-1.136702	-1.177905	-1.112768	-1.102038	-1.110768		

Table S332: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>-S-CH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.369759	-0.286971	-0.315311	-0.302646	-0.337443	-0.272932	-0.280855	-0.301641	-0.360730
(3,-1)	-0.369759	-0.286971	-0.315311	-0.302646	-0.337443	-0.272932	-0.280855	-0.301641	-0.360730
(3,-1)	-1.142663	-1.044034	-1.091011	-1.054853	-1.101422	-0.955763	-1.067352	-0.984618	-0.884149
(3,-1)	-1.140895	-1.040322	-1.086938	-1.051564	-1.098623	-0.958460	-1.063324	-0.983000	-0.878449
(3,-1)	-1.140895	-1.040322	-1.086938	-1.051564	-1.098623	-0.958460	-1.063324	-0.983000	-0.878449
(3,-1)	-1.142663	-1.044034	-1.091011	-1.054853	-1.101422	-0.955763	-1.067352	-0.984618	-0.884149
(3,-1)	-1.140895	-1.040322	-1.086938	-1.051564	-1.098623	-0.958460	-1.063324	-0.983000	-0.878449
(3,-1)	-1.140895	-1.040322	-1.086938	-1.051564	-1.098623	-0.958460	-1.063324	-0.983000	-0.878449
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.369759	-1.151824	-0.381593	-0.336708	-0.329784	-0.235751	-0.280586	-0.355878	-0.330269
(3,-1)	-0.369759	0.296187	-0.381593	-0.336708	-0.329784	-0.235751	-0.280586	-0.355878	-0.330269
(3,-1)	-1.142663	-1.142986	-1.059242	-1.111688	-1.082988	-1.049803	-0.955786	-1.109188	-1.074505
(3,-1)	-1.140895	-1.050474	-1.053228	-1.108304	-1.080386	-1.050075	-0.955320	-1.107138	-1.071266
(3,-1)	-1.140895	-1.049096	-1.053228	-1.108304	-1.080386	-1.050075	-0.955320	-1.107138	-1.071266
(3,-1)	-1.142663		-1.059242	-1.111688	-1.082988	-1.049803	-0.955786	-1.109188	-1.074505
(3,-1)	-1.140895		-1.053228	-1.108304	-1.080386	-1.050075	-0.955320	-1.107138	-1.071266
(3,-1)	-1.140895		-1.053228	-1.108304	-1.080386	-1.050075	-0.955320	-1.107138	-1.071266
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.369759	-0.250494	-0.313518	-0.346877	-0.333948	-0.345277	-0.342649	-0.328727	-0.317957
(3,-1)	-0.369759	-0.250494	-0.313518	-0.346877	-0.333948	-0.345277	-0.342649	-0.328727	-0.317957
(3,-1)	-1.142663	-1.041355	-1.172810	-1.263187	-1.449185	-1.097160	-1.094586	-1.082542	-1.058196
(3,-1)	-1.140895	-1.039463	-1.169007	-1.259878	-1.445129	-1.096017	-1.092936	-1.080151	-1.054931
(3,-1)	-1.140895	-1.039463	-1.169007	-1.259878	-1.445129	-1.096017	-1.092936	-1.080151	-1.054931
(3,-1)	-1.142663	-1.041355	-1.172810	-1.263187	-1.449185	-1.097160	-1.094586	-1.082542	-1.058196
(3,-1)	-1.140895	-1.039463	-1.169007	-1.259878	-1.445129	-1.096017	-1.092936	-1.080151	-1.054931
(3,-1)	-1.140895	-1.039463	-1.169007	-1.259878	-1.445129	-1.096017	-1.092936	-1.080151	-1.054931
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.369759	-1.157658	-0.297135	-0.431648	-0.344551	-0.348787	-0.359631		
(3,-1)	-0.369759	0.227507	-0.297135	-0.431648	-0.344551	-0.348787	-0.359631		
(3,-1)	-1.142663	-1.096464	-1.160051	-1.193687	-1.126610	-1.116149	-1.124815		
(3,-1)	-1.140895	-1.021215	-1.151460	-1.192152	-1.123856	-1.114145	-1.122858		
(3,-1)	-1.140895	-1.020610	-1.151460	-1.192152	-1.123856	-1.114145	-1.122858		
(3,-1)	-1.142663		-1.160051	-1.193687	-1.126610	-1.116149	-1.124815		
(3,-1)	-1.140895		-1.151460	-1.192152	-1.123856	-1.114145	-1.122858		
(3,-1)	-1.140895		-1.151460	-1.192152	-1.123856	-1.114145	-1.122858		



Table S333: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>2</sub>C=CHF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.224177	-1.084574	-1.150922	-1.108355	-1.164145	-1.085530	-1.115333	-1.157399	-1.246843
(3,-1)	0.022027	-0.194295	-0.205298	-0.154364	-0.013625	-0.181471	-0.049171	0.087882	0.453257
(3,-1)	-1.276939	-1.178160	-1.224829	-1.185807	-1.241909	-1.073706	-1.207031	-1.062359	-0.955591
(3,-1)	-1.183769	-1.092730	-1.138031	-1.099584	-1.149456	-0.994772	-1.115033	-1.012890	-0.933171
(3,-1)	-1.181854	-1.090695	-1.135618	-1.097329	-1.147000	-0.994789	-1.111950	-1.013418	-0.935035
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.224177	-0.634293	-1.157198	-1.182077	-1.152742	-1.133808	-1.148766	-1.199287	-1.109487
(3,-1)	0.022027	-0.324201	0.422064	-0.124788	-0.051066	0.133088	-0.057538	0.078398	-0.014456
(3,-1)	-1.276939	-1.062915	-1.226166	-1.254606	-1.224885	-1.174900	-1.044564	-1.261535	-1.232132
(3,-1)	-1.183769	-1.062915	-1.106888	-1.162606	-1.132235	-1.090314	-0.986377	-1.161629	-1.127602
(3,-1)	-1.181854	-0.977621	-1.103170	-1.160223	-1.130013	-1.088712	-0.986806	-1.158440	-1.125067
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.224177	-1.119071	-1.210649	-1.271346	-1.229263	-1.105189	-1.139443	-1.163959	-1.115219
(3,-1)	0.022027	0.033890	0.032431	-0.031306	-0.009350	-0.002544	-0.041318	-0.055984	-0.046935
(3,-1)	-1.276939	-1.178818	-1.323728	-1.419512	-1.588813	-1.245234	-1.242895	-1.229097	-1.201389
(3,-1)	-1.183769	-1.085834	-1.229013	-1.320918	-1.513952	-1.146110	-1.144798	-1.132937	-1.107063
(3,-1)	-1.181854	-1.084196	-1.228555	-1.320090	-1.516301	-1.142981	-1.142108	-1.130637	-1.104181
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.224177	-0.639913	-1.204393	-1.341492	-1.199109	-1.193267	-1.213250		
(3,-1)	0.022027	-0.300319	-0.025688	0.284910	-0.072943	0.033602	0.017751		
(3,-1)	-1.276939	-1.022899	-1.339748	-1.363549	-1.271626	-1.264458	-1.273119		
(3,-1)	-1.183769	-1.022899	-1.232338	-1.253324	-1.177058	-1.166992	-1.174336		
(3,-1)	-1.181854	-0.949399	-1.228481	-1.250881	-1.174632	-1.164610	-1.172014		

Table S334: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>-CH<sub>2</sub>-Cl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.718537	-0.592505	-0.645535	-0.618220	-0.670502	-0.569139	-0.600427	-0.686457	-0.658454
(3,-1)	-0.315587	-0.230128	-0.250502	-0.243302	-0.280525	-0.216318	-0.223611	-0.228488	-0.303028
(3,-1)	-1.212327	-1.104633	-1.152525	-1.115404	-1.166227	-1.009991	-1.131245	-1.026104	-0.904834
(3,-1)	-1.212327	-1.104633	-1.152525	-1.115404	-1.166227	-1.009991	-1.131245	-1.026104	-0.904834
(3,-1)	-1.112554	-1.014559	-1.061382	-1.025644	-1.070559	-0.936773	-1.034501	-0.962609	-0.860277
(3,-1)	-1.139385	-1.041029	-1.089033	-1.052445	-1.098005	-0.959868	-1.063138	-0.980433	-0.876079
(3,-1)	-1.139385	-1.041029	-1.089033	-1.052445	-1.098005	-0.959868	-1.063138	-0.980433	-0.876079
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.718537	-1.109978	-0.676633	-0.673049	-0.654903	-0.640179	-0.663571	-0.694448	-0.639826
(3,-1)	-0.315587	-0.407389	-0.338610	-0.273869	-0.272466	-0.171864	-0.208744	-0.299282	-0.278943
(3,-1)	-1.212327	-1.106949	-1.130637	-1.176727	-1.147664	-1.108175	-1.001312	-1.178304	-1.144257
(3,-1)	-1.212327	-1.062269	-1.130637	-1.176727	-1.147664	-1.108175	-1.001312	-1.178304	-1.144257
(3,-1)	-1.112554	-1.049407	-1.026292	-1.081605	-1.053108	-1.018875	-0.934959	-1.077605	-1.042915
(3,-1)	-1.139385		-1.055542	-1.109229	-1.079975	-1.043284	-0.952240	-1.105460	-1.071070
(3,-1)	-1.139385		-1.055542	-1.109229	-1.079975	-1.043284	-0.952240	-1.105460	-1.071070
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.718537	-0.566354	-0.676544	-0.702419	-0.659045	-0.663616	-0.664822	-0.651784	-0.630698
(3,-1)	-0.315587	-0.190553	-0.247539	-0.282169	-0.296328	-0.295009	-0.285106	-0.263876	-0.259246
(3,-1)	-1.212327	-1.105970	-1.237098	-1.332118	-1.510919	-1.166523	-1.163473	-1.149816	-1.123164
(3,-1)	-1.212327	-1.105970	-1.237098	-1.332118	-1.510919	-1.166523	-1.163473	-1.149816	-1.123164
(3,-1)	-1.112554	-1.016565	-1.139764	-1.226116	-1.412636	-1.065138	-1.063697	-1.052482	-1.028516
(3,-1)	-1.139385	-1.041972	-1.167704	-1.256133	-1.441554	-1.091983	-1.090570	-1.079429	-1.054953
(3,-1)	-1.139385	-1.041972	-1.167704	-1.256133	-1.441554	-1.091983	-1.090570	-1.079429	-1.054953
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.718537	-1.120640	-0.652587	-0.802394	-0.684251	-0.683670	-0.700554		
(3,-1)	-0.315587	-0.390479	-0.216694	-0.374608	-0.283252	-0.292729	-0.300388		
(3,-1)	-1.212327	-1.066565	-1.233918	-1.269728	-1.192728	-1.183405	-1.192535		
(3,-1)	-1.212327	-1.029498	-1.233918	-1.269728	-1.192728	-1.183405	-1.192536		
(3,-1)	-1.112554	-1.019086	-1.118437	-1.162095	-1.096572	-1.085926	-1.094736		
(3,-1)	-1.139385		-1.150520	-1.190230	-1.124025	-1.112881	-1.121790		
(3,-1)	-1.139385		-1.150520	-1.190230	-1.124025	-1.112881	-1.121791		

Table S335: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>2</sub>C=CHCl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.179989	-1.049259	-1.112203	-1.071320	-1.123874	-1.049766	-1.075602	-1.100484	-1.207248
(3,-1)	-0.398919	-0.311723	-0.335962	-0.325206	-0.370093	-0.296384	-0.299120	-0.292919	-0.394723
(3,-1)	-1.239863	-1.148724	-1.191588	-1.154974	-1.207882	-1.038022	-1.171517	-1.052308	-0.955061
(3,-1)	-1.193744	-1.102415	-1.147943	-1.110356	-1.160901	-1.003432	-1.125000	-1.018462	-0.933837
(3,-1)	-1.181888	-1.089709	-1.134399	-1.097039	-1.147285	-0.993497	-1.110430	-1.012029	-0.928297
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.179989	-1.072173	-1.111370	-1.141359	-1.112862	-1.063738	-1.088890	-1.154366	-1.074029
(3,-1)	-0.398919	-0.799536	-0.427888	-0.364262	-0.360890	-0.229127	-0.275958	-0.392337	-0.367030
(3,-1)	-1.239863	-1.083380	-1.178888	-1.218857	-1.190762	-1.148469	-1.028682	-1.224408	-1.190703
(3,-1)	-1.193744	-1.081802	-1.123163	-1.172982	-1.143628	-1.100536	-0.992617	-1.173872	-1.140323
(3,-1)	-1.181888	-1.073851	-1.106076	-1.159575	-1.130388	-1.089022	-0.986018	-1.159793	-1.126345
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.179989	-1.069360	-1.165240	-1.234129	-1.208371	-1.065933	-1.099455	-1.123099	-1.076459
(3,-1)	-0.398919	-0.252688	-0.342292	-0.390051	-0.414798	-0.380012	-0.373895	-0.352854	-0.343514
(3,-1)	-1.239863	-1.139768	-1.287421	-1.383145	-1.563707	-1.211493	-1.208377	-1.194251	-1.164660
(3,-1)	-1.193744	-1.097451	-1.239544	-1.332863	-1.522267	-1.159488	-1.157334	-1.144884	-1.117730
(3,-1)	-1.181888	-1.085029	-1.226880	-1.319920	-1.512495	-1.147390	-1.145161	-1.132254	-1.104146
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.179989	-1.088222	-1.168104	-1.282634	-1.156420	-1.149955	-1.169931		
(3,-1)	-0.398919	-0.822419	-0.317397	-0.487328	-0.374273	-0.384720	-0.396855		
(3,-1)	-1.239863	-1.047234	-1.301937	-1.318440	-1.234580	-1.227377	-1.235806		
(3,-1)	-1.193744	-1.046160	-1.246515	-1.266777	-1.187666	-1.178514	-1.186512		
(3,-1)	-1.181888	-1.038249	-1.230274	-1.253324	-1.174628	-1.165571	-1.174026		

Table S336: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>2</sub>C=CHCN system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.166457	-1.020413	-1.085004	-1.042642	-1.092727	-1.021500	-1.044245	-1.063885	-1.165081
(3,-1)	-0.988336	-0.774541	-0.824174	-0.794105	-0.854660	-0.763821	-0.780029	-0.867522	-0.853200
(3,-1)	-1.234547	-1.124256	-1.169347	-1.131426	-1.182815	-1.021865	-1.147611	-1.029372	-0.940874
(3,-1)	-1.238616	-1.121067	-1.166305	-1.128240	-1.179787	-1.019906	-1.143775	-1.028991	-0.940129
(3,-1)	-1.278346	-1.117468	-1.160362	-1.123035	-1.171871	-1.009082	-1.137364	-1.025629	-0.938759
(3,-1)	-0.636416	-0.796093	-0.721353	-0.632845	-0.483566	-1.040257	-0.752096	-0.221040	0.162644
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.166457	0.120478	-1.073923	-1.111576	-1.080947	-1.018901	-1.049564	-1.118993	-1.043877
(3,-1)	-0.988336	-0.648497	-0.833558	-0.859880	-0.841584	-0.830732	-0.850821	-0.881294	-0.815024
(3,-1)	-1.234547	-0.648497	-1.150909	-1.195047	-1.165528	-1.119152	-1.004500	-1.197278	-1.164496
(3,-1)	-1.238616	-1.016629	-1.146723	-1.192282	-1.162672	-1.117138	-1.004763	-1.194618	-1.161679
(3,-1)	-1.278346	-1.016629	-1.137362	-1.184639	-1.155191	-1.108633	-0.999167	-1.185440	-1.149863
(3,-1)	-0.636416	-0.957872	0.259722	-0.642797	-0.532044	-0.665548	-0.746563	-0.291814	-0.519535
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.166457	-1.027424	-1.133280	-1.201541	-1.183834	-1.030645	-1.064601	-1.087863	-1.046003
(3,-1)	-0.988336	-0.734955	-0.888517	-0.915448	-0.894464	-0.843986	-0.851523	-0.844219	-0.809618
(3,-1)	-1.234547	-1.117528	-1.260946	-1.356563	-1.540407	-1.182202	-1.180006	-1.167437	-1.140254
(3,-1)	-1.238616	-1.116585	-1.258439	-1.353767	-1.538196	-1.180447	-1.178030	-1.164893	-1.137338
(3,-1)	-1.278346	-1.105352	-1.248523	-1.342600	-1.528165	-1.170689	-1.169489	-1.157296	-1.129410
(3,-1)	-0.636416	-0.247319	-0.401190	-0.605643	-0.378433	-0.424709	-0.541298	-0.626431	-0.808175
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.166457	0.014973	-1.135939	-1.239303	-1.124046	-1.114535	-1.134989		
(3,-1)	-0.988336	-0.659993	-0.881443	-1.029563	-0.873208	-0.877422	-0.894984		
(3,-1)	-1.234547	-0.659993	-1.274876	-1.292452	-1.208110	-1.199337	-1.206863		
(3,-1)	-1.238616	-0.985828	-1.269867	-1.290567	-1.205864	-1.197067	-1.205067		
(3,-1)	-1.278346	-0.985828	-1.264622	-1.272544	-1.199166	-1.189544	-1.197751		
(3,-1)	-0.636416	-0.935220	-0.593514	-0.235885	-0.546060	-0.422050	-0.473916		

Table S337: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>–CO–CH<sub>3</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.259132	-0.564833	-0.550857	-0.455050	-0.351708	-0.694618	-0.452078	-0.032430	0.232227
(3,-1)	-0.754743	-0.615721	-0.666414	-0.640214	-0.699067	-0.587500	-0.623292	-0.719259	-0.677785
(3,-1)	-0.754743	-0.615721	-0.666414	-0.640214	-0.699067	-0.587500	-0.623292	-0.719259	-0.677785
(3,-1)	-1.155279	-1.058257	-1.106607	-1.068791	-1.114626	-0.973199	-1.080917	-0.990583	-0.890359
(3,-1)	-1.155279	-1.058257	-1.106607	-1.068791	-1.114626	-0.973199	-1.080917	-0.990583	-0.890359
(3,-1)	-1.096287	-0.999587	-1.046092	-1.010058	-1.054599	-0.924894	-1.019315	-0.950401	-0.856775
(3,-1)	-1.096287	-0.999587	-1.046092	-1.010058	-1.054599	-0.924894	-1.019315	-0.950401	-0.856775
(3,-1)	-1.096287	-0.999587	-1.046092	-1.010058	-1.054599	-0.924894	-1.019315	-0.950401	-0.856775
(3,-1)	-1.096287	-0.999587	-1.046092	-1.010058	-1.054599	-0.924894	-1.019315	-0.950401	-0.856775
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.259132	0.035126	0.351235	-0.493458	-0.381648	-0.271313	-0.426290	-0.182071	-0.364645
(3,-1)	-0.754743	-0.487091	-0.695737	-0.700261	-0.684288	-0.689406	-0.700686	-0.727843	-0.665984
(3,-1)	-0.754743	-2.601007	-0.695737	-0.700261	-0.684288	-0.689406	-0.700686	-0.727843	-0.665984
(3,-1)	-1.155279	-0.678518	-1.073987	-1.126930	-1.096519	-1.057100	-0.962540	-1.122611	-1.087787
(3,-1)	-1.155279	-1.028908	-1.073987	-1.126930	-1.096519	-1.057100	-0.962540	-1.122611	-1.087787
(3,-1)	-1.096287	-0.979910	-1.005779	-1.066200	-1.037300	-1.005024	-0.921437	-1.060796	-1.025487
(3,-1)	-1.096287	-0.979910	-1.005779	-1.066200	-1.037300	-1.005024	-0.921437	-1.060796	-1.025487
(3,-1)	-1.096287		-1.005779	-1.066200	-1.037300	-1.005024	-0.921437	-1.060796	-1.025487
(3,-1)	-1.096287		-1.005779	-1.066200	-1.037300	-1.005024	-0.921437	-1.060796	-1.025487
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.259132	-0.062859	-0.249664	-0.508969	-0.388323	-0.313993	-0.380795	-0.392366	-0.571445
(3,-1)	-0.754743	-0.599019	-0.716209	-0.739861	-0.694726	-0.696662	-0.696871	-0.682081	-0.658646
(3,-1)	-0.754743	-0.599019	-0.716209	-0.739861	-0.694726	-0.696662	-0.696871	-0.682081	-0.658646
(3,-1)	-1.155279	-1.054294	-1.185049	-1.276609	-1.458977	-1.108928	-1.107665	-1.096396	-1.072266
(3,-1)	-1.155279	-1.054294	-1.185049	-1.276609	-1.458977	-1.108928	-1.107665	-1.096396	-1.072266
(3,-1)	-1.096287	-0.998168	-1.124387	-1.209926	-1.399495	-1.049168	-1.047795	-1.036229	-1.013152
(3,-1)	-1.096287	-0.998168	-1.124387	-1.209926	-1.399495	-1.049168	-1.047795	-1.036229	-1.013152
(3,-1)	-1.096287	-0.998168	-1.124387	-1.209926	-1.399495	-1.049168	-1.047795	-1.036229	-1.013152
(3,-1)	-1.096287	-0.998168	-1.124387	-1.209926	-1.399495	-1.049168	-1.047795	-1.036229	-1.013152
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.259132	-0.089212	-0.479761	-0.175203	-0.404229	-0.288184	-0.311043		
(3,-1)	-0.754743	-0.579870	-0.694672	-0.847873	-0.712356	-0.715953	-0.731006		
(3,-1)	-0.754743	-2.639141	-0.694672	-0.847873	-0.712356	-0.715953	-0.731006		
(3,-1)	-1.155279	-0.690038	-1.178692	-1.209115	-1.140284	-1.128450	-1.137280		
(3,-1)	-1.155279	-0.996592	-1.178692	-1.209115	-1.140284	-1.128450	-1.137280		
(3,-1)	-1.096287	-0.956219	-1.102848	-1.145660	-1.080509	-1.069468	-1.077814		
(3,-1)	-1.096287	-0.956219	-1.102848	-1.145660	-1.080509	-1.069468	-1.077813		
(3,-1)	-1.096287		-1.102848	-1.145660	-1.080509	-1.069468	-1.077814		
(3,-1)	-1.096287		-1.102848	-1.145660	-1.080509	-1.069468	-1.077813		

Table S338: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>COOH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.383932	-0.632480	-0.633822	-0.524998	-0.447003	-0.772255	-0.541307	-0.102606	0.159641
(3,-1)	-0.721423	-0.803100	-0.845164	-0.794855	-0.767755	-0.834438	-0.788694	-0.593621	-0.422992
(3,-1)	-2.734752	-2.609816	-2.576597	-2.568302	-2.645681	-2.415007	-2.646961	-2.643700	-2.739978
(3,-1)	-0.796223	-0.648849	-0.703539	-0.675579	-0.736392	-0.625559	-0.660652	-0.756032	-0.702570
(3,-1)	-1.169302	-1.069497	-1.119066	-1.080483	-1.127033	-0.981099	-1.093160	-0.997063	-0.898620
(3,-1)	-1.123428	-1.024533	-1.072376	-1.034853	-1.080274	-0.942173	-1.045404	-0.966577	-0.874184
(3,-1)	-1.123428	-1.024533	-1.072376	-1.034853	-1.080274	-0.942173	-1.045404	-0.966577	-0.874184
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.383932	0.236402	0.282780	-0.597118	-0.477386	-0.358169	-0.518391	-0.286649	-0.477243
(3,-1)	-0.721423	-0.138963	-0.336616	-0.851438	-0.784726	-0.617454	-0.731326	-0.684668	-0.799685
(3,-1)	-2.734752	-0.687470	-2.513313	-2.652078	-2.655681	-2.635095	-2.548694	-2.768037	-2.377285
(3,-1)	-0.796223	-1.033765	-0.728039	-0.738290	-0.721228	-0.735316	-0.739248	-0.766579	-0.700292
(3,-1)	-1.169302	-0.985638	-1.089313	-1.139784	-1.108736	-1.065957	-0.968618	-1.135833	-1.101442
(3,-1)	-1.123428	-0.985638	-1.032770	-1.092818	-1.062571	-1.026856	-0.937375	-1.087517	-1.052329
(3,-1)	-1.123428	-0.985638	-1.032770	-1.092818	-1.062571	-1.026856	-0.937375	-1.087517	-1.052329
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.383932	-0.158468	-0.366834	-0.634059	-0.545927	-0.420348	-0.487581	-0.494510	-0.683227
(3,-1)	-0.721423	-0.664666	-0.705627	-0.832774	-0.797514	-0.739835	-0.781994	-0.790258	-0.834762
(3,-1)	-2.734752	-2.631788	-2.555715	-2.661215	-2.695098	-2.729137	-2.723841	-2.708148	-2.651105
(3,-1)	-0.796223	-0.640103	-0.761729	-0.783100	-0.738099	-0.729970	-0.732268	-0.719735	-0.696112
(3,-1)	-1.169302	-1.067782	-1.199044	-1.290513	-1.475087	-1.121107	-1.119962	-1.108564	-1.084322
(3,-1)	-1.123428	-1.022597	-1.152429	-1.240171	-1.430648	-1.075726	-1.074301	-1.062187	-1.038559
(3,-1)	-1.123428	-1.022597	-1.152429	-1.240171	-1.430648	-1.075726	-1.074301	-1.062187	-1.038559
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.383932	0.108932	-0.612541	-0.347674	-0.500225	-0.386829	-0.409905		
(3,-1)	-0.721423	-0.193050	-0.752662	-0.630712	-0.823717	-0.745578	-0.751516		
(3,-1)	-2.734752	-0.699557	-2.934255	-2.894111	-2.669730	-2.705983	-2.673247		
(3,-1)	-0.796223	-1.001192	-0.734320	-0.896015	-0.752127	-0.755821	-0.770425		
(3,-1)	-1.169302	-0.961473	-1.193706	-1.222920	-1.153889	-1.141729	-1.150716		
(3,-1)	-1.123428	-0.961473	-1.139097	-1.173552	-1.107612	-1.095790	-1.104806		
(3,-1)	-1.123428	-0.961473	-1.139097	-1.173552	-1.107612	-1.095790	-1.104806		

Table S339: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>COF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.159489	-0.485881	-0.477245	-0.364440	-0.281348	-0.624251	-0.390221	0.068029	0.355661
(3,-1)	-0.379248	-0.481304	-0.510061	-0.475359	-0.398186	-0.502801	-0.441630	-0.319346	-0.062459
(3,-1)	-0.844421	-0.657365	-0.712797	-0.684555	-0.746068	-0.635459	-0.669251	-0.764428	-0.711855
(3,-1)	-1.174903	-1.074926	-1.124479	-1.085597	-1.132892	-0.985636	-1.099397	-0.999552	-0.903022
(3,-1)	-1.117175	-1.030094	-1.078312	-1.040423	-1.086409	-0.946689	-1.051988	-0.969471	-0.879029
(3,-1)	-1.085900	-1.030094	-1.078312	-1.040423	-1.086409	-0.946689	-1.051988	-0.969471	-0.879029
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.159489	-0.666780	0.489418	-0.435403	-0.311070	-0.233369	-0.377143	-0.107675	-0.300189
(3,-1)	-0.379248	-0.278859	-0.025388	-0.474179	-0.414989	-0.296297	-0.417974	-0.308478	-0.385744
(3,-1)	-0.844421	0.317791	-0.738156	-0.748128	-0.731104	-0.744907	-0.748082	-0.777279	-0.709442
(3,-1)	-1.174903	-1.026387	-1.095986	-1.145813	-1.114553	-1.070947	-0.971013	-1.142216	-1.108276
(3,-1)	-1.117175	-0.992431	-1.039794	-1.099087	-1.068532	-1.031485	-0.939952	-1.094003	-1.058755
(3,-1)	-1.085900	-0.992431	-1.039794	-1.099087	-1.068532	-1.031485	-0.939952	-1.094003	-1.058755
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.159489	0.037226	-0.184325	-0.471350	-0.356513	-0.259633	-0.323762	-0.326330	-0.536765
(3,-1)	-0.379248	-0.315087	-0.316275	-0.374671	-0.311256	-0.378454	-0.406458	-0.417699	-0.428591
(3,-1)	-0.844421	-0.651173	-0.772827	-0.794309	-0.748648	-0.737615	-0.741001	-0.729458	-0.705240
(3,-1)	-1.174903	-1.072708	-1.205982	-1.297632	-1.482435	-1.127525	-1.126301	-1.114641	-1.090503
(3,-1)	-1.117175	-1.027215	-1.158946	-1.247292	-1.437954	-1.082361	-1.080800	-1.068462	-1.044737
(3,-1)	-1.085900	-1.027215	-1.158946	-1.247292	-1.437954	-1.082361	-1.080800	-1.068462	-1.044737
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.159489	-0.676261	-0.473590	-0.166871	-0.331077	-0.213129	-0.239541		
(3,-1)	-0.379248	-0.264244	-0.377538	-0.091746	-0.441877	-0.350174	-0.355095		
(3,-1)	-0.844421	0.202548	-0.741601	-0.911668	-0.763540	-0.767792	-0.782103		
(3,-1)	-1.174903	-0.994028	-1.202910	-1.230416	-1.160020	-1.147956	-1.156820		
(3,-1)	-1.117175	-0.966582	-1.149186	-1.180776	-1.113976	-1.102087	-1.111020		
(3,-1)	-1.085900	-0.966582	-1.149186	-1.180776	-1.113976	-1.102087	-1.111019		

Table S340: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>COCl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.775247	-0.631675	-0.683455	-0.657179	-0.716156	-0.609038	-0.640612	-0.735146	-0.696068
(3,-1)	-0.287264	-0.184208	-0.198186	-0.195054	-0.240784	-0.164072	-0.177891	-0.185208	-0.258648
(3,-1)	-0.109153	-0.392219	-0.368817	-0.267865	-0.181982	-0.525201	-0.277456	0.162926	0.478024
(3,-1)	-1.166325	-1.067179	-1.115911	-1.077863	-1.124701	-0.976910	-1.091079	-0.995105	-0.896344
(3,-1)	-1.134221	-1.035851	-1.084204	-1.046732	-1.092560	-0.952893	-1.058613	-0.973249	-0.882618
(3,-1)	-1.134221	-1.035851	-1.084204	-1.046732	-1.092560	-0.952893	-1.058613	-0.973249	-0.882618
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.775247	-0.638560	-0.713958	-0.717395	-0.701719	-0.705243	-0.716477	-0.746025	-0.682843
(3,-1)	-0.287264	-0.597621	-0.297572	-0.231132	-0.235102	-0.137482	-0.167088	-0.268127	-0.241937
(3,-1)	-0.109153	-0.985825	0.568566	-0.327546	-0.214016	-0.122147	-0.282068	-0.014396	-0.203023
(3,-1)	-1.166325	-0.998827	-1.086937	-1.136981	-1.106447	-1.064511	-0.966672	-1.133482	-1.099245
(3,-1)	-1.134221	-0.998827	-1.048132	-1.104668	-1.074513	-1.037208	-0.943780	-1.099732	-1.064789
(3,-1)	-1.134221	-0.323398	-1.048132	-1.104668	-1.074513	-1.037208	-0.943780	-1.099732	-1.064789
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.775247	-0.616897	-0.732849	-0.756319	-0.704108	-0.712629	-0.713977	-0.700243	-0.676323
(3,-1)	-0.287264	-0.164809	-0.218944	-0.254613	-0.286191	-0.267411	-0.253252	-0.227895	-0.220519
(3,-1)	-0.109153	0.140047	-0.087092	-0.357799	-0.249961	-0.170994	-0.231404	-0.230142	-0.432128
(3,-1)	-1.166325	-1.063786	-1.196388	-1.288473	-1.471195	-1.119615	-1.118345	-1.106888	-1.082179
(3,-1)	-1.134221	-1.031614	-1.164462	-1.252672	-1.441592	-1.087342	-1.086065	-1.074436	-1.050246
(3,-1)	-1.134221	-1.031614	-1.164462	-1.252672	-1.441592	-1.087342	-1.086065	-1.074436	-1.050246
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.775247	-0.641027	-0.705141	-0.874610	-0.730811	-0.735381	-0.750117		
(3,-1)	-0.287264	-0.602819	-0.193039	-0.362235	-0.237770	-0.255518	-0.257748		
(3,-1)	-0.109153	-0.956946	-0.360293	-0.058801	-0.225709	-0.116358	-0.140569		
(3,-1)	-1.166325	-0.965617	-1.193839	-1.220755	-1.150826	-1.139130	-1.147978		
(3,-1)	-1.134221	-0.965617	-1.155922	-1.186071	-1.118919	-1.107144	-1.115715		
(3,-1)	-1.134221	-0.299740	-1.155922	-1.186071	-1.118919	-1.107144	-1.115715		



Table S341: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>Cl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.720717	-0.596104	-0.646659	-0.620543	-0.673171	-0.575675	-0.601870	-0.690016	-0.659958
(3,-1)	-0.669034	-0.552095	-0.602564	-0.576214	-0.625225	-0.534274	-0.556334	-0.635245	-0.622413
(3,-1)	-1.120139	-1.023455	-1.069818	-1.034167	-1.078958	-0.943584	-1.043638	-0.969743	-0.865661
(3,-1)	-1.135824	-1.039245	-1.083805	-1.048935	-1.094399	-0.954354	-1.059585	-0.978463	-0.863297
(3,-1)	-1.135824	-1.039245	-1.083805	-1.048935	-1.094399	-0.954354	-1.059585	-0.978463	-0.863297
(3,-1)	-0.314677	-0.229564	-0.249694	-0.242566	-0.279799	-0.217372	-0.222846	-0.227687	-0.301968
(3,-1)	-1.112047	-1.015746	-1.062331	-1.027047	-1.071328	-0.941336	-1.036103	-0.963405	-0.858001
(3,-1)	-1.112047	-1.015746	-1.062331	-1.027047	-1.071328	-0.941336	-1.036103	-0.963405	-0.858001
(3,-1)	-1.199920	-1.093723	-1.141360	-1.104794	-1.155291	-1.002685	-1.120364	-1.017815	-0.896196
(3,-1)	-1.199920	-1.093723	-1.141360	-1.104794	-1.155291	-1.002685	-1.120364	-1.017815	-0.896196
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.720717	-0.492885	-0.679286	-0.675025	-0.658042	-0.640448	-0.666437	-0.695896	-0.642273
(3,-1)	-0.669034	-2.508645	-0.636425	-0.628219	-0.610371	-0.577471	-0.611861	-0.646311	-0.597752
(3,-1)	-1.120139	-0.637331	-1.034574	-1.089805	-1.061389	-1.026668	-0.942052	-1.085830	-1.050798
(3,-1)	-1.135824	-1.019810	-1.049869	-1.104757	-1.077062	-1.039957	-0.952463	-1.102309	-1.066444
(3,-1)	-1.135824	-0.657278	-1.049869	-1.104757	-1.077062	-1.039957	-0.952463	-1.102309	-1.066444
(3,-1)	-0.314677	-0.979253	-0.337545	-0.273205	-0.271874	-0.171004	-0.208422	-0.298196	-0.278395
(3,-1)	-1.112047	-0.981502	-1.026087	-1.081878	-1.053696	-1.020886	-0.935293	-1.077582	-1.042681
(3,-1)	-1.112047	-0.992097	-1.026087	-1.081878	-1.053696	-1.020886	-0.935293	-1.077582	-1.042681
(3,-1)	-1.199920	-0.963956	-1.117436	-1.165312	-1.136710	-1.098736	-0.993436	-1.166429	-1.132096
(3,-1)	-1.199920	-0.976882	-1.117436	-1.165312	-1.136710	-1.098736	-0.993436	-1.166429	-1.132096
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.720717	-0.565082	-0.676308	-0.703005	-0.657270	-0.666715	-0.667796	-0.654363	-0.633077
(3,-1)	-0.669034	-0.518845	-0.624260	-0.653059	-0.620654	-0.617570	-0.618930	-0.605835	-0.587355
(3,-1)	-1.120139	-1.023926	-1.148040	-1.235364	-1.421677	-1.072747	-1.071600	-1.060970	-1.036476
(3,-1)	-1.135824	-1.039048	-1.160493	-1.250326	-1.434405	-1.088952	-1.087753	-1.077006	-1.052688
(3,-1)	-1.135824	-1.039048	-1.160493	-1.250326	-1.434405	-1.088952	-1.087753	-1.077006	-1.052688
(3,-1)	-0.314677	-0.189379	-0.247090	-0.281871	-0.296479	-0.294145	-0.284415	-0.263261	-0.258703
(3,-1)	-1.112047	-1.017254	-1.138912	-1.225735	-1.411626	-1.064519	-1.063076	-1.052219	-1.028508
(3,-1)	-1.112047	-1.017254	-1.138912	-1.225735	-1.411626	-1.064519	-1.063076	-1.052219	-1.028508
(3,-1)	-1.199920	-1.094323	-1.225057	-1.320113	-1.498542	-1.154830	-1.151762	-1.138462	-1.112286
(3,-1)	-1.199920	-1.094323	-1.225057	-1.320113	-1.498542	-1.154830	-1.151762	-1.138462	-1.112286
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.720717	-0.565509	-0.654212	-0.805826	-0.685153	-0.685604	-0.701766		
(3,-1)	-0.669034	-2.555676	-0.603669	-0.748725	-0.637357	-0.635878	-0.652387		
(3,-1)	-1.120139	-0.642224	-1.128577	-1.169365	-1.104523	-1.093925	-1.102727		
(3,-1)	-1.135824	-0.979214	-1.145900	-1.185994	-1.119064	-1.109172	-1.117262		
(3,-1)	-1.135824	-0.660068	-1.145900	-1.185994	-1.119064	-1.109172	-1.117263		
(3,-1)	-0.314677	-0.951801	-0.216629	-0.374293	-0.282111	-0.291636	-0.299292		
(3,-1)	-1.112047	-0.953605	-1.113839	-1.160230	-1.096818	-1.086161	-1.094792		
(3,-1)	-1.112047	-0.962996	-1.113839	-1.160230	-1.096818	-1.086161	-1.094792		
(3,-1)	-1.199920	-0.936566	-1.220592	-1.257421	-1.180695	-1.171526	-1.180243		
(3,-1)	-1.199920	-0.948234	-1.220592	-1.257421	-1.180695	-1.171526	-1.180243		

Table S342: Laplacian of the density value (a.u.) at the considered critical points for the  $(\text{CH}_3)_2\text{CH-OH}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.613779	-0.614403	-0.648123	-0.635649	-0.648376	-0.626957	-0.626105	-0.567004	-0.444434
(3,-1)	-2.687357	-2.577409	-2.533808	-2.529869	-2.603562	-2.360538	-2.598883	-2.592750	-2.696950
(3,-1)	-0.727074	-0.599371	-0.650900	-0.624256	-0.678093	-0.576334	-0.605899	-0.696341	-0.658372
(3,-1)	-1.165820	-1.057930	-1.102409	-1.067741	-1.117649	-0.971641	-1.081928	-0.987624	-0.845691
(3,-1)	-0.746106	-0.618627	-0.672440	-0.644495	-0.697936	-0.597100	-0.627259	-0.717660	-0.672846
(3,-1)	-1.117394	-1.020455	-1.068000	-1.031952	-1.076739	-0.945194	-1.041896	-0.966039	-0.861206
(3,-1)	-1.119316	-1.022906	-1.070357	-1.034231	-1.078833	-0.947211	-1.044220	-0.967911	-0.862618
(3,-1)	-1.128599	-1.031757	-1.079058	-1.042542	-1.087444	-0.951823	-1.052741	-0.974118	-0.868835
(3,-1)	-1.096135	-1.000783	-1.047329	-1.012153	-1.055787	-0.928828	-1.020292	-0.953370	-0.847032
(3,-1)	-1.108911	-1.013262	-1.060243	-1.024730	-1.068739	-0.939539	-1.033690	-0.960834	-0.857308
(3,-1)	-1.106936	-1.010887	-1.057423	-1.021880	-1.066389	-0.936877	-1.031004	-0.959604	-0.856656
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.613779	-0.458207	-0.392838	-0.671419	-0.654005	-0.502303	-0.573421	-0.613889	-0.664565
(3,-1)	-2.687357	-0.451150	-2.451689	-2.605216	-2.611461	-2.577164	-2.479323	-2.709272	-2.325742
(3,-1)	-0.727074	-1.070986	-0.680898	-0.680229	-0.662909	-0.655206	-0.675775	-0.702187	-0.645474
(3,-1)	-1.165820	-0.653013	-1.075673	-1.127358	-1.100530	-1.063815	-0.968342	-1.130345	-1.094795
(3,-1)	-0.746106	-1.008288	-0.699802	-0.700876	-0.682308	-0.676813	-0.695938	-0.721252	-0.664234
(3,-1)	-1.117394	-1.008288	-1.029619	-1.087726	-1.058864	-1.025283	-0.938486	-1.083042	-1.048238
(3,-1)	-1.119316	-1.008900	-1.032246	-1.089922	-1.060952	-1.027364	-0.940369	-1.085290	-1.050338
(3,-1)	-1.128599	-1.008900	-1.042176	-1.098917	-1.069665	-1.033551	-0.947189	-1.094260	-1.059935
(3,-1)	-1.096135	-0.990043	-1.008804	-1.066445	-1.038317	-1.006360	-0.926154	-1.061474	-1.026106
(3,-1)	-1.108911	-0.990043	-1.024035	-1.079559	-1.051155	-1.016758	-0.933401	-1.074725	-1.039855
(3,-1)	-1.106936	-0.977261	-1.020829	-1.077308	-1.048925	-1.015702	-0.932279	-1.072896	-1.038226
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.613779	-0.596517	-0.586732	-0.629974	-0.629538	-0.627186	-0.649821	-0.657199	-0.650742
(3,-1)	-2.687357	-2.558827	-2.544036	-2.631800	-2.738978	-2.680580	-2.671143	-2.652702	-2.591251
(3,-1)	-0.727074	-0.573448	-0.686486	-0.711960	-0.665366	-0.671911	-0.673100	-0.659644	-0.638258
(3,-1)	-1.165820	-1.066813	-1.178912	-1.276071	-1.446040	-1.117864	-1.115233	-1.102592	-1.078402
(3,-1)	-0.746106	-0.593157	-0.707240	-0.731513	-0.683773	-0.689629	-0.691787	-0.679428	-0.658182
(3,-1)	-1.117394	-1.021416	-1.144742	-1.232421	-1.418122	-1.070330	-1.068863	-1.057948	-1.034376
(3,-1)	-1.119316	-1.023028	-1.146973	-1.234763	-1.419882	-1.072552	-1.071039	-1.060118	-1.036374
(3,-1)	-1.128599	-1.031701	-1.156554	-1.245029	-1.430973	-1.080926	-1.079834	-1.069221	-1.045243
(3,-1)	-1.096135	-1.002214	-1.121426	-1.207279	-1.392962	-1.048034	-1.046958	-1.036674	-1.013506
(3,-1)	-1.108911	-1.014729	-1.136242	-1.222578	-1.408921	-1.060688	-1.059695	-1.049588	-1.026273
(3,-1)	-1.106936	-1.012269	-1.134963	-1.221121	-1.407011	-1.059640	-1.058359	-1.047728	-1.024419
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.613779	-0.542197	-0.563456	-0.466940	-0.678451	-0.648870	-0.644268		
(3,-1)	-2.687357	-0.539711	-2.886038	-2.825166	-2.625466	-2.660965	-2.630450		
(3,-1)	-0.727074	-1.027640	-0.663961	-0.813283	-0.690848	-0.691392	-0.707782		
(3,-1)	-1.165820	-0.659231	-1.172900	-1.220092	-1.143371	-1.135774	-1.144003		
(3,-1)	-0.746106	-0.970734	-0.683055	-0.832734	-0.711315	-0.710688	-0.727467		
(3,-1)	-1.117394	-0.970734	-1.123700	-1.166668	-1.102313	-1.091211	-1.099874		
(3,-1)	-1.119316	-0.973207	-1.126390	-1.168589	-1.104410	-1.093166	-1.101941		
(3,-1)	-1.128599	-0.973207	-1.140384	-1.178340	-1.113388	-1.102108	-1.111104		
(3,-1)	-1.096135	-0.961222	-1.096200	-1.143748	-1.081016	-1.070204	-1.078747		
(3,-1)	-1.108911	-0.961222	-1.113048	-1.157490	-1.094000	-1.083028	-1.091492		
(3,-1)	-1.106936	-0.948560	-1.112410	-1.156513	-1.091596	-1.080831	-1.089242		

Table S343: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{CH}_3\text{-CH}_2\text{-O-CH}_3$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.617945	-0.646275	-0.686524	-0.665845	-0.661691	-0.650186	-0.652899	-0.563852	-0.382437
(3,-1)	-0.619100	-0.653286	-0.700972	-0.675115	-0.667236	-0.663631	-0.661666	-0.564062	-0.361736
(3,-1)	-1.212734	-1.102403	-1.155592	-1.115776	-1.165431	-1.016256	-1.132643	-1.017608	-0.896753
(3,-1)	-0.744768	-0.615528	-0.671768	-0.642654	-0.695988	-0.595978	-0.626490	-0.713966	-0.671123
(3,-1)	-1.152289	-1.044887	-1.091957	-1.056530	-1.105800	-0.968777	-1.069873	-0.978429	-0.845056
(3,-1)	-1.152289	-1.044887	-1.091957	-1.056530	-1.105800	-0.968777	-1.069873	-0.978429	-0.845056
(3,-1)	-1.153787	-1.044677	-1.095046	-1.058099	-1.107174	-0.974692	-1.071635	-0.978660	-0.854801
(3,-1)	-1.153787	-1.044677	-1.095046	-1.058099	-1.107174	-0.974692	-1.071635	-0.978660	-0.854801
(3,-1)	-1.128748	-1.030864	-1.078268	-1.041715	-1.086628	-0.950957	-1.051445	-0.973796	-0.869565
(3,-1)	-1.128748	-1.030864	-1.078268	-1.041715	-1.086628	-0.950957	-1.051445	-0.973796	-0.869565
(3,-1)	-1.108455	-1.012591	-1.059316	-1.023710	-1.067743	-0.935719	-1.032294	-0.961132	-0.859206
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.617945	-0.841141	-0.353119	-0.702169	-0.670768	-0.507715	-0.592054	-0.611409	-0.687670
(3,-1)	-0.619100	-0.841141	-0.342478	-0.713591	-0.675965	-0.507628	-0.597453	-0.610970	-0.694463
(3,-1)	-1.212734	-0.841141	-1.139370	-1.178199	-1.146577	-1.101777	-0.995079	-1.177171	-1.148151
(3,-1)	-0.744768	-0.944581	-0.697030	-0.699635	-0.680017	-0.676714	-0.693417	-0.720052	-0.662337
(3,-1)	-1.152289	-1.022262	-1.066193	-1.115924	-1.088308	-1.055125	-0.958340	-1.117573	-1.082220
(3,-1)	-1.152289	-1.022262	-1.066193	-1.115924	-1.088308	-1.055125	-0.958340	-1.117573	-1.082220
(3,-1)	-1.153787	-0.944581	-1.070070	-1.118171	-1.089137	-1.056338	-0.956295	-1.117784	-1.084487
(3,-1)	-1.153787	-1.022262	-1.070070	-1.118171	-1.089137	-1.056338	-0.956295	-1.117784	-1.084487
(3,-1)	-1.128748	-1.022262	-1.042135	-1.098168	-1.068839	-1.033806	-0.945904	-1.094086	-1.059691
(3,-1)	-1.128748	-0.944581	-1.042135	-1.098168	-1.068839	-1.033806	-0.945904	-1.094086	-1.059691
(3,-1)	-1.108455	-1.022262	-1.024283	-1.078712	-1.050219	-1.015928	-0.933211	-1.074373	-1.039357
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.617945	-0.619041	-0.608076	-0.663407	-0.667656	-0.637693	-0.667023	-0.677773	-0.676368
(3,-1)	-0.619100	-0.624349	-0.616628	-0.675017	-0.683699	-0.641188	-0.672451	-0.684318	-0.684156
(3,-1)	-1.212734	-1.111280	-1.233918	-1.327880	-1.496099	-1.164122	-1.161828	-1.148972	-1.124229
(3,-1)	-0.744768	-0.593624	-0.707563	-0.731350	-0.687104	-0.687312	-0.689569	-0.677556	-0.656387
(3,-1)	-1.152289	-1.054759	-1.168293	-1.263504	-1.431614	-1.105180	-1.102386	-1.089225	-1.066192
(3,-1)	-1.152289	-1.054759	-1.168293	-1.263504	-1.431614	-1.105180	-1.102386	-1.089225	-1.066192
(3,-1)	-1.153787	-1.054977	-1.172303	-1.266778	-1.435188	-1.105642	-1.102725	-1.089310	-1.066479
(3,-1)	-1.153787	-1.054977	-1.172303	-1.266778	-1.435188	-1.105642	-1.102725	-1.089310	-1.066479
(3,-1)	-1.128748	-1.032386	-1.155932	-1.243733	-1.429025	-1.081328	-1.079736	-1.068226	-1.044189
(3,-1)	-1.128748	-1.032386	-1.155932	-1.243733	-1.429025	-1.081328	-1.079736	-1.068226	-1.044189
(3,-1)	-1.108455	-1.014402	-1.135843	-1.221388	-1.406256	-1.060692	-1.059520	-1.048970	-1.025472
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.617945	-0.806464	-0.590227	-0.470805	-0.701358	-0.653010	-0.654146		
(3,-1)	-0.619100	-0.806464	-0.597290	-0.486755	-0.708834	-0.653434	-0.656246		
(3,-1)	-1.212734	-0.806464	-1.229458	-1.268587	-1.194786	-1.183148	-1.194222		
(3,-1)	-0.744768	-0.916606	-0.682802	-0.831250	-0.710751	-0.709231	-0.726703		
(3,-1)	-1.152289	-0.985904	-1.155168	-1.207844	-1.131653	-1.123082	-1.131872		
(3,-1)	-1.152289	-0.985904	-1.155168	-1.207844	-1.131653	-1.123082	-1.131872		
(3,-1)	-1.153787	-0.916606	-1.155874	-1.209351	-1.134571	-1.124801	-1.134564		
(3,-1)	-1.153787	-0.985904	-1.155874	-1.209351	-1.134571	-1.124801	-1.134565		
(3,-1)	-1.128748	-0.985904	-1.136497	-1.177573	-1.113377	-1.102049	-1.111238		
(3,-1)	-1.128748	-0.916606	-1.136497	-1.177573	-1.113377	-1.102049	-1.111237		
(3,-1)	-1.108455	-0.985904	-1.112729	-1.156677	-1.093254	-1.082305	-1.090950		

Table S344: Laplacian of the density value (a.u.) at the considered critical points for the  $(\text{CH}_3)_3\text{N}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.851920	-0.683747	-0.731833	-0.715769	-0.787840	-0.656807	-0.702916	-0.748188	-0.887955
(3,-1)	-0.851920	-0.683747	-0.731833	-0.715769	-0.787840	-0.656807	-0.702916	-0.748188	-0.887955
(3,-1)	-0.851920	-0.683747	-0.731833	-0.715769	-0.787840	-0.656807	-0.702916	-0.748188	-0.887955
(3,-1)	-1.080995	-0.981556	-1.027568	-0.993896	-1.039515	-0.917221	-1.003103	-0.936654	-0.819028
(3,-1)	-1.158825	-1.055555	-1.106000	-1.068594	-1.115577	-0.978213	-1.080859	-0.988657	-0.872228
(3,-1)	-1.158825	-1.055555	-1.106000	-1.068594	-1.115577	-0.978213	-1.080859	-0.988657	-0.872228
(3,-1)	-1.080995	-0.981556	-1.027568	-0.993896	-1.039515	-0.917221	-1.003103	-0.936654	-0.819028
(3,-1)	-1.158826	-1.055555	-1.106000	-1.068594	-1.115577	-0.978213	-1.080859	-0.988657	-0.872228
(3,-1)	-1.158823	-1.055555	-1.106000	-1.068594	-1.115577	-0.978213	-1.080859	-0.988657	-0.872228
(3,-1)	-1.080995	-0.981556	-1.027568	-0.993896	-1.039515	-0.917221	-1.003103	-0.936654	-0.819028
(3,-1)	-1.158823	-1.055555	-1.106000	-1.068594	-1.115577	-0.978213	-1.080859	-0.988657	-0.872228
(3,-1)	-1.158826	-1.055555	-1.106000	-1.068594	-1.115577	-0.978213	-1.080859	-0.988657	-0.872228
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.851920	0.351996	-0.870584	-0.775727	-0.773106	-0.618288	-0.673996	-0.834417	-0.740938
(3,-1)	-0.851920	0.023197	-0.870584	-0.775727	-0.773106	-0.618288	-0.673996	-0.834417	-0.740938
(3,-1)	-0.851920	0.023197	-0.870584	-0.775727	-0.773106	-0.618288	-0.673996	-0.834417	-0.740938
(3,-1)	-1.080995	-0.995683	-0.992371	-1.048703	-1.022270	-1.000264	-0.913795	-1.047812	-1.009692
(3,-1)	-1.158825	-0.995683	-1.079071	-1.127013	-1.097307	-1.058641	-0.964323	-1.124107	-1.091129
(3,-1)	-1.158825	-0.800967	-1.079071	-1.127013	-1.097307	-1.058641	-0.964323	-1.124107	-1.091129
(3,-1)	-1.080995	-1.129928	-0.992371	-1.048703	-1.022270	-1.000264	-0.913795	-1.047812	-1.009692
(3,-1)	-1.158826	-1.129928	-1.079071	-1.127013	-1.097307	-1.058641	-0.964323	-1.124107	-1.091129
(3,-1)	-1.158823	-1.072679	-1.079071	-1.127013	-1.097307	-1.058641	-0.964323	-1.124107	-1.091129
(3,-1)	-1.080995	-1.072679	-0.992371	-1.048703	-1.022270	-1.000264	-0.913795	-1.047812	-1.009692
(3,-1)	-1.158823	-1.072679	-1.079071	-1.127013	-1.097307	-1.058641	-0.964323	-1.124107	-1.091129
(3,-1)	-1.158826	-1.072679	-1.079071	-1.127013	-1.097307	-1.058641	-0.964323	-1.124107	-1.091129
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.851920	-0.685743	-0.727062	-0.786442	-0.758402	-0.790857	-0.783757	-0.765645	-0.735400
(3,-1)	-0.851920	-0.685743	-0.727062	-0.786442	-0.758402	-0.790857	-0.783757	-0.765645	-0.735400
(3,-1)	-0.851920	-0.685743	-0.727062	-0.786442	-0.758402	-0.790857	-0.783757	-0.765645	-0.735400
(3,-1)	-1.080995	-0.986308	-1.100953	-1.189495	-1.363604	-1.035928	-1.033120	-1.020913	-0.999289
(3,-1)	-1.158825	-1.061426	-1.182201	-1.273683	-1.450807	-1.110468	-1.108946	-1.097656	-1.073258
(3,-1)	-1.158825	-1.061426	-1.182201	-1.273683	-1.450807	-1.110468	-1.108946	-1.097656	-1.073258
(3,-1)	-1.080995	-0.986308	-1.100953	-1.189495	-1.363604	-1.035928	-1.033120	-1.020913	-0.999289
(3,-1)	-1.158826	-1.061426	-1.182201	-1.273683	-1.450807	-1.110468	-1.108946	-1.097656	-1.073258
(3,-1)	-1.158823	-1.061426	-1.182201	-1.273683	-1.450807	-1.110468	-1.108946	-1.097656	-1.073258
(3,-1)	-1.158826	-1.061426	-1.182201	-1.273683	-1.450807	-1.110468	-1.108946	-1.097656	-1.073258
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.851920	0.348700	-0.707331	-0.992388	-0.795005	-0.815434	-0.818975		
(3,-1)	-0.851920	-0.075885	-0.707331	-0.992388	-0.795005	-0.815434	-0.819007		
(3,-1)	-0.851920	-0.075885	-0.707331	-0.992388	-0.795005	-0.815434	-0.819006		
(3,-1)	-1.080995	-1.007720	-1.073612	-1.132542	-1.063287	-1.054465	-1.062458		
(3,-1)	-1.158825	-1.007720	-1.168835	-1.212122	-1.142263	-1.131114	-1.140873		
(3,-1)	-1.158825	-0.814384	-1.168835	-1.212122	-1.142263	-1.131114	-1.140874		
(3,-1)	-1.080995	-1.090553	-1.073612	-1.132542	-1.063287	-1.054465	-1.062475		
(3,-1)	-1.158826	-1.090553	-1.168835	-1.212122	-1.142263	-1.131114	-1.140958		
(3,-1)	-1.158823	-1.038702	-1.168835	-1.212122	-1.142263	-1.131114	-1.140880		
(3,-1)	-1.080995	-1.038702	-1.073612	-1.132542	-1.063287	-1.054465	-1.062475		
(3,-1)	-1.158823	-1.038702	-1.168835	-1.212122	-1.142263	-1.131114	-1.140881		
(3,-1)	-1.158826	-1.038702	-1.168835	-1.212122	-1.142263	-1.131114	-1.140959		

Table S345: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>4</sub>O system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.353044	0.345984	0.348419	0.349135	0.356100	0.335748	0.347071	0.364956	0.375682
(3,-1)	-0.264042	-0.492628	-0.502097	-0.440955	-0.316393	-0.529119	-0.390070	-0.153618	0.162437
(3,-1)	-0.264042	-0.492628	-0.502097	-0.440955	-0.316393	-0.529119	-0.390070	-0.153618	0.162437
(3,-1)	-1.078208	-0.950712	-1.009802	-0.971532	-1.021896	-0.956688	-0.967089	-1.004018	-1.080021
(3,-1)	-1.078208	-0.950712	-1.009802	-0.971532	-1.021896	-0.956688	-0.967089	-1.004018	-1.080021
(3,-1)	-0.883307	-0.748830	-0.803924	-0.769940	-0.824253	-0.742163	-0.755884	-0.797387	-0.854498
(3,-1)	-1.281686	-1.168863	-1.212222	-1.173906	-1.228171	-1.071118	-1.192324	-1.055244	-0.969626
(3,-1)	-1.281686	-1.168863	-1.212222	-1.173906	-1.228171	-1.071118	-1.192324	-1.055244	-0.969626
(3,-1)	-1.210943	-1.112680	-1.154079	-1.117552	-1.166151	-1.013030	-1.131288	-1.021657	-0.944461
(3,-1)	-1.210943	-1.112680	-1.154079	-1.117552	-1.166151	-1.013030	-1.131288	-1.021657	-0.944461
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.353044	0.241978	0.359755	0.352086	0.353784	0.362205	0.351830	0.358167	0.339224
(3,-1)	-0.264042	-0.480559	0.159603	-0.437052	-0.352231	-0.195069	-0.352049	-0.204406	-0.372075
(3,-1)	-0.264042	-0.480559	0.159603	-0.437052	-0.352231	-0.195069	-0.352049	-0.204406	-0.372075
(3,-1)	-1.078208	-0.942965	-1.004491	-1.037635	-1.010590	-0.959133	-0.991408	-1.047993	-0.970941
(3,-1)	-1.078208	-0.942965	-1.004491	-1.037635	-1.010590	-0.959133	-0.991408	-1.047993	-0.970941
(3,-1)	-0.883307	-0.942965	-0.821450	-0.834489	-0.811183	-0.720862	-0.776684	-0.850844	-0.792177
(3,-1)	-1.281686	-1.064983	-1.199949	-1.241143	-1.211811	-1.160377	-1.037054	-1.244354	-1.214246
(3,-1)	-1.281686	-1.064983	-1.199949	-1.241143	-1.211811	-1.160377	-1.037054	-1.244354	-1.214246
(3,-1)	-1.210943	-1.058943	-1.127563	-1.178430	-1.149751	-1.102404	-0.997460	-1.176868	-1.143705
(3,-1)	-1.210943	-1.058943	-1.127563	-1.178430	-1.149751	-1.102404	-0.997460	-1.176868	-1.143705
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.353044	0.341342	0.361012	0.362694	0.343919	0.364789	0.358570	0.353492	0.345737
(3,-1)	-0.264042	-0.287564	-0.284650	-0.392067	-0.351261	-0.270459	-0.331740	-0.364424	-0.405959
(3,-1)	-0.264042	-0.287564	-0.284650	-0.392067	-0.351261	-0.270459	-0.331740	-0.364424	-0.405959
(3,-1)	-1.078208	-0.932360	-1.049013	-1.111924	-1.079543	-0.965816	-0.996966	-1.015453	-0.978230
(3,-1)	-1.078208	-0.932360	-1.049013	-1.111924	-1.079543	-0.965816	-0.996966	-1.015453	-0.978230
(3,-1)	-0.883307	-0.706641	-0.838159	-0.889782	-0.890782	-0.794923	-0.812103	-0.813667	-0.783547
(3,-1)	-1.281686	-1.159546	-1.313977	-1.411396	-1.594847	-1.227073	-1.226416	-1.214049	-1.188014
(3,-1)	-1.281686	-1.159546	-1.313977	-1.411396	-1.594847	-1.227073	-1.226416	-1.214049	-1.188014
(3,-1)	-1.210943	-1.097624	-1.244512	-1.340185	-1.529496	-1.158764	-1.159175	-1.149241	-1.124488
(3,-1)	-1.210943	-1.097624	-1.244512	-1.340185	-1.529496	-1.158764	-1.159175	-1.149241	-1.124488
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.353044	0.239008	0.368366	0.366180	0.353356	0.356185	0.349560		
(3,-1)	-0.264042	-0.479301	-0.309143	-0.077838	-0.387913	-0.280282	-0.287959		
(3,-1)	-0.264042	-0.479301	-0.309143	-0.077838	-0.387913	-0.280282	-0.287959		
(3,-1)	-1.078208	-0.958331	-1.050735	-1.167282	-1.046765	-1.040135	-1.061740		
(3,-1)	-1.078208	-0.860074	-1.050735	-1.167282	-1.046765	-1.040135	-1.061740		
(3,-1)	-0.883307	-0.958331	-0.833146	-0.979006	-0.841933	-0.839193	-0.857716		
(3,-1)	-1.281686	-1.034302	-1.331256	-1.348655	-1.255287	-1.248071	-1.255132		
(3,-1)	-1.281686	-1.034302	-1.331256	-1.348655	-1.255287	-1.248071	-1.255132		
(3,-1)	-1.210943	-1.024584	-1.253463	-1.266493	-1.191447	-1.182405	-1.189365		
(3,-1)	-1.210943	-1.024584	-1.253463	-1.266493	-1.191447	-1.182405	-1.189365		

Table S346: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>4</sub>S system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.239953	0.235258	0.237201	0.238180	0.243002	0.227514	0.237178	0.252172	0.258431
(3,-1)	-0.503032	-0.409730	-0.446000	-0.426160	-0.463642	-0.408511	-0.402783	-0.403952	-0.493678
(3,-1)	-0.503032	-0.409730	-0.446000	-0.426160	-0.463642	-0.408511	-0.402783	-0.403952	-0.493678
(3,-1)	-1.018966	-0.894818	-0.950621	-0.915136	-0.965212	-0.896935	-0.907588	-0.930587	-1.025493
(3,-1)	-0.939177	-0.799110	-0.855939	-0.821396	-0.878029	-0.790967	-0.808689	-0.869098	-0.903313
(3,-1)	-1.018966	-0.894818	-0.950621	-0.915136	-0.965212	-0.896935	-0.907588	-0.930587	-1.025493
(3,-1)	-1.212759	-1.110003	-1.149253	-1.114458	-1.165062	-1.007313	-1.128362	-1.023550	-0.946696
(3,-1)	-1.212759	-1.110003	-1.149253	-1.114458	-1.165062	-1.007313	-1.128362	-1.023550	-0.946696
(3,-1)	-1.197906	-1.097470	-1.138750	-1.103216	-1.152345	-0.997270	-1.116330	-1.013021	-0.928291
(3,-1)	-1.197906	-1.097470	-1.138750	-1.103216	-1.152345	-0.997270	-1.116330	-1.013021	-0.928291
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.239953	0.342796	0.245795	0.239494	0.241032	0.251039	0.240474	0.244138	0.229299
(3,-1)	-0.503032	-1.802304	-0.509520	-0.469869	-0.457103	-0.327120	-0.381345	-0.483481	-0.455284
(3,-1)	-0.503032	-0.534740	-0.509520	-0.469869	-0.457103	-0.327120	-0.381345	-0.483481	-0.455284
(3,-1)	-1.018966	-0.534740	-0.953789	-0.978101	-0.953373	-0.870460	-0.910949	-0.989608	-0.921766
(3,-1)	-0.939177	-0.932117	-0.866879	-0.887905	-0.864487	-0.803925	-0.849209	-0.905273	-0.842639
(3,-1)	-1.018966	-0.932117	-0.953789	-0.978101	-0.953373	-0.870460	-0.910949	-0.989608	-0.921766
(3,-1)	-1.212759	-0.822100	-1.123001	-1.175300	-1.148591	-1.108231	-0.998802	-1.177905	-1.142761
(3,-1)	-1.212759	-1.080036	-1.123001	-1.175300	-1.148591	-1.108231	-0.998802	-1.177905	-1.142761
(3,-1)	-1.197906	-1.080036	-1.113631	-1.163603	-1.135958	-1.091792	-0.988560	-1.164117	-1.129812
(3,-1)	-1.197906	-1.059088	-1.113631	-1.163603	-1.135958	-1.091792	-0.988560	-1.164117	-1.129812
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.239953	0.232031	0.246239	0.246553	0.231277	0.251298	0.245703	0.241390	0.235842
(3,-1)	-0.503032	-0.365132	-0.448156	-0.495175	-0.502765	-0.457695	-0.465076	-0.459656	-0.442218
(3,-1)	-0.503032	-0.365132	-0.448156	-0.495175	-0.502765	-0.457695	-0.465076	-0.459656	-0.442218
(3,-1)	-1.018966	-0.863506	-0.987123	-1.054858	-1.045686	-0.915230	-0.942564	-0.956994	-0.921074
(3,-1)	-0.939177	-0.764788	-0.903403	-0.949999	-0.942886	-0.849129	-0.865399	-0.866678	-0.834024
(3,-1)	-1.018966	-0.863506	-0.987123	-1.054858	-1.045686	-0.915230	-0.942564	-0.956994	-0.921074
(3,-1)	-1.212759	-1.093002	-1.247032	-1.343651	-1.537949	-1.164662	-1.162342	-1.149607	-1.122408
(3,-1)	-1.212759	-1.093002	-1.247032	-1.343651	-1.537949	-1.164662	-1.162342	-1.149607	-1.122408
(3,-1)	-1.197906	-1.086592	-1.228313	-1.323765	-1.510686	-1.148766	-1.147688	-1.136483	-1.110497
(3,-1)	-1.197906	-1.086592	-1.228313	-1.323765	-1.510686	-1.148766	-1.147688	-1.136483	-1.110497
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.239953	0.339540	0.252328	0.248570	0.240848	0.242952	0.238139		
(3,-1)	-0.503032	-1.822644	-0.438122	-0.583894	-0.473800	-0.475087	-0.487083		
(3,-1)	-0.503032	-0.628428	-0.438122	-0.583894	-0.473800	-0.475087	-0.487083		
(3,-1)	-1.018966	-0.628428	-0.995518	-1.103723	-0.987166	-0.982025	-1.002981		
(3,-1)	-0.939177	-0.945558	-0.899471	-1.038293	-0.895087	-0.892765	-0.911825		
(3,-1)	-1.018966	-0.945558	-0.995518	-1.103723	-0.987166	-0.982025	-1.002981		
(3,-1)	-1.212759	-0.837809	-1.258481	-1.271541	-1.188774	-1.182003	-1.189055		
(3,-1)	-1.212759	-1.046674	-1.258481	-1.271541	-1.188774	-1.182003	-1.189055		
(3,-1)	-1.197906	-1.046674	-1.236265	-1.254870	-1.176777	-1.168610	-1.175651		
(3,-1)	-1.197906	-1.026375	-1.236265	-1.254870	-1.176777	-1.168610	-1.175651		

Table S347: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>4</sub>H<sub>4</sub>NH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.344058	0.337138	0.339363	0.340567	0.347173	0.325245	0.339485	0.357945	0.367957
(3,-1)	-2.128618	-1.993291	-1.956299	-1.943885	-2.021424	-1.765159	-1.953983	-1.934362	-2.004402
(3,-1)	-0.775361	-0.867557	-0.900519	-0.855529	-0.808769	-0.890535	-0.852619	-0.644721	-0.379300
(3,-1)	-0.775361	-0.867557	-0.900519	-0.855529	-0.808769	-0.890535	-0.852619	-0.644721	-0.379300
(3,-1)	-1.011474	-0.887742	-0.944981	-0.908289	-0.957604	-0.890941	-0.899626	-0.935751	-1.014405
(3,-1)	-1.011474	-0.887742	-0.944981	-0.908289	-0.957604	-0.890941	-0.899626	-0.935751	-1.014405
(3,-1)	-0.906083	-0.776252	-0.830971	-0.796553	-0.849222	-0.770834	-0.782879	-0.821105	-0.886000
(3,-1)	-1.227695	-1.120867	-1.162539	-1.126042	-1.177424	-1.026081	-1.139904	-1.027072	-0.945936
(3,-1)	-1.227695	-1.120867	-1.162539	-1.126042	-1.177424	-1.026081	-1.139904	-1.027072	-0.945936
(3,-1)	-1.197645	-1.099991	-1.140926	-1.105153	-1.153029	-1.003198	-1.117557	-1.014312	-0.934368
(3,-1)	-1.197645	-1.099991	-1.140926	-1.105153	-1.153029	-1.003198	-1.117557	-1.014312	-0.934368
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.344058	0.163874	0.351326	0.342681	0.344704	0.355781	0.343083	0.349472	0.329136
(3,-1)	-2.128618	-1.002354	-1.865342	-2.018687	-2.017986	-2.014898	-1.833626	-2.089025	-1.789817
(3,-1)	-0.775361	-1.002354	-0.366470	-0.898358	-0.836366	-0.698493	-0.785614	-0.716047	-0.860117
(3,-1)	-0.775361	-0.927568	-0.366470	-0.898358	-0.836366	-0.698493	-0.785614	-0.716047	-0.860117
(3,-1)	-1.011474	-0.927549	-0.943498	-0.971855	-0.945875	-0.880087	-0.918831	-0.981891	-0.911255
(3,-1)	-1.011474	-0.927568	-0.943498	-0.971855	-0.945875	-0.880087	-0.918831	-0.981891	-0.911255
(3,-1)	-0.906083	-0.927549	-0.841717	-0.860370	-0.836456	-0.751116	-0.802629	-0.874398	-0.814656
(3,-1)	-1.227695	-1.069905	-1.138122	-1.189366	-1.161274	-1.116065	-1.005743	-1.190109	-1.156910
(3,-1)	-1.227695	-1.100021	-1.138122	-1.189366	-1.161274	-1.116065	-1.005743	-1.190109	-1.156910
(3,-1)	-1.197645	-1.100021	-1.111152	-1.164748	-1.136697	-1.092435	-0.990294	-1.162818	-1.128932
(3,-1)	-1.197645	-1.058114	-1.111152	-1.164748	-1.136697	-1.092435	-0.990294	-1.162818	-1.128932
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.344058	0.333660	0.351852	0.352806	0.332963	0.357017	0.350174	0.345000	0.336258
(3,-1)	-2.128618	-1.906191	-2.066048	-2.218653	-2.421310	-2.046891	-2.037754	-2.005475	-1.958737
(3,-1)	-0.775361	-0.779535	-0.781090	-0.884046	-0.830531	-0.753496	-0.823614	-0.860669	-0.893137
(3,-1)	-0.775361	-0.779535	-0.781090	-0.884046	-0.830531	-0.753496	-0.823614	-0.860669	-0.893137
(3,-1)	-1.011474	-0.856194	-0.979743	-1.042575	-1.022757	-0.905910	-0.934171	-0.949098	-0.914420
(3,-1)	-1.011474	-0.856194	-0.979743	-1.042575	-1.022757	-0.905910	-0.934171	-0.949098	-0.914420
(3,-1)	-0.906083	-0.732700	-0.865947	-0.922114	-0.920887	-0.815867	-0.835055	-0.839105	-0.807895
(3,-1)	-1.227695	-1.111054	-1.261084	-1.358066	-1.549650	-1.173021	-1.172660	-1.161491	-1.135394
(3,-1)	-1.227695	-1.111054	-1.261084	-1.358066	-1.549650	-1.173021	-1.172660	-1.161491	-1.135394
(3,-1)	-1.197645	-1.086463	-1.230743	-1.326594	-1.518071	-1.145325	-1.145467	-1.135585	-1.110724
(3,-1)	-1.197645	-1.086463	-1.230743	-1.326594	-1.518071	-1.145325	-1.145467	-1.135585	-1.110724
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.344058	0.164475	0.359302	0.355335	0.344662	0.347597	0.340714		
(3,-1)	-2.128618	-1.086425	-2.200307	-2.217072	-2.057998	-2.089230	-2.064929		
(3,-1)	-0.775361	-1.086425	-0.785707	-0.664036	-0.874434	-0.797579	-0.813819		
(3,-1)	-0.775361	-0.948064	-0.785707	-0.664036	-0.874434	-0.797579	-0.813819		
(3,-1)	-1.011474	-0.950151	-0.982690	-1.098304	-0.980144	-0.973806	-0.995218		
(3,-1)	-1.011474	-0.948064	-0.982690	-1.098304	-0.980144	-0.973806	-0.995218		
(3,-1)	-0.906083	-0.950151	-0.866196	-0.999062	-0.867424	-0.863579	-0.883296		
(3,-1)	-1.227695	-1.031532	-1.269450	-1.290119	-1.203183	-1.195727	-1.202497		
(3,-1)	-1.227695	-1.054657	-1.269450	-1.290119	-1.203183	-1.195727	-1.202498		
(3,-1)	-1.197645	-1.054657	-1.234887	-1.251610	-1.178105	-1.169232	-1.176402		
(3,-1)	-1.197645	-1.022693	-1.234887	-1.251610	-1.178105	-1.169232	-1.176402		

Table S348: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>5</sub>H<sub>5</sub>N system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.163805	0.162389	0.160749	0.163238	0.165401	0.157947	0.163373	0.168121	0.164350
(3,-1)	-1.212958	-1.101824	-1.164631	-1.133897	-1.197275	-1.098280	-1.121229	-1.033173	-0.986504
(3,-1)	-1.212958	-1.101824	-1.164631	-1.133897	-1.197275	-1.098280	-1.121229	-1.033173	-0.986504
(3,-1)	-1.028882	-0.891153	-0.950463	-0.913267	-0.968376	-0.885613	-0.903224	-0.960408	-0.997072
(3,-1)	-1.038816	-0.895939	-0.954034	-0.917637	-0.975181	-0.888286	-0.908073	-0.972385	-1.000739
(3,-1)	-1.028882	-0.891153	-0.950463	-0.913267	-0.968376	-0.885613	-0.903224	-0.960408	-0.997072
(3,-1)	-1.038816	-0.895939	-0.954034	-0.917637	-0.975181	-0.888286	-0.908073	-0.972385	-1.000739
(3,-1)	-1.210055	-1.106986	-1.149395	-1.113370	-1.163572	-1.003760	-1.127121	-1.018257	-0.921886
(3,-1)	-1.242018	-1.131907	-1.176825	-1.139686	-1.192339	-1.028538	-1.156373	-1.034154	-0.924414
(3,-1)	-1.242018	-1.131907	-1.176825	-1.139686	-1.192339	-1.028538	-1.156373	-1.034154	-0.924414
(3,-1)	-1.197135	-1.098844	-1.140314	-1.104407	-1.152042	-0.996029	-1.116858	-1.014309	-0.919874
(3,-1)	-1.197135	-1.098844	-1.140314	-1.104407	-1.152042	-0.996029	-1.116858	-1.014309	-0.919874
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.163805	-0.614495	0.169678	0.162693	0.165470	0.174335	0.164642	0.169165	0.156457
(3,-1)	-1.212958		-0.874258	-1.214054	-1.191066	-0.973596	-1.024095	-1.179832	-1.148909
(3,-1)	-1.212958		-0.874258	-1.214054	-1.191066	-0.973596	-1.024095	-1.179832	-1.148909
(3,-1)	-1.028882		-0.948969	-0.980729	-0.954904	-0.902145	-0.939185	-0.993620	-0.926114
(3,-1)	-1.038816		-0.950680	-0.986726	-0.962056	-0.924434	-0.956796	-1.002022	-0.931883
(3,-1)	-1.028882		-0.948969	-0.980729	-0.954904	-0.902145	-0.939185	-0.993620	-0.926114
(3,-1)	-1.038816		-0.950680	-0.986726	-0.962056	-0.924434	-0.956796	-1.002022	-0.931883
(3,-1)	-1.210055		-1.129354	-1.174885	-1.146963	-1.101244	-0.994528	-1.177275	-1.143531
(3,-1)	-1.242018		-1.167622	-1.203962	-1.175375	-1.127077	-1.013019	-1.208909	-1.176853
(3,-1)	-1.242018		-1.167622	-1.203962	-1.175375	-1.127077	-1.013019	-1.208909	-1.176853
(3,-1)	-1.197135		-1.112643	-1.163881	-1.135599	-1.090771	-0.988641	-1.163202	-1.129323
(3,-1)	-1.197135		-1.112643	-1.163881	-1.135599	-1.090771	-0.988641	-1.163202	-1.129323
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.163805	0.171087	0.171372	0.166858	0.168399	0.168338	0.167090	0.166860	0.165154
(3,-1)	-1.212958	-1.070848	-1.158219	-1.283180	-1.259379	-1.149695	-1.183169	-1.185887	-1.168535
(3,-1)	-1.212958	-1.070848	-1.158219	-1.283180	-1.259379	-1.149695	-1.183169	-1.185887	-1.168535
(3,-1)	-1.028882	-0.863887	-1.005229	-1.057155	-1.051060	-0.927286	-0.949184	-0.956813	-0.921048
(3,-1)	-1.038816	-0.872488	-1.016150	-1.065546	-1.049580	-0.936005	-0.957242	-0.964085	-0.927941
(3,-1)	-1.028882	-0.863887	-1.005229	-1.057155	-1.051060	-0.927286	-0.949184	-0.956813	-0.921048
(3,-1)	-1.038816	-0.872488	-1.016150	-1.065546	-1.049580	-0.936005	-0.957242	-0.964085	-0.927941
(3,-1)	-1.210055	-1.100693	-1.237232	-1.333474	-1.514046	-1.163418	-1.161198	-1.148576	-1.121863
(3,-1)	-1.242018	-1.131424	-1.264860	-1.361606	-1.531755	-1.194880	-1.192132	-1.178740	-1.151066
(3,-1)	-1.242018	-1.131424	-1.264860	-1.361606	-1.531755	-1.194880	-1.192132	-1.178740	-1.151066
(3,-1)	-1.197135	-1.088650	-1.226465	-1.320857	-1.506047	-1.147403	-1.146638	-1.135721	-1.110034
(3,-1)	-1.197135	-1.088650	-1.226465	-1.320857	-1.506047	-1.147403	-1.146638	-1.135721	-1.110034
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.163805	-0.613122	0.172715	0.169045	0.164028	0.166909	0.163516		
(3,-1)	-1.212958		-1.165036	-1.228057	-1.229720	-1.218737	-1.230815		
(3,-1)	-1.212958		-1.165036	-1.228057	-1.229720	-1.218737	-1.230815		
(3,-1)	-1.028882		-1.006779	-1.121276	-0.991154	-0.986385	-1.007660		
(3,-1)	-1.038816		-1.016849	-1.133460	-0.997269	-0.994346	-1.015143		
(3,-1)	-1.028882		-1.006779	-1.121276	-0.991154	-0.986385	-1.007660		
(3,-1)	-1.038816		-1.016849	-1.133460	-0.997269	-0.994346	-1.015143		
(3,-1)	-1.210055		-1.246802	-1.271716	-1.188087	-1.179986	-1.187276		
(3,-1)	-1.242018		-1.278198	-1.306743	-1.217770	-1.209859	-1.217541		
(3,-1)	-1.242018		-1.278198	-1.306743	-1.217770	-1.209859	-1.217541		
(3,-1)	-1.197135		-1.233702	-1.247056	-1.177586	-1.168404	-1.176589		
(3,-1)	-1.197135		-1.233702	-1.247056	-1.177586	-1.168404	-1.176589		



Table S349: Laplacian of the density value (a.u.) at the considered critical points for the SH<sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.674617	-0.625035	-0.647291	-0.627423	-0.654948	-0.609180	-0.623561	-0.630442	-0.558383
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.674617	-1.263132	-0.636033	-0.662709	-0.647004	-0.642389	-0.612122	-0.656992	-0.646389
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.674617	-0.610866	-0.697892	-0.742578	-0.849359	-0.651713	-0.653070	-0.646141	-0.636387
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.674617	-1.290093	-0.668370	-0.724122	-0.672577	-0.668266	-0.673679		

Table S350: Laplacian of the density value (a.u.) at the considered critical points for the  $C_2H_3^\bullet$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.337500	-1.197194	-1.264428	-1.219575	-1.270683	-1.223331	-1.236643	-1.226830	-1.358317
(3,-1)	-1.118487	-1.027771	-1.071675	-1.037612	-1.083962	-0.937156	-1.046687	-0.979285	-0.893635
(3,-1)	-1.163160	-1.070848	-1.117323	-1.080686	-1.128460	-0.975794	-1.091900	-1.002134	-0.916950
(3,-1)	-1.188136	-1.109004	-1.147313	-1.113385	-1.156406	-1.008090	-1.128318	-1.014822	-0.948601
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.337500	-0.584615	-1.253922	-1.295245	-1.264217	-1.205394	-1.217154	-1.301656	-1.220512
(3,-1)	-1.118487	-0.993341	-1.039831	-1.096275	-1.069805	-1.040042	-0.950227	-1.094861	-1.059510
(3,-1)	-1.163160	-0.992128	-1.088390	-1.141051	-1.112213	-1.074757	-0.974391	-1.141070	-1.103984
(3,-1)	-1.188136	-0.992128	-1.110654	-1.170079	-1.143673	-1.104601	-0.994101	-1.167631	-1.163708
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.337500	-1.262212	-1.332532	-1.405512	-1.405060	-1.205067	-1.246485	-1.279224	-1.228289
(3,-1)	-1.118487	-1.025128	-1.160288	-1.246618	-1.442126	-1.085611	-1.083082	-1.069481	-1.042926
(3,-1)	-1.163160	-1.067675	-1.202735	-1.295598	-1.483346	-1.127818	-1.125385	-1.112469	-1.084733
(3,-1)	-1.188136	-1.083784	-1.245634	-1.308818	-1.495730	-1.154394	-1.153003	-1.142037	-1.116262
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.337500	-0.600938	-1.322380	-1.471131	-1.310711	-1.300935	-1.315163		
(3,-1)	-1.118487	-0.966729	-1.155402	-1.182599	-1.110731	-1.104661	-1.111611		
(3,-1)	-1.163160	-0.966082	-1.205921	-1.224699	-1.156433	-1.148280	-1.156179		
(3,-1)	-1.188136	-0.966082	-1.279269	-1.246110	-1.186155	-1.180024	-1.186090		

Table S351: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>CO• system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.659186	-0.551675	-0.596781	-0.573212	-0.625039	-0.527120	-0.556273	-0.637152	-0.614573
(3,-1)	-1.126502	-1.038300	-1.085519	-1.048621	-1.094731	-0.958323	-1.060730	-0.976568	-0.879151
(3,-1)	-1.123733	-1.035876	-1.084314	-1.046242	-1.091226	-0.956344	-1.057839	-0.972765	-0.881085
(3,-1)	-1.123733	-1.035876	-1.084314	-1.046242	-1.091226	-0.956344	-1.057839	-0.972765	-0.881085
(3,-1)	0.256647	-0.126722	-0.080627	0.007106	0.135143	-0.262950	0.022065	0.420509	0.784164
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.659186	-0.132231	-0.630628	-0.626845	-0.612736	-0.597466	-0.615145	-0.651210	-0.593898
(3,-1)	-1.126502	-2.638031	-1.046876	-1.107147	-1.077729	-1.044548	-0.949292	-1.103614	-1.069189
(3,-1)	-1.123733	-1.068820	-1.047987	-1.104181	-1.073304	-1.036817	-0.944100	-1.098962	-1.064962
(3,-1)	-1.123733	-1.121934	-1.047987	-1.104181	-1.073304	-1.036817	-0.944100	-1.098962	-1.064962
(3,-1)	0.256647	0.853028	-0.007780	0.097918	0.143947	-0.006708	0.327520	0.131609	
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.659186	-0.531771	-0.624214	-0.650330	-0.593771	-0.622363	-0.621992	-0.607563	-0.589057
(3,-1)	-1.126502	-1.034986	-1.166225	-1.256357	-1.440627	-1.092283	-1.090121	-1.077158	-1.054337
(3,-1)	-1.123733	-1.031405	-1.163163	-1.251980	-1.441983	-1.087200	-1.085543	-1.073194	-1.049019
(3,-1)	-1.123733	-1.031405	-1.163163	-1.251980	-1.441983	-1.087200	-1.085543	-1.073194	-1.049019
(3,-1)	0.256647	0.428330	0.252835	-0.000109	0.169740	0.149128	0.095902	0.096602	-0.104703
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.659186	-0.224276	-0.586389	-0.767034	-0.639266	-0.643083	-0.655555		
(3,-1)	-1.126502	-2.677292	-1.160029	-1.193148	-1.120882	-1.110407	-1.118618		
(3,-1)	-1.123733	-1.025808	-1.153230	-1.182373	-1.118496	-1.106094	-1.115793		
(3,-1)	-1.123733	-1.068950	-1.153230	-1.182373	-1.118496	-1.106094	-1.115793		
(3,-1)	0.256647		-0.015799	0.311174	0.102472	0.217622	0.207430		

Table S352: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>2</sub>COH• system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.420914	-0.534845	-0.559166	-0.509766	-0.398079	-0.578866	-0.448822	-0.267286	0.009773
(3,-1)	-2.736144	-2.690505	-2.650580	-2.641988	-2.714387	-2.477866	-2.712264	-2.717856	-2.802739
(3,-1)	-1.180331	-1.088377	-1.132477	-1.097207	-1.143380	-0.996608	-1.113665	-1.004957	-0.914423
(3,-1)	-1.232362	-1.139585	-1.186291	-1.148830	-1.195875	-1.042460	-1.168531	-1.041586	-0.955553
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.420914	-0.389472	-0.003050	-0.510620	-0.442569	-0.289277	-0.431304	-0.292497	-0.470846
(3,-1)	-2.736144	-0.970823	-2.563125	-2.719279	-2.720654	-2.696892	-2.606087	-2.833446	-2.430712
(3,-1)	-1.180331	-1.030006	-1.101283	-1.155595	-1.128038	-1.101350	-0.987626	-1.152706	-1.149602
(3,-1)	-1.232362	-1.030006	-1.165370	-1.209099	-1.179515	-1.148160	-1.024825	-1.206407	-1.204721
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.420914	-0.370393	-0.399447	-0.490999	-0.478106	-0.380087	-0.422192	-0.437704	-0.472145
(3,-1)	-2.736144	-2.689333	-2.631107	-2.735184	-2.789119	-2.796353	-2.788938	-2.771298	-2.705084
(3,-1)	-1.180331	-1.079196	-1.224507	-1.295619	-1.467586	-1.143825	-1.140016	-1.126288	-1.103135
(3,-1)	-1.232362	-1.129437	-1.280258	-1.350536	-1.520867	-1.196765	-1.193204	-1.179546	-1.155163
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.420914	-0.503690	-0.419385	-0.199558	-0.470649	-0.379198	-0.374447		
(3,-1)	-2.736144	-0.942517	-3.001733	-2.927262	-2.739141	-2.770592	-2.743457		
(3,-1)	-1.180331	-0.992913	-1.242340	-1.242417	-1.173533	-1.165104	-1.172827		
(3,-1)	-1.232362	-0.992913	-1.302807	-1.295074	-1.227327	-1.217374	-1.226044		

Table S353: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>O• system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.683464	-0.740294	-0.781589	-0.748901	-0.696171	-0.776057	-0.725750	-0.555610	-0.306888
(3,-1)	-1.097732	-0.989269	-1.042818	-1.006361	-1.059341	-0.927834	-1.024595	-0.947262	-0.851434
(3,-1)	-1.165059	-1.067369	-1.118551	-1.080042	-1.129418	-0.995375	-1.095146	-0.993842	-0.873739
(3,-1)	-1.165059	-1.067369	-1.118551	-1.080042	-1.129418	-0.995375	-1.095146	-0.993842	-0.873739
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.683464	-0.608569	-0.278467	-0.763031	-0.704207	-0.529002	-0.628113	-0.590383	-0.711936
(3,-1)	-1.097732	-0.394791	-1.022561	-1.070911	-1.043439	-1.013320	-0.920138	-1.071015	-1.037511
(3,-1)	-1.165059	-1.013603	-1.095867	-1.142021	-1.111455	-1.075356	-0.970208	-1.141275	-1.110276
(3,-1)	-1.165059	-1.013603	-1.095867	-1.142021	-1.111455	-1.075356	-0.970208	-1.141275	-1.110276
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.683464	-0.629672	-0.629868	-0.711108	-0.695295	-0.635852	-0.683578	-0.709850	-0.728755
(3,-1)	-1.097732	-1.006968	-1.127495	-1.214524	-1.389362	-1.063564	-1.059568	-1.044120	-1.022989
(3,-1)	-1.165059	-1.075100	-1.196246	-1.290554	-1.458461	-1.129808	-1.126673	-1.112315	-1.089415
(3,-1)	-1.165059	-1.075100	-1.196246	-1.290554	-1.458461	-1.129808	-1.126673	-1.112315	-1.089415
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.683464	-0.613638	-0.619173	-0.383955	-0.737611	-0.641913	-0.660361		
(3,-1)	-1.097732	-0.504038	-1.115387	-1.175821	-1.088624	-1.082275	-1.090445		
(3,-1)	-1.165059	-0.978885	-1.187728	-1.233550	-1.159009	-1.148409	-1.159142		
(3,-1)	-1.165059	-0.978885	-1.187728	-1.233550	-1.159009	-1.148409	-1.159143		

Table S354: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>CH<sub>2</sub>O• system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.646651	-0.514371	-0.621086	-0.594511	-0.646540	-0.497789	-0.576062	-0.664470	-0.632369
(3,-1)	-0.599357	-0.735279	-0.772936	-0.745667	-0.695008	-0.767868	-0.722742	-0.565142	-0.321048
(3,-1)	-1.179391	-1.070320	-1.086618	-1.050550	-1.104261	-0.986636	-1.068967	-0.979357	-0.869051
(3,-1)	-1.179391	-1.070320	-1.086618	-1.050550	-1.104261	-0.986636	-1.068967	-0.979357	-0.869051
(3,-1)	-1.123747	-1.028029	-1.059125	-1.023196	-1.068372	-0.945697	-1.032722	-0.965805	-0.859920
(3,-1)	-1.146435	-1.057268	-1.084361	-1.047429	-1.091972	-0.968123	-1.057305	-0.977011	-0.872553
(3,-1)	-1.146435	-1.057268	-1.084361	-1.047429	-1.091972	-0.968123	-1.057305	-0.977011	-0.872553
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.646651	-0.342745	-0.653337	-0.648842	-0.631226	-0.623982	-0.642667	-0.623731	-0.614456
(3,-1)	-0.599357	-0.966560	-0.282068	-0.756503	-0.703801	-0.536123	-0.631010	-0.591723	-0.705958
(3,-1)	-1.179391	-1.015198	-1.070126	-1.115476	-1.088286	-1.053170	-0.955465	-1.143660	-1.084244
(3,-1)	-1.179391	-1.015198	-1.070126	-1.115476	-1.088286	-1.053170	-0.955465	-1.143660	-1.084244
(3,-1)	-1.123747		-1.020856	-1.079517	-1.050941	-1.019449	-0.937886	-1.089350	-1.040066
(3,-1)	-1.146435		-1.047698	-1.103711	-1.073934	-1.038136	-0.949422	-1.113330	-1.065416
(3,-1)	-1.146435		-1.047698	-1.103711	-1.073934	-1.038136	-0.949422	-1.113330	-1.065416
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.646651	-0.547311	-0.650930	-0.675902	-0.623907	-0.641656	-0.641656	-0.580555	-0.608350
(3,-1)	-0.599357	-0.630129	-0.623606	-0.701041	-0.673122	-0.635126	-0.681805	-0.706047	-0.726607
(3,-1)	-1.179391	-1.051639	-1.173676	-1.264950	-1.438419	-1.108511	-1.104887	-1.114812	-1.067434
(3,-1)	-1.179391	-1.051639	-1.173676	-1.264950	-1.438419	-1.108511	-1.104887	-1.114812	-1.067434
(3,-1)	-1.123747	-1.017264	-1.137645	-1.222994	-1.411595	-1.061486	-1.060327	-1.064542	-1.026695
(3,-1)	-1.146435	-1.037197	-1.161413	-1.249174	-1.434817	-1.086072	-1.084656	-1.087920	-1.049319
(3,-1)	-1.146435	-1.037197	-1.161413	-1.249174	-1.434817	-1.086072	-1.084656	-1.087920	-1.049319
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.646651	-0.341849	-0.625334	-0.776351	-0.660006	-0.659688	-0.676586		
(3,-1)	-0.599357	-0.942189	-0.613968	-0.375613	-0.733290	-0.644023	-0.658008		
(3,-1)	-1.179391	-0.984415	-1.169164	-1.218545	-1.133413	-1.127027	-1.135227		
(3,-1)	-1.179391	-0.984415	-1.169164	-1.218545	-1.133413	-1.127027	-1.135227		
(3,-1)	-1.123747		-1.109716	-1.160036	-1.094537	-1.083968	-1.092347		
(3,-1)	-1.146435		-1.142508	-1.181857	-1.118578	-1.106782	-1.116210		
(3,-1)	-1.146435		-1.142508	-1.181857	-1.118578	-1.106782	-1.116211		

Table S355: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>S<sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.352568	-0.280283	-0.308576	-0.296710	-0.331011	-0.265836	-0.275041	-0.289104	-0.354246
(3,-1)	-1.097675	-1.004677	-1.051853	-1.017163	-1.063649	-0.922769	-1.027457	-0.958819	-0.868759
(3,-1)	-1.149144	-1.059763	-1.106879	-1.070483	-1.117529	-0.971632	-1.082684	-0.996092	-0.892739
(3,-1)	-1.149144	-1.059763	-1.106879	-1.070483	-1.117529	-0.971632	-1.082684	-0.996092	-0.892739
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.352568	-0.663881	-0.377463	-0.329735	-0.323627	-0.233237	-0.268910	-0.348613	-0.325950
(3,-1)	-1.097675	-0.934970	-1.019289	-1.074074	-1.046904	-1.018712	-0.928649	-1.071666	-1.036692
(3,-1)	-1.149144	-0.982538	-1.075340	-1.128078	-1.099146	-1.066373	-0.967326	-1.126524	-1.091744
(3,-1)	-1.149144	-0.982538	-1.075340	-1.128078	-1.099146	-1.066373	-0.967326	-1.126524	-1.091744
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.352568	-0.243194	-0.311628	-0.345006	-0.339925	-0.338952	-0.335983	-0.321851	-0.312234
(3,-1)	-1.097675	-1.002511	-1.134780	-1.219982	-1.407718	-1.063175	-1.059245	-1.045406	-1.021263
(3,-1)	-1.149144	-1.056173	-1.188380	-1.280129	-1.464545	-1.115138	-1.112209	-1.098962	-1.073704
(3,-1)	-1.149144	-1.056173	-1.188380	-1.280129	-1.464545	-1.115138	-1.112209	-1.098962	-1.073704
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.352568	-0.688193	-0.291229	-0.423730	-0.338538	-0.343401	-0.353971		
(3,-1)	-1.097675	-0.913364	-1.116630	-1.161119	-1.089612	-1.080802	-1.088958		
(3,-1)	-1.149144	-0.953579	-1.175802	-1.212342	-1.143503	-1.133121	-1.142560		
(3,-1)	-1.149144	-0.953579	-1.175802	-1.212342	-1.143503	-1.133121	-1.142560		

Table S356: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>2</sub>H<sub>5</sub><sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.729342	-0.623012	-0.675875	-0.648133	-0.697783	-0.602371	-0.631590	-0.687365	-0.688294
(3,-1)	-1.061072	-0.970270	-1.016573	-0.983150	-1.026108	-0.895281	-0.991073	-0.936288	-0.838492
(3,-1)	-1.109776	-1.021861	-1.069247	-1.033008	-1.077248	-0.943495	-1.041631	-0.968416	-0.864840
(3,-1)	-1.109776	-1.021861	-1.069247	-1.033008	-1.077248	-0.943495	-1.041631	-0.968416	-0.864840
(3,-1)	-1.164793	-1.085701	-1.127060	-1.092866	-1.134489	-0.985304	-1.106172	-1.002587	-0.931391
(3,-1)	-1.164793	-1.085701	-1.127060	-1.092866	-1.134489	-0.985304	-1.106172	-1.002587	-0.931391
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.729342	-0.667308	-0.703984	-0.702471	-0.683959	-0.645951	-0.667347	-0.719946	-0.678287
(3,-1)	-1.061072	-0.667308	-0.980505	-1.037369	-1.011049	-0.985989	-0.907336	-1.033645	-0.997007
(3,-1)	-1.109776	-1.046599	-1.033883	-1.088691	-1.059564	-1.026834	-0.939475	-1.084835	-1.049245
(3,-1)	-1.109776	-0.987006	-1.033883	-1.088691	-1.059564	-1.026834	-0.939475	-1.084835	-1.049245
(3,-1)	-1.164793	-0.987006	-1.093818	-1.145382	-1.117689	-1.089672	-0.981053	-1.139856	-1.140543
(3,-1)	-1.164793	-0.925917	-1.093818	-1.145382	-1.117689	-1.089672	-0.981053	-1.139856	-1.140543
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.729342	-0.593775	-0.714492	-0.746537	-0.748658	-0.688044	-0.691678	-0.681350	-0.657816
(3,-1)	-1.061072	-0.973918	-1.092653	-1.173452	-1.359942	-1.024079	-1.021214	-1.008699	-0.985904
(3,-1)	-1.109776	-1.023422	-1.144372	-1.231847	-1.415452	-1.071869	-1.070038	-1.058294	-1.034146
(3,-1)	-1.109776	-1.023422	-1.144372	-1.231847	-1.415452	-1.071869	-1.070038	-1.058294	-1.034146
(3,-1)	-1.164793	-1.068181	-1.214312	-1.284216	-1.470394	-1.133698	-1.129232	-1.116322	-1.091985
(3,-1)	-1.164793	-1.068181	-1.214312	-1.284216	-1.470394	-1.133698	-1.129232	-1.116322	-1.091985
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.729342	-0.689260	-0.685878	-0.827067	-0.715996	-0.714958	-0.731977		
(3,-1)	-1.061072	-0.689260	-1.063385	-1.119826	-1.052995	-1.044160	-1.052148		
(3,-1)	-1.109776	-1.011377	-1.122357	-1.167265	-1.103858	-1.092550	-1.101928		
(3,-1)	-1.109776	-0.957589	-1.122357	-1.167265	-1.103858	-1.092550	-1.101928		
(3,-1)	-1.164793	-0.957589	-1.231368	-1.211830	-1.161585	-1.150669	-1.159470		
(3,-1)	-1.164793	-0.905390	-1.231368	-1.211830	-1.161585	-1.150669	-1.159470		



Table S357: Laplacian of the density value (a.u.) at the considered critical points for the  $(\text{CH}_3)_2\text{CH}^\bullet$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.749477	-0.625419	-0.676896	-0.649933	-0.700324	-0.604939	-0.632470	-0.692768	-0.690748
(3,-1)	-0.749477	-0.625419	-0.676896	-0.649933	-0.700324	-0.604939	-0.632470	-0.692768	-0.690748
(3,-1)	-1.158098	-1.069848	-1.108187	-1.076233	-1.118263	-0.971843	-1.088638	-0.992451	-0.911150
(3,-1)	-1.120623	-1.024371	-1.071291	-1.035155	-1.079578	-0.944160	-1.044198	-0.970196	-0.865498
(3,-1)	-1.120623	-1.024371	-1.071291	-1.035155	-1.079578	-0.944160	-1.044198	-0.970196	-0.865498
(3,-1)	-1.059057	-0.961816	-1.006849	-0.973910	-1.016994	-0.889241	-0.980717	-0.930005	-0.831163
(3,-1)	-1.100879	-1.003642	-1.050923	-1.015600	-1.059758	-0.931139	-1.023675	-0.956271	-0.852485
(3,-1)	-1.100879	-1.003642	-1.050923	-1.015600	-1.059758	-0.931139	-1.023675	-0.956271	-0.852485
(3,-1)	-1.059057	-0.961816	-1.006849	-0.973910	-1.016994	-0.889241	-0.980717	-0.930005	-0.831163
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.749477	-1.285328	-0.706953	-0.704146	-0.686407	-0.647550	-0.672604	-0.721758	-0.679510
(3,-1)	-0.749477	-1.285328	-0.706953	-0.704146	-0.686407	-0.647550	-0.672604	-0.721758	-0.679510
(3,-1)	-1.158098		-1.073098	-1.127447	-1.101951	-1.073934	-0.971596	-1.122511	-1.119750
(3,-1)	-1.120623		-1.036388	-1.090740	-1.061723	-1.027845	-0.942315	-1.087276	-1.051494
(3,-1)	-1.120623		-1.036388	-1.090740	-1.061723	-1.027845	-0.942315	-1.087276	-1.051494
(3,-1)	-1.059057		-0.968992	-1.027333	-1.001389	-0.978645	-0.901818	-1.024310	-0.986597
(3,-1)	-1.100879		-1.014331	-1.070535	-1.042310	-1.012195	-0.927825	-1.066737	-1.030238
(3,-1)	-1.100879		-1.014331	-1.070535	-1.042310	-1.012195	-0.927825	-1.066737	-1.030238
(3,-1)	-1.059057		-0.968992	-1.027333	-1.001389	-0.978645	-0.901818	-1.024310	-0.986597
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.749477	-0.592615	-0.714188	-0.747182	-0.744447	-0.691462	-0.694588	-0.683518	-0.660105
(3,-1)	-0.749477	-0.592615	-0.714188	-0.747182	-0.744447	-0.691462	-0.694588	-0.683518	-0.660105
(3,-1)	-1.158098	-1.051611	-1.192909	-1.264848	-1.449383	-1.116677	-1.112440	-1.099924	-1.076547
(3,-1)	-1.120623	-1.025375	-1.147091	-1.234667	-1.418091	-1.073644	-1.072043	-1.060931	-1.036498
(3,-1)	-1.120623	-1.025375	-1.147091	-1.234667	-1.418091	-1.073644	-1.072043	-1.060931	-1.036498
(3,-1)	-1.059057	-0.964922	-1.082614	-1.162986	-1.347660	-1.014595	-1.011811	-0.999427	-0.976816
(3,-1)	-1.100879	-1.006025	-1.125665	-1.211898	-1.395899	-1.053958	-1.052007	-1.040445	-1.017051
(3,-1)	-1.100879	-1.006025	-1.125665	-1.211898	-1.395899	-1.053958	-1.052007	-1.040445	-1.017051
(3,-1)	-1.059057	-0.964922	-1.082614	-1.162986	-1.347660	-1.014595	-1.011811	-0.999427	-0.976816
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.749477	-1.265086	-0.687007	-0.829696	-0.716484	-0.716074	-0.732502		
(3,-1)	-0.749477	-1.265086	-0.687007	-0.829696	-0.716484	-0.716074	-0.732502		
(3,-1)	-1.158098		-1.207291	-1.194393	-1.143200	-1.134149	-1.141454		
(3,-1)	-1.120623		-1.127083	-1.168926	-1.105490	-1.094246	-1.103550		
(3,-1)	-1.120623		-1.127083	-1.168926	-1.105490	-1.094246	-1.103551		
(3,-1)	-1.059057		-1.051226	-1.108027	-1.042489	-1.033773	-1.041578		
(3,-1)	-1.100879		-1.100064	-1.149429	-1.085525	-1.074862	-1.083720		
(3,-1)	-1.100879		-1.100064	-1.149429	-1.085525	-1.074862	-1.083720		
(3,-1)	-1.059057		-1.051226	-1.108027	-1.042489	-1.033773	-1.041579		

Table S358: Laplacian of the density value (a.u.) at the considered critical points for the NO<sub>2</sub><sup>•</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.262060	-1.147941	-1.182859	-1.164749	-1.252774	-1.026907	-1.094311	-1.031148	-1.226796
(3,-1)	-1.262060	-1.147941	-1.182859	-1.164749	-1.252774	-1.026907	-1.094311	-1.031148	-1.226796
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.262060		-1.282740	-1.240695	-1.237066	-0.850117	-0.942352	-1.315467	-1.109638
(3,-1)	-1.262060		-1.282740	-1.240695	-1.237066	-0.850117	-0.942352	-1.315467	-1.109638
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.262060	-1.005502	-1.255957	-1.398623	-1.703100	-1.212924	-1.220485	-1.195605	-1.132355
(3,-1)	-1.262060	-1.005502	-1.255957	-1.398623	-1.703100	-1.212924	-1.220485	-1.195605	-1.132355
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.262060		-1.209712	-1.454913	-1.237572	-1.258900	-1.296593		
(3,-1)	-1.262060		-1.209712	-1.454913	-1.237572	-1.258900	-1.296593		

Table S359: Laplacian of the density value (a.u.) at the considered critical points for the  $[\text{HON}_2]^\ddagger$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.059229	-0.997330	-1.016118	-1.003626	-1.078477	-0.896230	-0.927233	-0.872871	-1.020488
(3,-1)	-0.023372	-0.058131	-0.027095	-0.035953	-0.040579	-0.038169	-0.025767	-0.020769	-0.086549
(3,-1)	-2.071489	-1.932627	-1.998148	-1.942830	-2.010126	-1.911101	-1.942103	-1.645444	-2.112391
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.059229	-1.096173	-1.080999	-1.064350	-1.062799	-0.708642	-0.797587	-1.110467	-0.947181
(3,-1)	-0.023372	-0.064013	-0.041403	-0.035196	-0.041062	-0.033299	-0.026740	-0.035687	-0.019463
(3,-1)	-2.071489	-1.915964	-1.978750	-2.037697	-2.000443	-1.625781	-1.635481	-2.060742	-1.818447
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.059229	-0.814901	-1.062452	-1.181187	-1.450011	-1.041058	-1.042414	-1.011885	-0.979082
(3,-1)	-0.023372	-0.028545	-0.011363	-0.036295	0.000610	-0.031843	-0.037603	-0.039846	-0.053693
(3,-1)	-2.071489	-1.874302	-2.090986	-2.377990	-2.687781	-1.884528	-1.963810	-2.024679	-1.916801
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.059229	-1.070849	-1.014941	-1.242778	-1.027688	-1.035128	-1.045495		
(3,-1)	-0.023372	-0.028451	-0.029141	-0.007301	-0.013443	-0.017794	-0.002840		
(3,-1)	-2.071489	-1.983474	-2.101058	-2.304392	-2.022621	-2.002168	-2.035950		

Table S360: Laplacian of the density value (a.u.) at the considered critical points for the [HCiH]<sup>‡</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.229909	-0.237232	-0.225042	-0.228534	-0.236719	-0.182990	-0.228727	-0.232757	-0.294585
(3,-1)	-0.229909	-0.237232	-0.225042	-0.228534	-0.236719	-0.182990	-0.228727	-0.232757	-0.294585
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.229909	-0.246704	-0.260543	-0.232850	-0.235670	-0.195882	-0.192817	-0.239530	-0.215361
(3,-1)	-0.229909	-0.246704	-0.260543	-0.232850	-0.235670	-0.195882	-0.192817	-0.239530	-0.215361
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.229909	-0.208041	-0.191956	-0.214505	-0.196652	-0.259503	-0.250315	-0.241048	-0.230714
(3,-1)	-0.229909	-0.208041	-0.191956	-0.214505	-0.196652	-0.259503	-0.250315	-0.241048	-0.230714
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.229909	-0.251658	-0.192851	-0.237010	-0.236304	-0.241538	-0.241362		
(3,-1)	-0.229909	-0.251658	-0.192851	-0.237010	-0.236304	-0.241538	-0.241362		

Table S361: Laplacian of the density value (a.u.) at the considered critical points for the  $[\text{ClFCH}_3]^\ddagger$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.102830	0.182428	0.185839	0.173871	0.150818	0.167180	0.193352	0.173270	0.143733
(3,-1)	0.143616	0.131130	0.135772	0.135060	0.131454	0.131731	0.133911	0.145345	0.156796
(3,-1)	-1.237168	-1.179092	-1.225724	-1.184840	-1.232717	-1.086369	-1.208356	-1.060660	-0.990805
(3,-1)	-1.237280	-1.179200	-1.225840	-1.184949	-1.232829	-1.086477	-1.208729	-1.060804	-0.990934
(3,-1)	-1.237289	-1.179215	-1.225852	-1.184958	-1.232838	-1.086496	-1.208918	-1.060807	-0.990993
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.102830	0.142662	0.124751	0.159657	0.141222	0.141757	0.151430	0.123755	0.157146
(3,-1)	0.143616	0.144425	0.148119	0.133403	0.132824	0.138286	0.145530	0.130345	0.141643
(3,-1)	-1.237168	-1.145272	-1.207078	-1.244889	-1.209815	-1.171573	-1.038639	-1.240631	-1.230204
(3,-1)	-1.237280	-1.145359	-1.207156	-1.245003	-1.209922	-1.171768	-1.038809	-1.240736	-1.230319
(3,-1)	-1.237289	-1.145366	-1.207125	-1.245013	-1.209930	-1.171764	-1.038810	-1.240742	-1.230331
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.102830	0.145825	0.119018	0.125288	0.127017	0.127180	0.132576	0.143903	0.143732
(3,-1)	0.143616	0.135253	0.140731	0.131373	0.130549	0.134777	0.134409	0.133370	0.131320
(3,-1)	-1.237168	-1.158043	-1.311047	-1.393758	-1.570973	-1.221167	-1.219104	-1.209385	-1.186392
(3,-1)	-1.237280	-1.157988	-1.311279	-1.393871	-1.570963	-1.221375	-1.219344	-1.209716	-1.186482
(3,-1)	-1.237289	-1.157856	-1.311279	-1.393890	-1.570995	-1.221457	-1.219447	-1.209881	-1.186481
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.102830	0.128908	0.125305	0.114185	0.135478	0.097224	0.089162		
(3,-1)	0.143616	0.148529	0.132511	0.147536	0.133928	0.132823	0.134485		
(3,-1)	-1.237168	-1.089680	-1.329062	-1.276385	-1.258140	-1.241279	-1.249824		
(3,-1)	-1.237280	-1.089768	-1.329054	-1.276490	-1.258253	-1.241388	-1.249964		
(3,-1)	-1.237289	-1.089785	-1.329139	-1.276496	-1.258262	-1.241397	-1.249869		

Table S362: Laplacian of the density value (a.u.) at the considered critical points for the  $[\text{ClCH}_3\text{Cl}]^{-\ddagger}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.076662	0.077739	0.080041	0.077373	0.076776	0.070219	0.077164	0.093076	0.086999
(3,-1)	-1.381180	-1.238353	-1.296915	-1.254300	-1.325406	-1.145543	-1.282018	-1.128935	-1.024620
(3,-1)	-1.381314	-1.238471	-1.297040	-1.254420	-1.325536	-1.145668	-1.282686	-1.129065	-1.024737
(3,-1)	-1.381078	-1.238264	-1.296820	-1.254208	-1.325312	-1.145432	-1.282465	-1.128884	-1.024584
(3,-1)	0.076639	0.077734	0.080035	0.077366	0.076763	0.070220	0.077153	0.093068	0.086942
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.076662	0.088902	0.083291	0.078336	0.075463	0.079768	0.079716	0.074562	0.085164
(3,-1)	-1.381180	-1.217286	-1.311349	-1.336702	-1.306035	-1.253418	-1.112426	-1.350481	-1.328283
(3,-1)	-1.381314	-1.217382	-1.311471	-1.336831	-1.306162	-1.253605	-1.112586	-1.350606	-1.328414
(3,-1)	-1.381078	-1.217196	-1.311259	-1.336604	-1.305940	-1.253398	-1.112403	-1.350385	-1.328192
(3,-1)	0.076639	0.088882	0.083273	0.078325	0.075450	0.079733	0.079693	0.074542	0.085154
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.076662	0.075098	0.071234	0.067895	0.068828	0.078829	0.077428	0.076526	0.071398
(3,-1)	-1.381180	-1.264762	-1.420186	-1.517634	-1.715750	-1.351756	-1.343337	-1.321466	-1.280087
(3,-1)	-1.381314	-1.264475	-1.420433	-1.517710	-1.715518	-1.352143	-1.343791	-1.322117	-1.280169
(3,-1)	-1.381078	-1.264271	-1.420185	-1.517451	-1.715198	-1.351920	-1.343565	-1.321891	-1.279953
(3,-1)	0.076639	0.075081	0.071223	0.067884	0.068835	0.078805	0.077407	0.076509	0.071381
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.076662	0.079582	0.068413	0.083310	0.077248	0.074890	0.073436		
(3,-1)	-1.381180	-1.168557	-1.436846	-1.489998	-1.358873	-1.356272	-1.367633		
(3,-1)	-1.381314	-1.168653	-1.436829	-1.490152	-1.359004	-1.356402	-1.367725		
(3,-1)	-1.381078	-1.168478	-1.436568	-1.489880	-1.358774	-1.356172	-1.367492		
(3,-1)	0.076639	0.079563	0.068391	0.083288	0.077234	0.074872	0.073416		

Table S363: Laplacian of the density value (a.u.) at the considered critical points for the  $[\text{FCH}_3\text{Cl}]^{-\ddagger}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.163224	0.154432	0.156719	0.153946	0.156903	0.144483	0.156558	0.166829	0.196394
(3,-1)	-1.374308	-1.234892	-1.295047	-1.251032	-1.321297	-1.138462	-1.280247	-1.128064	-1.016409
(3,-1)	-1.374308	-1.234892	-1.295047	-1.251032	-1.321297	-1.138468	-1.280246	-1.128077	-1.016417
(3,-1)	0.025736	0.048275	0.048549	0.045625	0.036948	0.051056	0.038640	0.037751	0.024894
(3,-1)	-1.374308	-1.234892	-1.295047	-1.251032	-1.321297	-1.138468	-1.280246	-1.128077	-1.016417
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.163224	0.171061	0.162548	0.158511	0.156204	0.171508	0.162853	0.160964	0.162859
(3,-1)	-1.374308	-1.212278	-1.304846	-1.333494	-1.301348	-1.249493	-1.112988	-1.345670	-1.322856
(3,-1)	-1.374308	-1.212270	-1.304844	-1.333494	-1.301348	-1.249538	-1.113017	-1.345668	-1.322857
(3,-1)	0.025736	0.028282	0.028119	0.040450	0.035993	0.018847	0.024892	0.027321	0.043111
(3,-1)	-1.374308	-1.212270	-1.304844	-1.333494	-1.301348	-1.249538	-1.113017	-1.345668	-1.322857
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.163224	0.161109	0.162273	0.164428	0.153343	0.161297	0.160937	0.160190	0.155617
(3,-1)	-1.374308	-1.264067	-1.414278	-1.512244	-1.700441	-1.339983	-1.333350	-1.313939	-1.276734
(3,-1)	-1.374308	-1.264051	-1.414350	-1.512253	-1.700437	-1.339981	-1.333349	-1.313939	-1.276735
(3,-1)	0.025736	0.032423	0.043197	0.044009	0.071458	0.021895	0.026411	0.030009	0.031744
(3,-1)	-1.374308	-1.264051	-1.414350	-1.512253	-1.700437	-1.339981	-1.333349	-1.313939	-1.276735
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.163224	0.168683	0.168315	0.175179	0.158028	0.158316	0.156122		
(3,-1)	-1.374308	-1.166145	-1.424948	-1.475756	-1.354827	-1.350263	-1.359940		
(3,-1)	-1.374308	-1.166141	-1.424871	-1.475756	-1.354826	-1.350263	-1.360118		
(3,-1)	0.025736	0.032074	0.037609	0.026979	0.036141	0.029537	0.029410		
(3,-1)	-1.374308	-1.166141	-1.424871	-1.475756	-1.354826	-1.350263	-1.360117		

Table S364: Laplacian of the density value (a.u.) at the considered critical points for the  $[\text{HOCH}_3\text{F}]^{-\ddagger}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.116095	0.136238	0.138493	0.132715	0.124371	0.125696	0.132746	0.146352	0.136855
(3,-1)	-1.375569	-1.234624	-1.297202	-1.251627	-1.321943	-1.143324	-1.282431	-1.127136	-1.002280
(3,-1)	-1.369605	-1.226687	-1.289641	-1.244330	-1.314610	-1.137959	-1.273840	-1.123998	-0.998086
(3,-1)	-1.370152	-1.227264	-1.290216	-1.244887	-1.315159	-1.138473	-1.274368	-1.124360	-0.998511
(3,-1)	0.123676	0.123794	0.126898	0.122783	0.122859	0.114155	0.122290	0.141269	0.161309
(3,-1)	-2.467996	-2.477610	-2.412355	-2.415762	-2.469339	-2.234207	-2.460620	-2.469250	-2.548848
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.116095	0.131794	0.121377	0.130997	0.123343	0.124863	0.137678	0.118872	0.132171
(3,-1)	-1.375569	-1.215744	-1.306684	-1.335171	-1.301533	-1.250064	-1.116054	-1.346775	-1.326703
(3,-1)	-1.369605	-1.206038	-1.294343	-1.327609	-1.294269	-1.243565	-1.111927	-1.338537	-1.317166
(3,-1)	-1.370152	-1.206557	-1.294991	-1.328178	-1.294819	-1.244065	-1.112306	-1.339110	-1.317751
(3,-1)	0.123676	0.141080	0.129014	0.125789	0.121468	0.130977	0.131725	0.121259	0.132794
(3,-1)	-2.467996	-2.307894	-2.302694	-2.466058	-2.475121	-2.387630	-2.304845	-2.524128	-2.185312
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.116095	0.115748	0.108352	0.105330	0.104291	0.112536	0.118470	0.122711	0.121644
(3,-1)	-1.375569	-1.271671	-1.410059	-1.510000	-1.688659	-1.338380	-1.332290	-1.313816	-1.279355
(3,-1)	-1.369605	-1.265517	-1.402445	-1.503997	-1.684824	-1.330222	-1.324132	-1.305628	-1.270829
(3,-1)	-1.370152	-1.266037	-1.403039	-1.504564	-1.685441	-1.330766	-1.324673	-1.306145	-1.271386
(3,-1)	0.123676	0.117641	0.112139	0.111697	0.105343	0.122909	0.123050	0.122666	0.117670
(3,-1)	-2.467996	-2.381526	-2.469562	-2.516584	-2.727839	-2.521454	-2.505872	-2.485069	-2.427195
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.116095	0.121610	0.102838	0.132024	0.126298	0.118375	0.117281		
(3,-1)	-1.375569	-1.166834	-1.414846	-1.479587	-1.354850	-1.349388	-1.358463		
(3,-1)	-1.369605	-1.159683	-1.404040	-1.472415	-1.347961	-1.342671	-1.351970		
(3,-1)	-1.370152	-1.160158	-1.404730	-1.472974	-1.348536	-1.343230	-1.352532		
(3,-1)	0.123676	0.128988	0.111288	0.138698	0.124103	0.121271	0.119818		
(3,-1)	-2.467996	-2.361373	-2.701920	-2.609093	-2.487376	-2.516156	-2.491130		



Table S365: Laplacian of the density value (a.u.) at the considered critical points for the  $[\text{HN}_2]^\ddagger$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-2.609460	-2.413866	-2.507528	-2.439490	-2.528049	-2.368289	-2.453311	-2.177777	-2.538453
(3,-1)	-0.072300	-0.115385	-0.089736	-0.098186	-0.102094	-0.100840	-0.096911	-0.093587	-0.144849
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-2.609460	-2.378474	-2.403447	-2.561449	-2.515956	-2.150371	-2.146876	-2.588594	-2.276924
(3,-1)	-0.072300	-0.132073	-0.124993	-0.095634	-0.101599	-0.076149	-0.081564	-0.098995	-0.080598
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-2.609460	-2.435141	-2.607462	-2.939127	-3.112336	-2.400470	-2.480768	-2.539791	-2.419912
(3,-1)	-0.072300	-0.082235	-0.051471	-0.073827	-0.017912	-0.101629	-0.105691	-0.106674	-0.114238
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-2.609460	-2.441814	-2.719440	-2.849852	-2.557127	-2.540959	-2.586122		
(3,-1)	-0.072300	-0.093280	-0.069426	-0.074989	-0.080147	-0.085008	-0.076061		

Table S366: Laplacian of the density value (a.u.) at the considered critical points for the  $[\text{HCH}_2\text{CH}_2]^\ddagger$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-1.140563	-1.021892	-1.089339	-1.043034	-1.097961	-1.020291	-1.038853	-1.077133	-1.148256
(3,-1)	0.047242	0.034696	0.039998	0.037527	0.040894	0.030671	0.047893	0.043851	0.068454
(3,-1)	-1.212300	-1.124126	-1.173072	-1.132198	-1.183555	-1.026750	-1.144388	-1.037986	-0.942062
(3,-1)	-1.212407	-1.124226	-1.173176	-1.132298	-1.183659	-1.026844	-1.144494	-1.038066	-0.942153
(3,-1)	-1.201683	-1.113053	-1.160056	-1.120862	-1.170195	-1.013851	-1.133326	-1.029398	-0.938631
(3,-1)	-1.201666	-1.113035	-1.160039	-1.120846	-1.170177	-1.013835	-1.133307	-1.029390	-0.938613
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-1.140563	-1.057468	-1.063752	-1.115867	-1.082432	-1.041905	-1.055411	-1.118541	-1.038469
(3,-1)	0.047242	0.053563	0.052423	0.040747	0.038788	0.042089	0.047266	0.043565	0.050639
(3,-1)	-1.212300	-1.080442	-1.143031	-1.195524	-1.162786	-1.121299	-1.011615	-1.192226	-1.159446
(3,-1)	-1.212407	-1.080542	-1.143138	-1.195630	-1.162889	-1.121394	-1.011696	-1.192333	-1.159553
(3,-1)	-1.201683	-1.071645	-1.129073	-1.182539	-1.151137	-1.110857	-1.002921	-1.180668	-1.148527
(3,-1)	-1.201666	-1.071626	-1.129051	-1.182521	-1.151119	-1.110842	-1.002910	-1.180649	-1.148508
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-1.140563	-1.025925	-1.133071	-1.207749	-1.181562	-1.037517	-1.070044	-1.090375	-1.048317
(3,-1)	0.047242	0.043680	0.044661	0.038807	0.046572	0.046650	0.044427	0.043699	0.041558
(3,-1)	-1.212300	-1.119274	-1.257686	-1.355155	-1.541294	-1.178112	-1.177233	-1.165694	-1.137171
(3,-1)	-1.212407	-1.119376	-1.257800	-1.355272	-1.541420	-1.178213	-1.177337	-1.165800	-1.137274
(3,-1)	-1.201683	-1.109033	-1.247350	-1.340740	-1.529571	-1.167117	-1.165469	-1.153532	-1.124523
(3,-1)	-1.201666	-1.109017	-1.247329	-1.340719	-1.529553	-1.167101	-1.165452	-1.153514	-1.124504
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-1.140563	-1.078427	-1.141115	-1.263819	-1.119288	-1.107136	-1.123949		
(3,-1)	0.047242	0.060627	0.042067	0.045706	0.045029	0.044230	0.045384		
(3,-1)	-1.212300	-1.044791	-1.260894	-1.270997	-1.210150	-1.199214	-1.209435		
(3,-1)	-1.212407	-1.044889	-1.261018	-1.271108	-1.210258	-1.199321	-1.209543		
(3,-1)	-1.201683	-1.036896	-1.251087	-1.254829	-1.199931	-1.189387	-1.200079		
(3,-1)	-1.201666	-1.036876	-1.251062	-1.254811	-1.199913	-1.189368	-1.200059		

Table S367: Laplacian of the density value (a.u.) at the considered critical points for the [HCN]<sup>‡</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.693640	-1.163614	-1.100150	-1.018027	-0.861445	-1.368655	-1.076469	-0.595609	-0.142729
(3,-1)	-0.404788	-0.390100	-0.374515	-0.371115	-0.389914	-0.351968	-0.346648	-0.403828	-0.436395
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.693640	-0.327982	-0.151933	-1.004232	-0.894777	-0.913724	-1.028092	-0.636273	-0.873942
(3,-1)	-0.404788	-0.364574	-0.387467	-0.387417	-0.385727	-0.364443	-0.363053	-0.384894	-0.354606
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.693640	-0.465022	-0.709955	-0.921881	-0.725000	-0.809037	-0.899048	-0.943445	-1.155550
(3,-1)	-0.404788	-0.304374	-0.393364	-0.407544	-0.372826	-0.389370	-0.380429	-0.361664	-0.359874
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.693640	-0.414156	-0.990946	-0.524680	-0.891515	-0.759713	-0.812251		
(3,-1)	-0.404788	-0.362319	-0.329447	-0.443789	-0.395009	-0.400288	-0.388231		

Table S368: Laplacian of the density value (a.u.) at the considered critical points for the  $[\text{HOCH}_4]^\ddagger$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.041467	-0.079512	-0.051178	-0.062201	-0.051126	-0.089968	-0.046570	-0.016172	-0.102897
(3,-1)	-0.532596	-0.486621	-0.517191	-0.500251	-0.529952	-0.447320	-0.504464	-0.592038	-0.571387
(3,-1)	-1.159216	-1.072125	-1.119455	-1.081742	-1.126956	-0.986947	-1.093113	-0.998522	-0.905970
(3,-1)	-1.154246	-1.067670	-1.115227	-1.077746	-1.122455	-0.985942	-1.088593	-0.995340	-0.901439
(3,-1)	-1.156479	-1.069381	-1.116546	-1.078873	-1.124213	-0.982968	-1.090310	-0.996899	-0.904819
(3,-1)	-2.742377	-2.658674	-2.625767	-2.618362	-2.702969	-2.445620	-2.695269	-2.707380	-2.793959
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.041467	-0.056816	-0.050469	-0.048164	-0.055137	-0.048808	-0.039266	-0.041304	-0.013177
(3,-1)	-0.532596	-0.430969	-0.480531	-0.530548	-0.518129	-0.565077	-0.546761	-0.534029	-0.469112
(3,-1)	-1.159216	-1.021279	-1.081646	-1.138795	-1.108137	-1.071505	-0.969719	-1.132404	-1.102167
(3,-1)	-1.154246	-1.016456	-1.077197	-1.134084	-1.103569	-1.066997	-0.966313	-1.126780	-1.096900
(3,-1)	-1.156479	-1.018790	-1.078481	-1.136017	-1.105420	-1.069223	-0.968019	-1.129856	-1.099458
(3,-1)	-2.742377	-2.608459	-2.547201	-2.707117	-2.713915	-2.700358	-2.601862	-2.822591	-2.429529
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.041467	-0.031583	-0.018062	-0.048407	-0.009836	-0.042341	-0.046838	-0.053379	-0.057463
(3,-1)	-0.532596	-0.480191	-0.521002	-0.543756	-0.457300	-0.532185	-0.525898	-0.515047	-0.500120
(3,-1)	-1.159216	-1.065186	-1.202346	-1.292487	-1.480398	-1.123867	-1.120988	-1.107888	-1.082981
(3,-1)	-1.154246	-1.061537	-1.196980	-1.287470	-1.475753	-1.118283	-1.115539	-1.102764	-1.078120
(3,-1)	-1.156479	-1.062527	-1.199653	-1.289506	-1.477354	-1.121401	-1.118481	-1.105337	-1.080462
(3,-1)	-2.742377	-2.671346	-2.641640	-2.728856	-2.807200	-2.786895	-2.777174	-2.756180	-2.695282
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.041467	-0.023686	-0.059541	0.020404	-0.055800	-0.057651	-0.062707		
(3,-1)	-0.532596	-0.500617	-0.508862	-0.600479	-0.530626	-0.528396	-0.526298		
(3,-1)	-1.159216	-0.995324	-1.197514	-1.208190	-1.156070	-1.143545	-1.155136		
(3,-1)	-1.154246	-0.990348	-1.188115	-1.201820	-1.151237	-1.138578	-1.150090		
(3,-1)	-1.156479	-0.993310	-1.195226	-1.205760	-1.153234	-1.140841	-1.152288		
(3,-1)	-2.742377	-2.657812	-2.982787	-2.993857	-2.729401	-2.773157	-2.735126		

Table S369: Laplacian of the density value (a.u.) at the considered critical points for the [HHO]<sup>‡</sup> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.310752	-0.339036	-0.319602	-0.331061	-0.312547	-0.308488	-0.301502	-0.348815	-0.379401
(3,-1)	-0.480383	-0.467239	-0.482694	-0.474011	-0.496893	-0.383748	-0.509668	-0.526100	-0.582030
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.310752	-0.337747	-0.345444	-0.322176	-0.333192	-0.321906	-0.331544	-0.330628	-0.278431
(3,-1)	-0.480383	-0.466004	-0.412351	-0.488803	-0.480438	-0.569835	-0.510412	-0.503160	-0.474458
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.310752	-0.287468	-0.245937	-0.253352	-0.144474	-0.314489	-0.318351	-0.324604	-0.319532
(3,-1)	-0.480383	-0.483957	-0.499650	-0.526663	-0.417522	-0.518871	-0.508868	-0.504085	-0.483801
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.310752	-0.291123	-0.275168	-0.274648	-0.333779	-0.342352	-0.343218		
(3,-1)	-0.480383	-0.521164	-0.499985	-0.503967	-0.484634	-0.481499	-0.480517		

Table S370: Laplacian of the density value (a.u.) at the considered critical points for the  $[\text{HH}_2\text{S}]^\ddagger$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	-0.689313	-0.633069	-0.658590	-0.636212	-0.664996	-0.613083	-0.630721	-0.645928	-0.569308
(3,-1)	-0.419176	-0.374952	-0.392925	-0.379955	-0.403463	-0.387243	-0.357947	-0.412808	-0.440899
(3,-1)	-0.072513	-0.096818	-0.085606	-0.091704	-0.089182	-0.092235	-0.084866	-0.076356	-0.103988
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.689313	-0.619513	-0.648938	-0.674547	-0.656703	-0.648206	-0.627028	-0.667823	-0.650405
(3,-1)	-0.419176	-0.325034	-0.365369	-0.405514	-0.396298	-0.399754	-0.390258	-0.398051	-0.347666
(3,-1)	-0.072513	-0.104367	-0.107112	-0.084498	-0.088111	-0.051745	-0.058417	-0.086575	-0.083638
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	-0.689313	-0.630216	-0.700777	-0.742306	-0.831414	-0.657797	-0.661339	-0.656140	-0.643475
(3,-1)	-0.419176	-0.323530	-0.416382	-0.442134	-0.397713	-0.393859	-0.398428	-0.388736	-0.377261
(3,-1)	-0.072513	-0.080061	-0.056352	-0.064742	-0.055080	-0.083685	-0.086480	-0.088887	-0.089296
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	-0.689313	-0.611958	-0.673072	-0.738174	-0.684002	-0.678397	-0.683470		
(3,-1)	-0.419176	-0.378760	-0.392706	-0.463956	-0.416417	-0.416927	-0.426873		
(3,-1)	-0.072513	-0.070590	-0.064152	-0.056929	-0.079408	-0.079908	-0.078606		

Table S371: Laplacian of the density value (a.u.) at the considered critical points for the  $(\text{NH}_3)_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.037702	0.030764	0.033764	0.032766	0.034546	0.036297	0.033191	0.037107	0.042985
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.037702	0.040583	0.039334	0.034587	0.034013	0.035119	0.035383	0.034642	0.035650
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.037702	0.035837	0.040338	0.038105	0.041784	0.034788	0.034967	0.035092	0.034258
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.037702	0.040384	0.040450	0.038686	0.035500	0.035568	0.035614		

Table S372: Laplacian of the density value (a.u.) at the considered critical points for the (HF)<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.047762	0.040952	0.044120	0.043140	0.044898	0.046379	0.043261	0.047868	0.052942
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.047762	0.051058	0.049628	0.044909	0.044357	0.044258	0.044786	0.045456	0.045140
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.047762	0.046553	0.050827	0.048646	0.051248	0.044423	0.044811	0.045054	0.045050
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.047762	0.050783	0.050436	0.048769	0.045710	0.045767	0.045701		



Table S373: Laplacian of the density value (a.u.) at the considered critical points for the (H<sub>2</sub>O)<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.072320	0.063464	0.068654	0.066636	0.069587	0.067664	0.067857	0.078552	0.088611
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.072320	0.082623	0.078621	0.069937	0.068615	0.073165	0.072772	0.071007	0.071152
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.072320	0.071931	0.076712	0.073940	0.070022	0.070844	0.070708	0.070444	0.070593
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.072320	0.080482	0.078391	0.076281	0.070220	0.069973	0.069913		

Table S374: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{NH}_3 \cdots \text{H}_2\text{O}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.033772	0.029201	0.031118	0.030551	0.031926	0.031519	0.030874	0.034507	0.037675
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.033772	0.037490	0.035742	0.031713	0.031465	0.031024	0.032356	0.032265	0.031757
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.033772	0.032693	0.034912	0.032595	0.034147	0.031491	0.031763	0.032155	0.031788
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.033772	0.036864	0.036381	0.034706	0.032292	0.032526	0.032344		

Table S375: Laplacian of the density value (a.u.) at the considered critical points for the  $(\text{HCONH}_2)_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.095943	0.088272	0.093338	0.091579	0.093427	0.096173	0.092798	0.099762	0.099981
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.095943	0.103725	0.099826	0.093884	0.092684	0.089286	0.091159	0.093249	0.093374
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.095943	0.095103	0.098262	0.094888	0.097543	0.092130	0.092960	0.093465	0.097217
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.095943	0.102276	0.104929	0.097070	0.093903	0.093388	0.093301		

Table S376: Laplacian of the density value (a.u.) at the considered critical points for the (HCOOH)<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.008545	0.009084	0.008855	0.008770	0.008459	0.007918	0.008443	0.008595	0.007542
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.008545	0.008200	0.008389	0.008730	0.008607	0.008642	0.008669	0.008626	0.008788
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.008545	0.008824	0.008703	0.008832	0.008826	0.008844	0.008730	0.008633	0.008692
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.008545	0.008367	0.009123	0.008262	0.008650	0.008482	0.008613		

Table S377: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>2</sub>H<sub>4</sub>...F<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.009522	0.009921	0.009607	0.009562	0.009349	0.008949	0.009261	0.009826	0.008596
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.009522	0.009630	0.009288	0.009551	0.009490	0.009167	0.009812	0.009632	0.009716
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.009522	0.009733	0.009682	0.009744	0.009902	0.009686	0.009603	0.009569	0.009487
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.009522	0.009688	0.010420	0.009281	0.009557	0.009486	0.009514		

Table S378: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{NH}_3 \cdots \text{F}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.030773	0.031022	0.031072	0.030857	0.030912	0.031634	0.030006	0.030052	0.029248
(3,-1)	0.112585	0.101048	0.111517	0.106794	0.110503	0.108892	0.111527	0.125492	0.150143
(3,-1)	0.112585	0.101048	0.111517	0.106794	0.110503	0.108892	0.111527	0.125492	0.150143
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.030773	0.029091	0.028701	0.031129	0.031002	0.030838	0.030006	0.030637	0.029854
(3,-1)	0.112585	0.137641	0.127347	0.112616	0.109134	0.126558	0.123031	0.113747	0.115028
(3,-1)	0.112585	0.137641	0.127347	0.112616	0.109134	0.126558	0.123031	0.113747	0.115028
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.030773	0.030157	0.030192	0.031208	0.032987	0.030424	0.030528	0.030627	0.030662
(3,-1)	0.112585	0.114138	0.109115	0.107033	0.086637	0.113821	0.114148	0.113779	0.115002
(3,-1)	0.112585	0.114138	0.109115	0.107033	0.086637	0.113821	0.114148	0.113779	0.115002
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.030773	0.030292	0.031821	0.031364	0.031288	0.031301	0.030981		
(3,-1)	0.112585	0.130159	0.114296	0.121578	0.111870	0.110095	0.110896		
(3,-1)	0.112585	0.130159	0.114296	0.121578	0.111870	0.110095	0.110896		

Table S379: Laplacian of the density value (a.u.) at the considered critical points for the C<sub>2</sub>H<sub>2</sub>...ClF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.044296	0.035609	0.039626	0.037964	0.040351	0.038719	0.038655	0.044799	0.052381
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.044296	0.049180	0.047155	0.040671	0.039562	0.044309	0.044339	0.041245	0.043529
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.044296	0.041602	0.045653	0.043653	0.046039	0.041919	0.041755	0.041471	0.039969
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.044296	0.047474	0.045885	0.045891	0.041665	0.041449	0.041926		

Table S380: Laplacian of the density value (a.u.) at the considered critical points for the HCN...CIF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.136280	0.119365	0.124853	0.121904	0.125750	0.109688	0.124658	0.142111	0.161850
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.136280	0.145247	0.138634	0.126562	0.124384	0.139318	0.139450	0.129046	0.136784
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.136280	0.129075	0.125107	0.119123	0.109286	0.133027	0.131463	0.129778	0.122194
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.136280	0.138919	0.122221	0.141048	0.128470	0.128476	0.126964		



Table S381: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{NH}_3 \cdots \text{Cl}_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.080247	0.069813	0.072175	0.071719	0.074541	0.074852	0.071694	0.078004	0.083871
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.080247	0.081913	0.081660	0.074260	0.074432	0.077402	0.077155	0.077353	0.075818
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.080247	0.079059	0.081052	0.078064	0.075408	0.077000	0.077078	0.076345	0.076000
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.080247	0.081649	0.077838	0.082766	0.075939	0.077204	0.076777		

Table S382: Laplacian of the density value (a.u.) at the considered critical points for the H<sub>2</sub>O...ClF system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.061107	0.054162	0.055083	0.055329	0.056796	0.055856	0.054758	0.060355	0.064120
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.061107	0.061324	0.061158	0.056178	0.056736	0.058816	0.057580	0.058753	0.056846
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.061107	0.059564	0.061928	0.059405	0.059222	0.059041	0.058795	0.058283	0.057388
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.061107	0.061559	0.062322	0.061308	0.057662	0.058719	0.058270		

Table S383: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{NH}_3 \cdots \text{ClF}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.011322	0.011541	0.011363	0.011218	0.011014	0.009865	0.010912	0.011352	0.010301
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.011322	0.011474	0.010845	0.011315	0.011165	0.010912	0.011359	0.011288	0.011355
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.011322	0.011637	0.011455	0.011650	0.012011	0.011327	0.011321	0.011326	0.011408
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.011322	0.011570	0.012178	0.011141	0.011316	0.011188	0.011303		

Table S384: Laplacian of the density value (a.u.) at the considered critical points for the  $(\text{H}_2\text{S})_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.017509	0.016959	0.016774	0.016868	0.017035	0.017189	0.016594	0.017833	0.018239
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.017509	0.017924	0.017561	0.016966	0.017102	0.017284	0.017218	0.016903	0.016674
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.017509	0.016745	0.017196	0.017284	0.018038	0.016945	0.017003	0.017049	0.016817
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.017509	0.018014	0.018870	0.017636	0.017193	0.017391	0.017147		

Table S385: Laplacian of the density value (a.u.) at the considered critical points for the (HCl)<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.094481	0.084685	0.086988	0.086902	0.089707	0.088713	0.086464	0.093071	0.097650
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.094481	0.097269	0.097052	0.089026	0.089557	0.089740	0.089477	0.092448	0.089384
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.094481	0.093216	0.095671	0.092534	0.093730	0.090299	0.090716	0.090558	0.090281
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.094481	0.096807	0.094355	0.096418	0.090575	0.091911	0.090733		

Table S386: Laplacian of the density value (a.u.) at the considered critical points for the HCl $\cdots$ H<sub>2</sub>S system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+3)	0.014562	0.015406	0.014588	0.014608	0.014448	0.012859	0.014160	0.015198	0.014995
(3,+1)	0.015067	0.015456	0.015041	0.015042	0.014994	0.014753	0.014717	0.015777	0.015121
(3,+1)	0.015067	0.015456	0.015041	0.015042	0.014994	0.014753	0.014717	0.015777	0.015121
(3,+1)	0.015067	0.015456	0.015041	0.015042	0.014994	0.014753	0.014717	0.015777	0.015121
(3,+1)	0.015067	0.015456	0.015041	0.015042	0.014994	0.014753	0.014717	0.015777	0.015121
(3,-1)	0.016072	0.016107	0.016063	0.015994	0.016080	0.016531	0.015740	0.016687	0.016041
(3,-1)	0.016072	0.016107	0.016063	0.015994	0.016080	0.016531	0.015740	0.016687	0.016041
(3,-1)	0.016087	0.016120	0.016078	0.016009	0.016096	0.016553	0.015755	0.016702	0.016057
(3,-1)	0.016087	0.016120	0.016078	0.016009	0.016096	0.016553	0.015755	0.016702	0.016057
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+3)	0.014562	0.015354	0.014701	0.014690	0.014713	0.014431	0.015603	0.015088	0.014960
(3,+1)	0.015067	0.015547	0.015124	0.015120	0.015141	0.015001	0.015534	0.015074	0.015039
(3,+1)	0.015067	0.015547	0.015124	0.015120	0.015141	0.015001	0.015534	0.015074	0.015039
(3,+1)	0.015067	0.015547	0.015124	0.015120	0.015141	0.015001	0.015534	0.015074	0.015039
(3,+1)	0.015067	0.015547	0.015124	0.015120	0.015141	0.015001	0.015534	0.015074	0.015039
(3,-1)	0.016072	0.016345	0.016067	0.016145	0.016127	0.015881	0.015972	0.015674	0.015775
(3,-1)	0.016072	0.016345	0.016067	0.016145	0.016127	0.015881	0.015972	0.015674	0.015775
(3,-1)	0.016087	0.016360	0.016084	0.016160	0.016142	0.015897	0.015985	0.015688	0.015790
(3,-1)	0.016087	0.016360	0.016084	0.016160	0.016142	0.015897	0.015985	0.015688	0.015790
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+3)	0.014562	0.014947	0.015142	0.015238	0.015910	0.015057	0.014928	0.014800	0.014513
(3,+1)	0.015067	0.014941	0.015369	0.015506	0.016131	0.015060	0.015065	0.015099	0.014905
(3,+1)	0.015067	0.014941	0.015369	0.015506	0.016131	0.015060	0.015065	0.015099	0.014905
(3,+1)	0.015067	0.014941	0.015369	0.015506	0.016131	0.015060	0.015065	0.015099	0.014905
(3,+1)	0.015067	0.014941	0.015369	0.015506	0.016131	0.015060	0.015065	0.015099	0.014905
(3,-1)	0.016072	0.015590	0.016206	0.016364	0.017049	0.015561	0.015735	0.015942	0.015861
(3,-1)	0.016072	0.015590	0.016206	0.016364	0.017049	0.015561	0.015735	0.015942	0.015861
(3,-1)	0.016087	0.015603	0.016220	0.016379	0.017064	0.015575	0.015749	0.015957	0.015875
(3,-1)	0.016087	0.015603	0.016220	0.016379	0.017064	0.015575	0.015749	0.015957	0.015875
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+3)	0.014562	0.015610	0.016037	0.014848	0.014884	0.014957	0.014880		
(3,+1)	0.015067	0.015686	0.016342	0.015328	0.015281	0.015353	0.015224		
(3,+1)	0.015067	0.015686	0.016342	0.015328	0.015281	0.015353	0.015224		
(3,+1)	0.015067	0.015686	0.016342	0.015328	0.015281	0.015353	0.015224		
(3,+1)	0.015067	0.015686	0.016342	0.015328	0.015281	0.015353	0.015224		
(3,-1)	0.016072	0.016218	0.017079	0.016577	0.016264	0.016334	0.016147		
(3,-1)	0.016072	0.016218	0.017079	0.016577	0.016264	0.016334	0.016147		
(3,-1)	0.016087	0.016233	0.017094	0.016593	0.016280	0.016349	0.016162		
(3,-1)	0.016087	0.016233	0.017094	0.016593	0.016280	0.016349	0.016162		

Table S387: Laplacian of the density value (a.u.) at the considered critical points for the  $\text{CH}_3\text{Cl}\cdots\text{HCl}$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.013388	0.014071	0.013880	0.013657	0.013147	0.011894	0.013231	0.013473	0.011490
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.013388	0.013651	0.012805	0.013645	0.013371	0.013063	0.013465	0.013424	0.013958
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.013388	0.014013	0.013601	0.013807	0.014152	0.013800	0.013646	0.013527	0.013844
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.013388	0.013732	0.014708	0.012751	0.013542	0.013224	0.013512		

Table S388: Laplacian of the density value (a.u.) at the considered critical points for the HCN $\cdots$ CH<sub>3</sub>SH system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.020664	0.021344	0.021047	0.020912	0.020743	0.020512	0.020361	0.020961	0.019841
(3,-1)	0.098767	0.089395	0.096958	0.093889	0.097621	0.093047	0.095493	0.106606	0.115769
(3,-1)	0.098767	0.089395	0.096958	0.093889	0.097621	0.093047	0.095493	0.106606	0.115769
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.020664	0.019876	0.019309	0.021029	0.020919	0.020543	0.020710	0.020660	0.020559
(3,-1)	0.098767	0.110078	0.107798	0.098289	0.096136	0.102102	0.099219	0.099712	0.098681
(3,-1)	0.098767	0.110078	0.107798	0.098289	0.096136	0.102102	0.099219	0.099712	0.098681
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,+1)	0.020664	0.020318	0.020474	0.021234	0.022032	0.020665	0.020721	0.020772	0.020597
(3,-1)	0.098767	0.100755	0.109235	0.107149	0.104021	0.098400	0.098345	0.097774	0.098509
(3,-1)	0.098767	0.100755	0.109235	0.107149	0.104021	0.098400	0.098345	0.097774	0.098509
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,+1)	0.020664	0.020614	0.021764	0.020941	0.021143	0.021102	0.020988		
(3,-1)	0.098767	0.107974	0.106381	0.105964	0.098026	0.097176	0.097376		
(3,-1)	0.098767	0.107974	0.106381	0.105964	0.098026	0.097176	0.097376		



Table S389: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>3</sub>SH...HCl system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.102338	0.091975	0.093965	0.093762	0.096569	0.097209	0.093662	0.099201	0.104810
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.102338	0.101928	0.101879	0.096097	0.096543	0.097799	0.096546	0.098754	0.096943
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.102338	0.100796	0.104507	0.101560	0.102826	0.097175	0.097745	0.097615	0.098271
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.102338	0.102900	0.102057	0.103495	0.097879	0.099248	0.098179		

Table S390: Laplacian of the density value (a.u.) at the considered critical points for the HeNe system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.036699	0.031768	0.033874	0.033380	0.034524	0.038027	0.033389	0.035578	0.039435
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.036699	0.037865	0.037359	0.034413	0.034210	0.033395	0.033257	0.034229	0.033931
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.036699	0.035568	0.037822	0.036201	0.040018	0.033544	0.033988	0.034393	0.034328
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.036699	0.038208	0.039064	0.037154	0.035077	0.035273	0.034986		

Table S391: Laplacian of the density value (a.u.) at the considered critical points for the HeAr system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.024731	0.021357	0.022612	0.022456	0.023268	0.028003	0.022463	0.023263	0.026469
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.024731	0.024924	0.025375	0.023076	0.023097	0.022031	0.022145	0.022684	0.022537
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.024731	0.023787	0.024627	0.023346	0.024370	0.022645	0.022994	0.023115	0.023216
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.024731	0.025440	0.024749	0.025222	0.023561	0.023827	0.023638		

Table S392: Laplacian of the density value (a.u.) at the considered critical points for the Ne<sub>2</sub> system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.006704	0.006917	0.006748	0.006688	0.006560	0.006084	0.006454	0.006679	0.006262
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.006704	0.006396	0.006597	0.006727	0.006659	0.006687	0.006756	0.006722	0.006649
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.006704	0.006819	0.006796	0.006919	0.006953	0.006730	0.006722	0.006702	0.006649
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.006704	0.006559	0.007008	0.006683	0.006715	0.006647	0.006697		

Table S393: Laplacian of the density value (a.u.) at the considered critical points for the NeAr system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.081961	0.073955	0.078585	0.076957	0.079461	0.078972	0.077807	0.086026	0.090815
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.081961	0.087513	0.085661	0.079632	0.078619	0.078153	0.078130	0.080202	0.078953
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.081961	0.081531	0.087759	0.085074	0.087519	0.079188	0.079390	0.079429	0.080326
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.081961	0.087551	0.090457	0.084808	0.079854	0.079712	0.079394		

Table S394: Laplacian of the density value (a.u.) at the considered critical points for the CH<sub>4</sub>...Ne system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.030906	0.027610	0.027402	0.027730	0.029031	0.027912	0.027040	0.029120	0.029346
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.030906	0.030083	0.029460	0.028655	0.029270	0.029274	0.029637	0.029745	0.029216
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.030906	0.029280	0.030328	0.030697	0.032527	0.030199	0.030070	0.029853	0.029167
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.030906	0.030537	0.032652	0.031946	0.029558	0.030383	0.030126		

Table S395: Laplacian of the density value (a.u.) at the considered critical points for the  $(\text{CH}_4)_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.012445	0.012666	0.012201	0.012272	0.012225	0.011933	0.011886	0.012806	0.011934
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.012445	0.012160	0.012186	0.012282	0.012362	0.012164	0.012192	0.012060	0.012279
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.012445	0.011643	0.012054	0.012472	0.012534	0.012192	0.012218	0.012224	0.012009
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.012445	0.012147	0.013715	0.012440	0.012367	0.012475	0.012327		

Table S396: Laplacian of the density value (a.u.) at the considered critical points for the  $(C_2H_2)_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.059750	0.052290	0.052649	0.052951	0.055840	0.055447	0.051866	0.054264	0.057277
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.059750	0.057710	0.057414	0.055181	0.056122	0.056328	0.055933	0.056622	0.056335
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.059750	0.056245	0.058211	0.058742	0.061149	0.056940	0.056965	0.056580	0.056255
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.059750	0.058399	0.059698	0.061458	0.056931	0.058450	0.057908		



Table S397: Laplacian of the density value (a.u.) at the considered critical points for the  $(C_2H_4)_2$  system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,-1)	0.045892	0.040862	0.043127	0.042342	0.043978	0.046341	0.042308	0.045108	0.050962
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	0.045892	0.048386	0.047311	0.043891	0.043500	0.042829	0.042391	0.043762	0.043826
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	$\omega$ B97	$\omega$ B97X	$\omega$ B97XD	N12-SX
(3,-1)	0.045892	0.044231	0.048395	0.047042	0.051749	0.042679	0.043107	0.043403	0.043601
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	$\omega$ B97X-2		
(3,-1)	0.045892	0.048915	0.050145	0.047648	0.044372	0.044582	0.044346		