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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

Éric Brémond,[*,†] Vincent Tognetti,[*,‡] Henry Chermette,[¶] Juan Carlos Sancho-García,[§] Laurent Joubert,[‡] and Carlo Adamo[‖,⊥]

† *Université de Paris, ITODYS, CNRS, F-75006 Paris, France*

‡ *Normandy University, COBRA UMR 6014 & FR 3038, Université de Rouen INSA Rouen, CNRS, F-76821 Mont St Aignan, France*

¶ *Université de Lyon, Institut des Sciences Analytiques, UMR 5280, CNRS, Université Lyon 1, 5 rue de la Doua, F-69100 Villeurbanne, France.*

§ *Departamento de Química Física, Universidad de Alicante, E-03080 Alicante, Spain*

‖ *Chimie ParisTech, PSL Research University, CNRS, Institute of Chemistry for Life and Health Sciences (i-CLeHS), UMR 8060, F-75005 Paris, France*

⊥ *Institut Universitaire de France, 103 Boulevard Saint Michel, F-75005 Paris, France*

E-mail: eric.bremond@u-paris.fr; vincent.tognetti@univ-rouen.fr

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: Na_2, Si_2, P_2, Si_2H_6, C_4H_6 (bicyclo[1.1.0]butane), C_4H_6 (cyclobutene), C_4H_8 (cyclobutane), C_4H_8 (isobutene), CCH. Due to integral storage limitations, we had to also to remove $(CH_3)_3C$ 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, ωB97X, ωB97XD, ωB97, 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

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

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

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

S3.2 Notes

- $\forall(\rho_1, \rho_2), \qquad 0 \leq S(\rho_1, \rho_2) \leq 1.$
- 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.

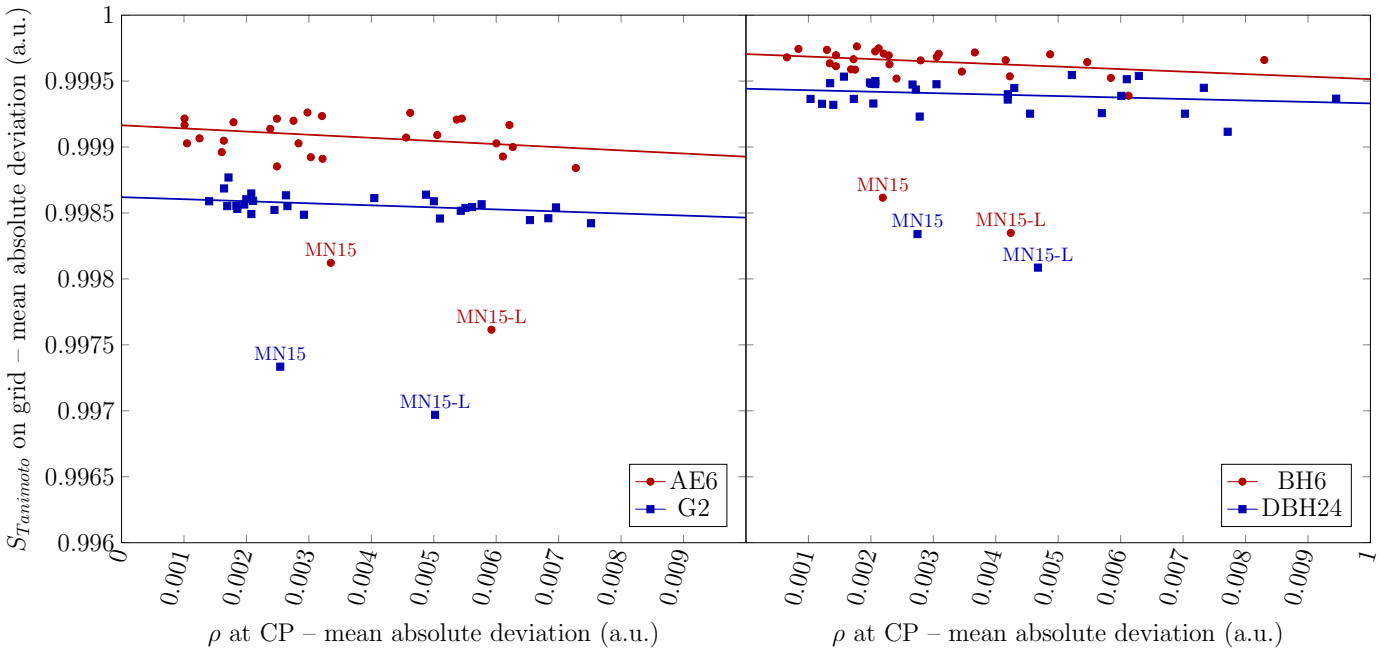

Figure S1: Correlation diagrams between the density errors computed at critical points and the S_{Tanimoto} criteria computed on an 'ultrafine' Becke-Lebedev integration grid. Except for MN15-L and MN15, the density error at critical points varies linearly with the S_{Tanimoto} criteria showing that 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

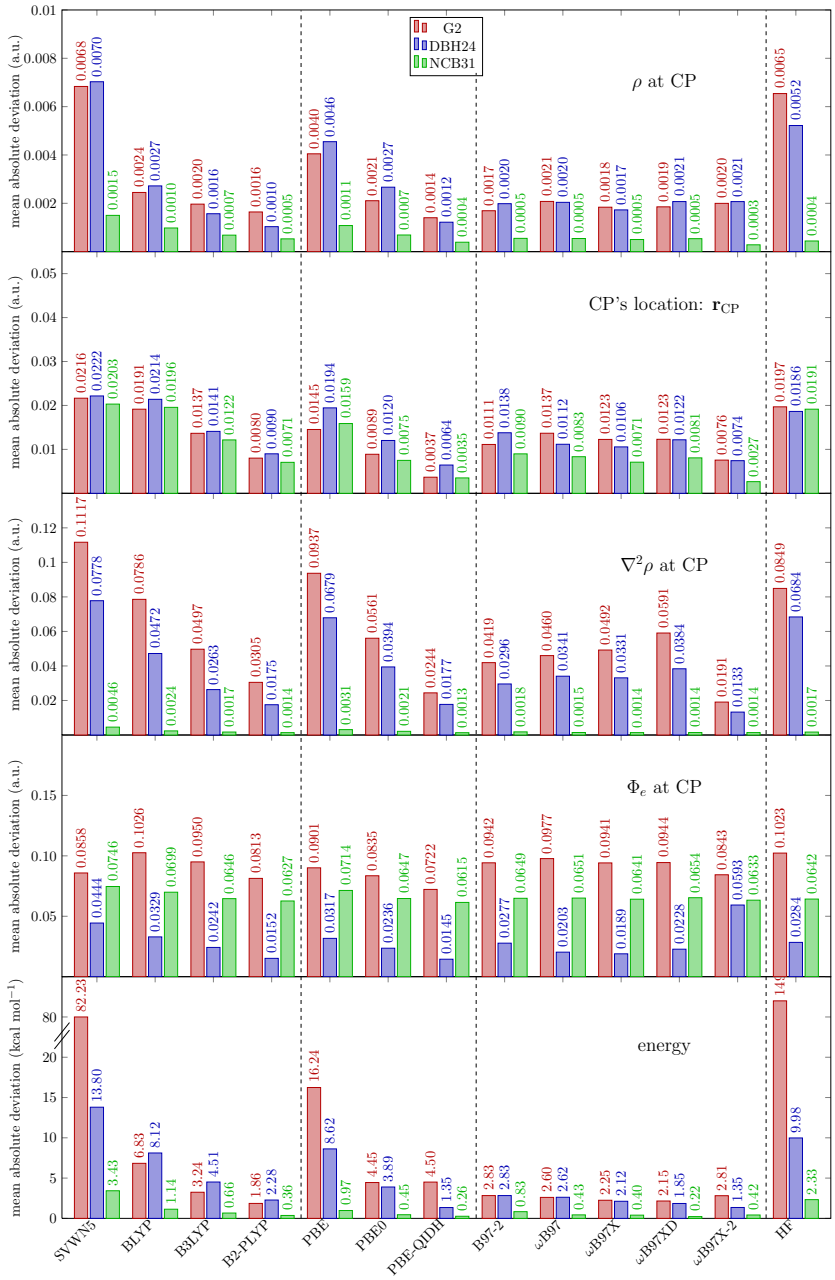

Figure S2: From top to down, mean absolute deviations (MADs) calculated over the density (ρ in a.u.), position ($\mathbf{r}_{\mathrm{CP}}$ in a.u.), Laplacian of the electron density ($\nabla^2\rho$ in a.u.), and electrostatic potential from electrons (Φ_e in a.u.) errors from the 746 critical points 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.

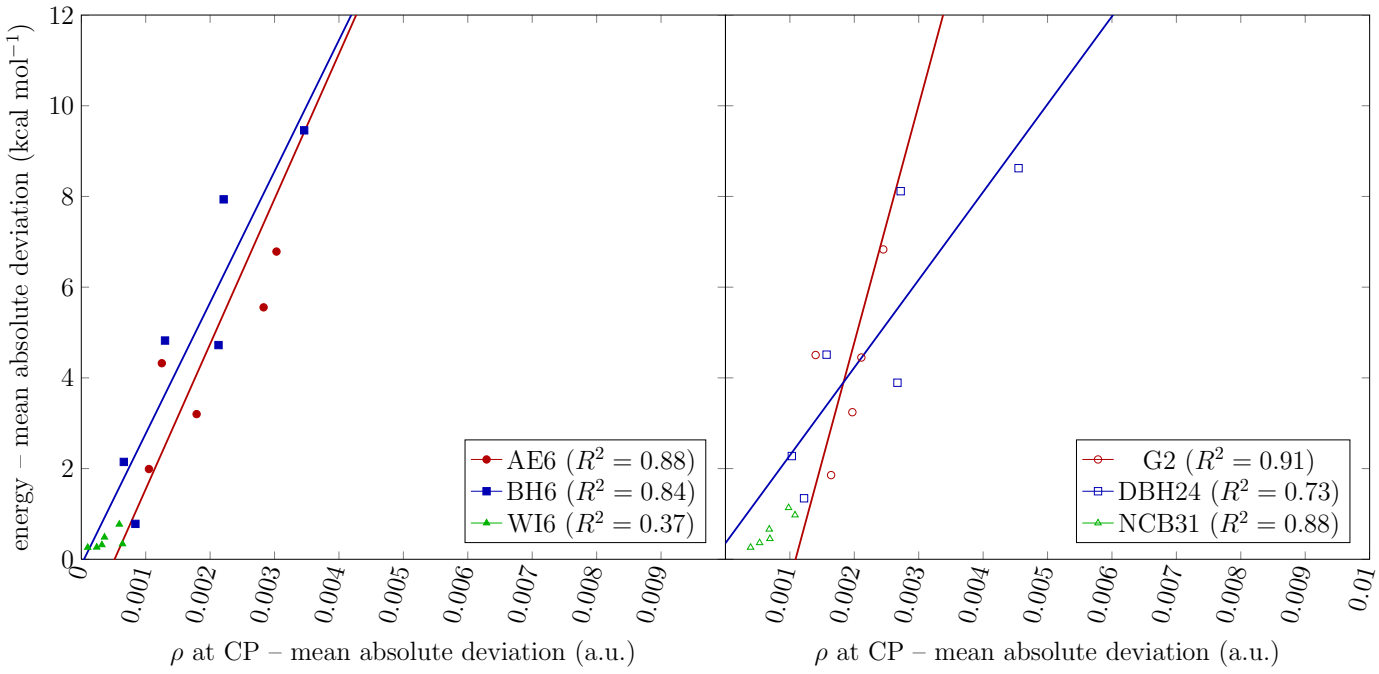

Figure S3: Correlation diagrams between the density and energy mean absolute deviation (MAD) criteria for PBE- (PBE, PBE0, PBE-QIDH) and BLYP-based (BLYP, B3LYP, B2-PLYP) nonempirical and minimally parameterized density functionals on the (red) atomization energy (left) AE6 and (right) G2, (blue) barrier 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.

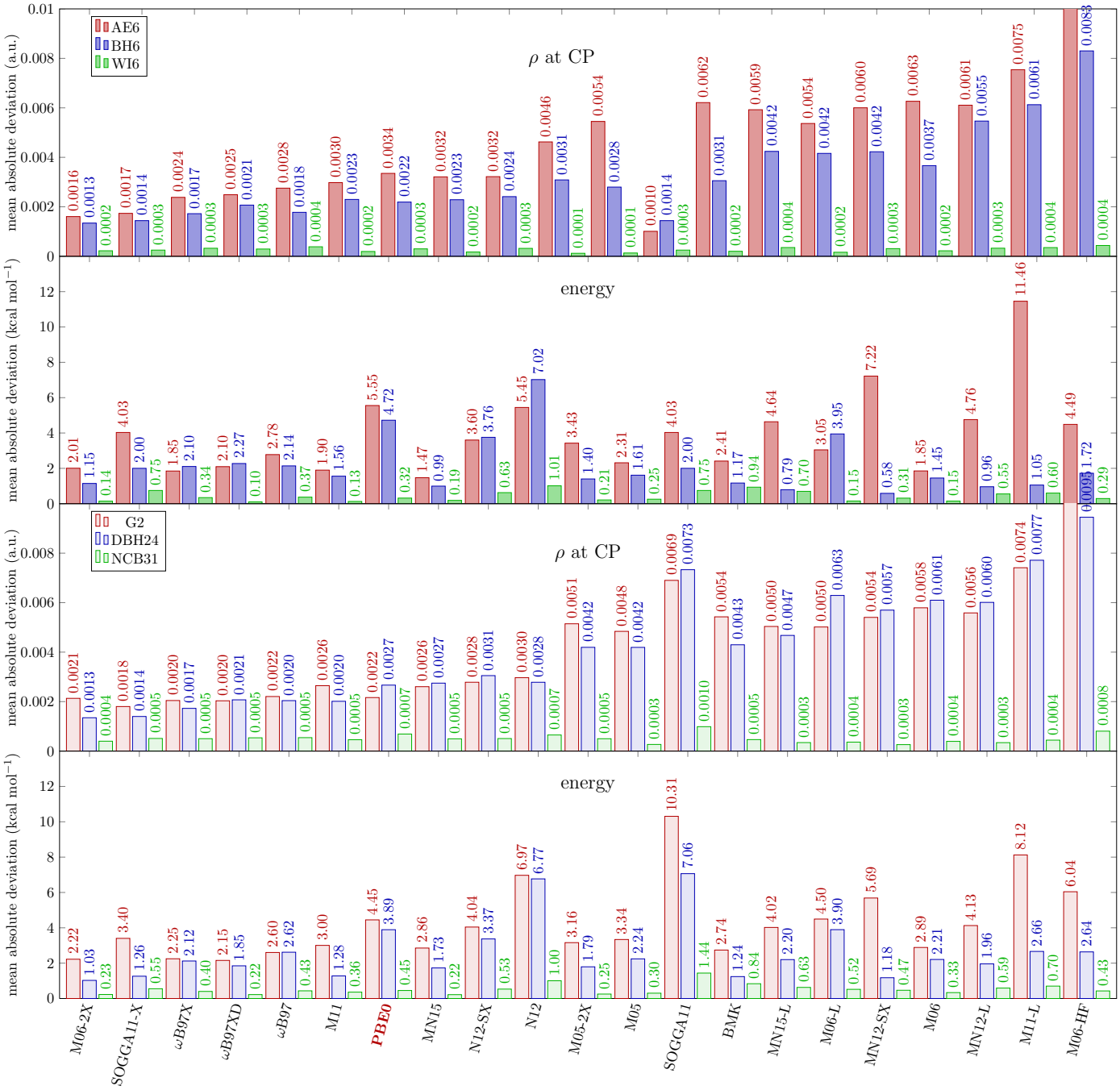

Figure S4: From top to down, for a selection of 20 highly parameterized density functionals (see Section S2), mean absolute deviations (MADs) calculated over the density (ρ in a.u.) errors from the 46 critical points gathered into the AE6, BH6 and WI6 representative databases, the corresponding energy (kcal mol^{-1}) 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.

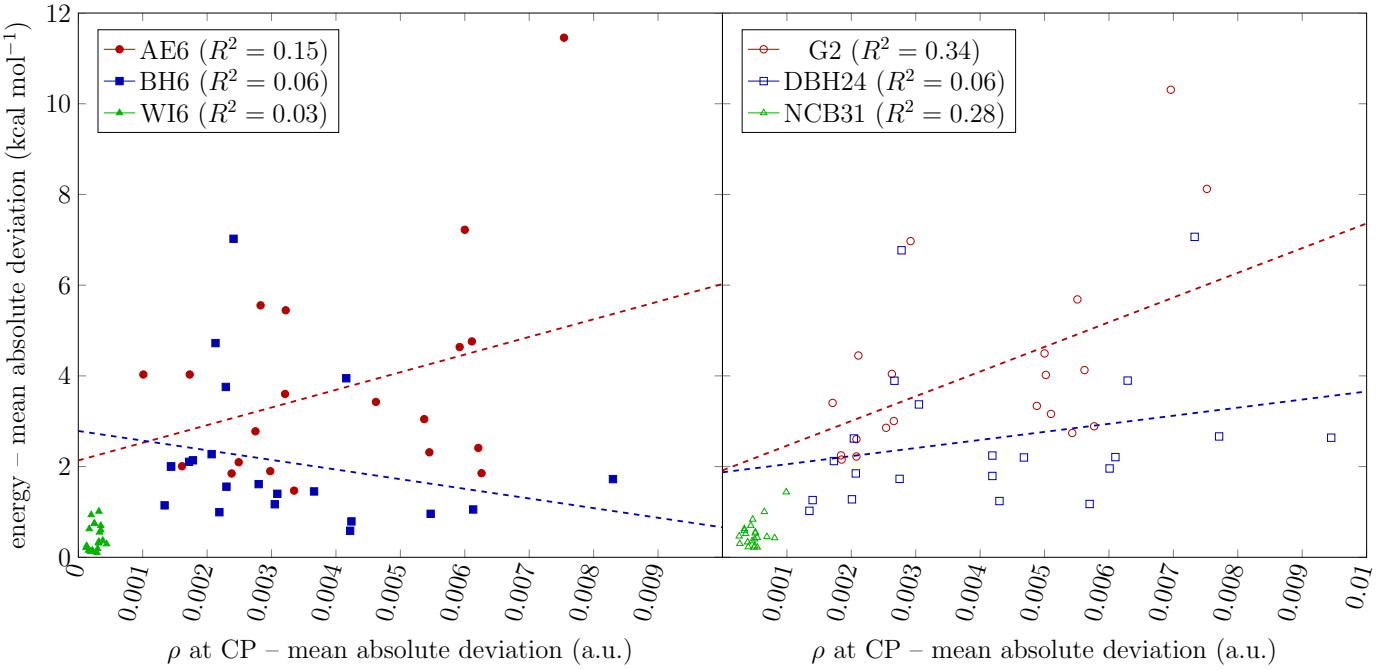

Figure S5: Correlation diagrams between the density and energy mean absolute deviation (MAD) criteria for a selection of 20 highly parameterized density functionals (see Section S2) on the (red) atomization energy (left) AE6 and (right) G2, (blue) barrier height (left) BH6 and (right) DBH24, and (green) 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

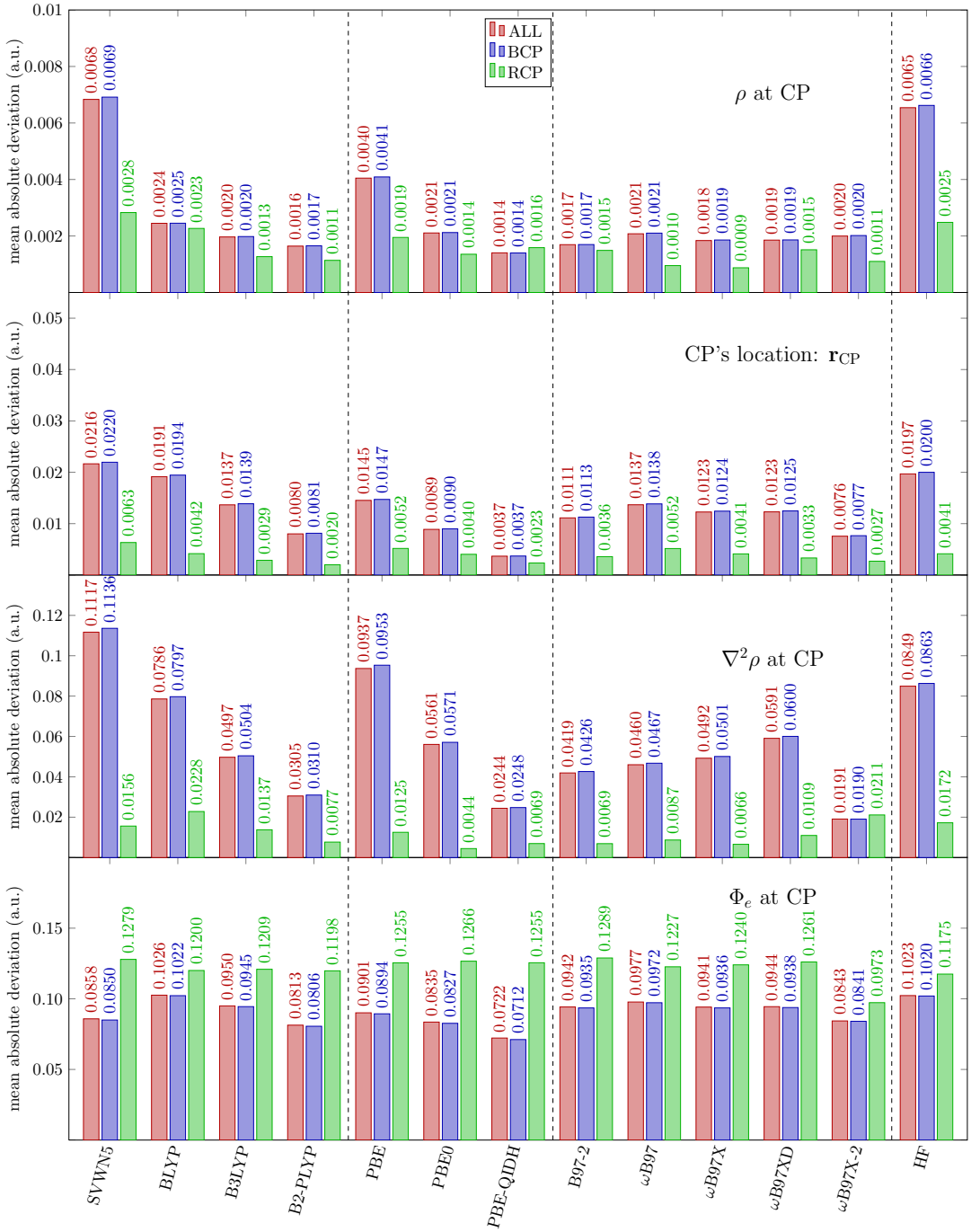

Figure S6: From top to down, mean absolute deviations (MADs) calculated over the density (ρ in a.u.), position ($\mathbf{r}_{\mathrm{CP}}$ in a.u.), Laplacian of the electron density ($\nabla^2\rho$ in a.u.), and electrostatic potential from electrons (Φ_e in a.u.) errors from the 727 bond and 19 ring 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.

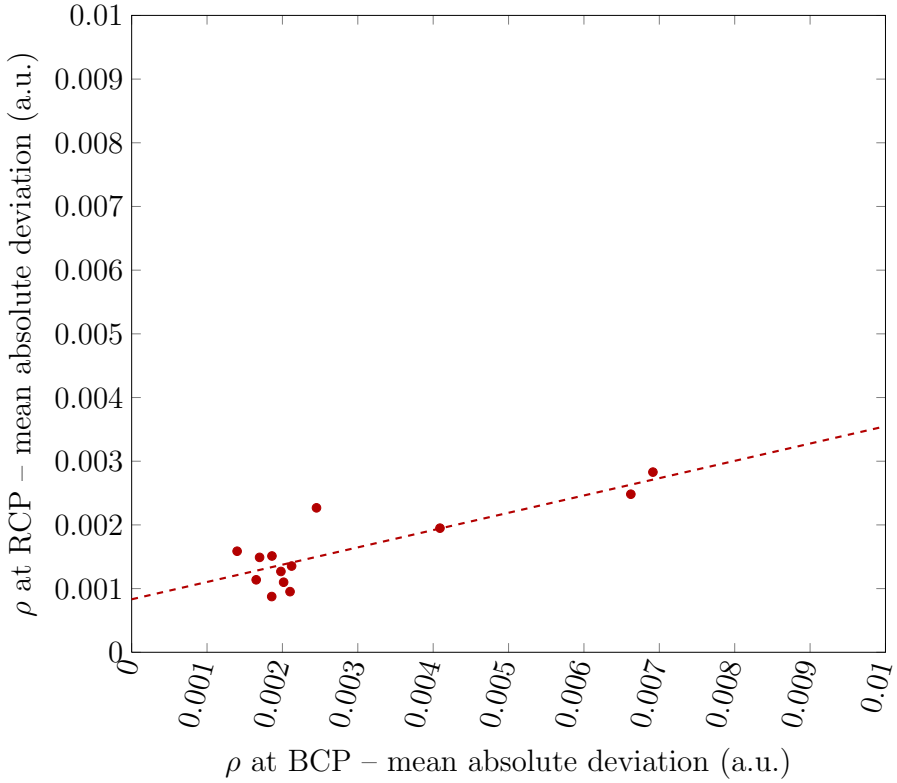

Figure S7: Correlation diagram between the density errors computed at the 727 bond and 19 ring critical points derived from the G2, DBH24, and NCB31 databases for PBE- (PBE, PBE0, PBE-QIDH) and BLYP-based (BLYP, B3LYP, B2-PLYP) nonempirical and minimally parameterized density functionals.

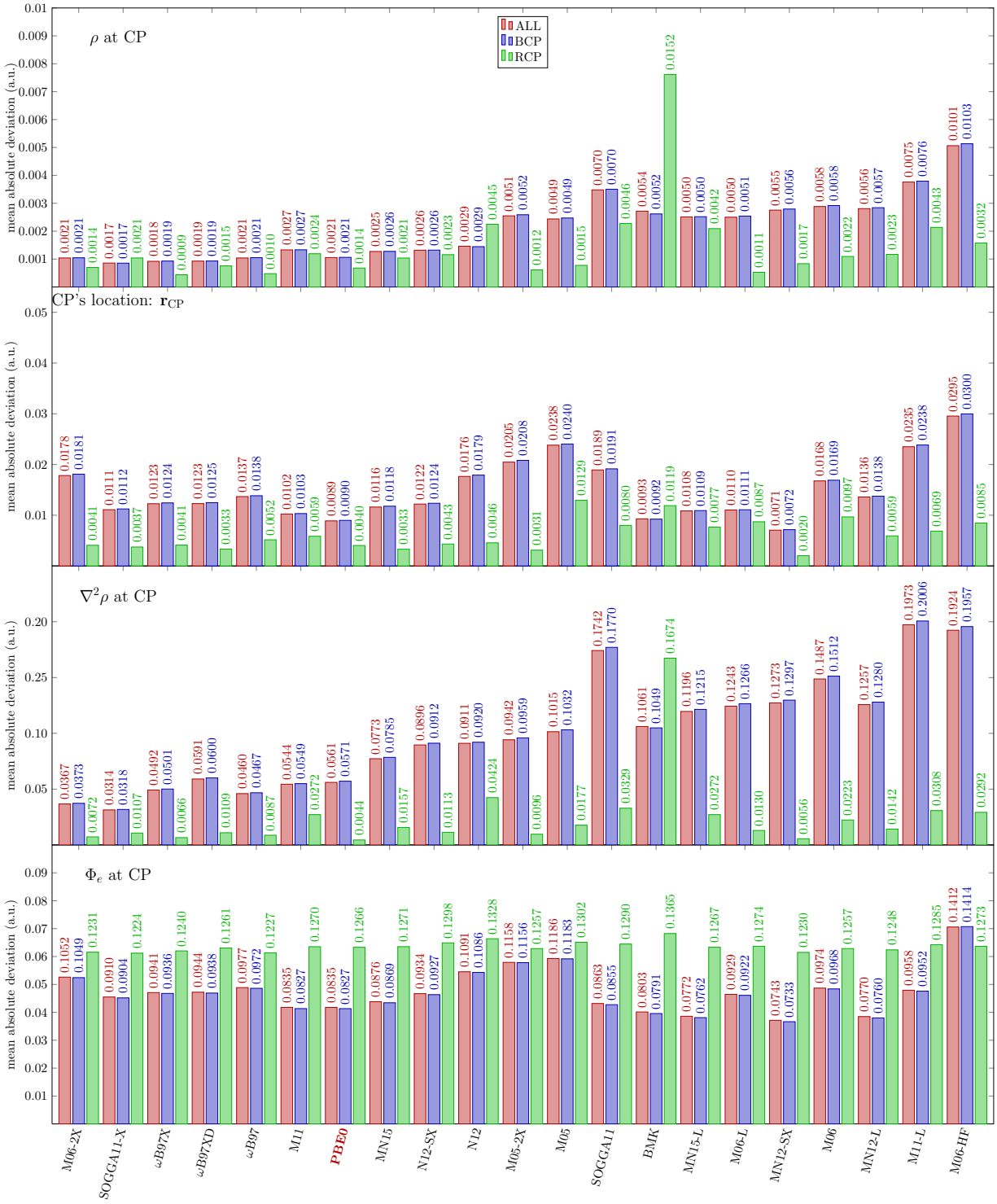

Figure S8: From top to down, mean absolute deviations (MADs) calculated over the density (ρ in a.u.), position ($\mathbf{r}_{CP}$ in a.u.), Laplacian of the electron density ($\nabla^2\rho$ in a.u.), and electrostatic potential from electrons (Φ_e in a.u.) errors from the 727 bond and 19 ring critical 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.

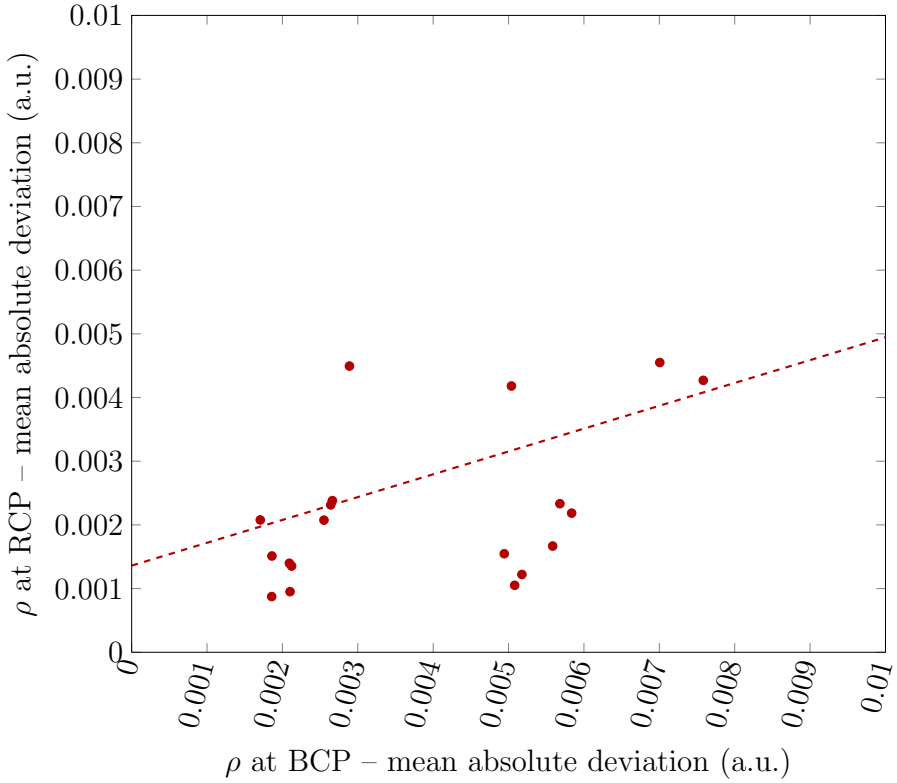

Figure S9: Correlation diagram between the density errors computed at the 727 bond and 19 ring critical points derived from the G2, DBH24, and NCB31 databases for a selection of 20 highly parameterized density functionals (see Section S2).

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_{Cosine})	0.999464	0.999474	0.999543	0.999524	0.999615	0.999541	0.999605	0.999522
MAD(S_{Tanimoto})	0.998841	0.998923	0.999072	0.999048	0.999216	0.998911	0.999208	0.998757
MAD(S_{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_{Cosine})	0.999487	0.999418	0.999598	0.999517	0.999637	0.999510	0.999591	0.999515
MAD(S_{Tanimoto})	0.998928	0.997615	0.999188	0.999028	0.999216	0.999000	0.999167	0.998122
MAD(S_{Dice})	0.999464	0.998805	0.999594	0.999513	0.999607	0.999499	0.999583	0.999060
	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	N12-SX
MAD(S_{Cosine})	0.999602	0.999508	0.999646	0.999493	0.999615	0.999579	0.999612	0.999638
MAD(S_{Tanimoto})	0.999167	0.998961	0.999259	0.998903	0.999199	0.999138	0.999215	0.999235
MAD(S_{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	ωB97X-2		
MAD(S_{Cosine})	0.999546	0.999644	0.999545	0.999516	0.999533	0.999435		
MAD(S_{Tanimoto})	0.999028	0.999262	0.999091	0.999028	0.999066	0.998853		
MAD(S_{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_{Cosine})	0.999803	0.999863	0.999791	0.999795	0.999855	0.999856	0.999830	0.999811
MAD(S_{Tanimoto})	0.999524	0.999708	0.999572	0.999589	0.999696	0.999519	0.999659	0.999389
MAD(S_{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_{Cosine})	0.999835	0.999808	0.999872	0.999876	0.999849	0.999868	0.999814	0.999807
MAD(S_{Tanimoto})	0.999644	0.998349	0.999737	0.999748	0.999657	0.999717	0.999613	0.998616
MAD(S_{Dice})	0.999822	0.999173	0.999868	0.999874	0.999828	0.999859	0.999807	0.999307
	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	N12-SX
MAD(S_{Cosine})	0.999859	0.999841	0.999867	0.999863	0.999894	0.999841	0.999866	0.999861
MAD(S_{Tanimoto})	0.999683	0.999635	0.999707	0.999660	0.999763	0.999666	0.999725	0.999695
MAD(S_{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	ωB97X-2		
MAD(S_{Cosine})	0.999816	0.999825	0.999852	0.999842	0.999872	0.999799		
MAD(S_{Tanimoto})	0.999536	0.999627	0.999703	0.999680	0.999744	0.999587		
MAD(S_{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_{Cosine})	0.999340	0.998996	0.999222	0.999005	0.999330	0.999089	0.999230	0.998929
MAD(S_{Tanimoto})	0.998553	0.997949	0.998421	0.998009	0.998646	0.998047	0.998457	0.997393
MAD(S_{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_{Cosine})	0.999140	0.999292	0.999160	0.999260	0.999131	0.999233	0.999337	0.998649
MAD(S_{Tanimoto})	0.998235	0.996508	0.998307	0.998511	0.998166	0.998432	0.998661	0.995610
MAD(S_{Dice})	0.999116	0.998251	0.999152	0.999255	0.999081	0.999215	0.999330	0.997799
	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	N12-SX
MAD(S_{Cosine})	0.999220	0.999005	0.999309	0.998956	0.999263	0.999309	0.999013	0.999001
MAD(S_{Tanimoto})	0.998377	0.997908	0.998559	0.997765	0.998475	0.998589	0.998011	0.997931
MAD(S_{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	ωB97X-2		
MAD(S_{Cosine})	0.999116	0.999306	0.999094	0.999279	0.999362	0.999185		
MAD(S_{Tanimoto})	0.998164	0.998578	0.998192	0.998551	0.998724	0.998349		
MAD(S_{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_{Cosine})	0.999249	0.999287	0.999324	0.999277	0.999302	0.999308	0.999302	0.999332
MAD(S_{Tanimoto})	0.998460	0.998523	0.998613	0.998552	0.998542	0.998487	0.998589	0.998422
MAD(S_{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_{Cosine})	0.999283	0.999245	0.999292	0.999304	0.999373	0.999308	0.999403	0.999270
MAD(S_{Tanimoto})	0.998545	0.996970	0.998564	0.998592	0.998639	0.998566	0.998769	0.997335
MAD(S_{Dice})	0.999260	0.998469	0.999267	0.999283	0.999310	0.999270	0.999377	0.998654
	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	N12-SX
MAD(S_{Cosine})	0.999292	0.999291	0.999260	0.999337	0.999359	0.999295	0.999273	0.999354
MAD(S_{Tanimoto})	0.998517	0.998492	0.998458	0.998542	0.998648	0.998553	0.998531	0.998634
MAD(S_{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	ωB97X-2		
MAD(S_{Cosine})	0.999323	0.999302	0.999212	0.999353	0.999296	0.999325		
MAD(S_{Tanimoto})	0.998538	0.998552	0.998446	0.998686	0.998589	0.998604		
MAD(S_{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_{Cosine})	0.999667	0.999729	0.999632	0.999745	0.999734	0.999702	0.999770	0.999686
MAD(S_{Tanimoto})	0.999253	0.999436	0.999253	0.999489	0.999449	0.999231	0.999539	0.999116
MAD(S_{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_{Cosine})	0.999713	0.999649	0.999770	0.999739	0.999703	0.999766	0.999667	0.999638
MAD(S_{Tanimoto})	0.999388	0.998086	0.999534	0.999474	0.999360	0.999514	0.999320	0.998340
MAD(S_{Dice})	0.999693	0.999041	0.999767	0.999737	0.999680	0.999757	0.999659	0.999169
	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	N12-SX
MAD(S_{Cosine})	0.999741	0.999766	0.999715	0.999719	0.999678	0.999691	0.999754	0.999753
MAD(S_{Tanimoto})	0.999448	0.999484	0.999400	0.999367	0.999330	0.999365	0.999500	0.999476
MAD(S_{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	ωB97X-2		
MAD(S_{Cosine})	0.999669	0.999751	0.999773	0.999684	0.999664	0.999745		
MAD(S_{Tanimoto})	0.999257	0.999480	0.999546	0.999365	0.999328	0.999477		
MAD(S_{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_{Cosine})	0.999825	0.999803	0.999834	0.999821	0.999816	0.999791	0.999788	0.999796
MAD(S_{Tanimoto})	0.999567	0.999557	0.999638	0.999627	0.999590	0.999378	0.999556	0.999387
MAD(S_{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_{Cosine})	0.999828	0.999742	0.999803	0.999837	0.999830	0.999839	0.999802	0.999754
MAD(S_{Tanimoto})	0.999611	0.998334	0.999581	0.999656	0.999578	0.999632	0.999574	0.998615
MAD(S_{Dice})	0.999805	0.999165	0.999790	0.999828	0.999789	0.999816	0.999787	0.999306
	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	N12-SX
MAD(S_{Cosine})	0.999820	0.999791	0.999812	0.999791	0.999791	0.999777	0.999816	0.999794
MAD(S_{Tanimoto})	0.999582	0.999509	0.999564	0.999491	0.999531	0.999515	0.999606	0.999530
MAD(S_{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	ωB97X-2		
MAD(S_{Cosine})	0.999834	0.999826	0.999809	0.999808	0.999811	0.999785		
MAD(S_{Tanimoto})	0.999559	0.999597	0.999608	0.999596	0.999612	0.999539		
MAD(S_{Dice})	0.999779	0.999798	0.999804	0.999798	0.999806	0.999769		

Table S7: Atomization energies (kcal mol^{-1}) 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_4	324.95	347.17	318.01	313.52	318.36	320.33	319.77	328.05
S_2	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_3H_4	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_4H_8	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_4	324.95	326.05	329.65	330.35	324.11	315.62	322.23	328.79
S_2	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_3H_4	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_4H_8	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	ωB97
SiH_4	324.95	320.33	324.84	323.30	320.81	316.62	316.42	324.55
S_2	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_3H_4	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_4H_8	1149.37	1149.73	1144.53	1153.29	1146.68	1148.28	1154.92	1151.48
	ref.	ωB97X	ωB97X-D	N12-SX	MN12-SX	M11	HF	B2-PLYP
SiH_4	324.95	324.66	324.07	320.30	325.13	324.79	256.84	322.66
S_2	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_3H_4	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_4H_8	1149.37	1150.53	1150.20	1149.00	1135.59	1147.14	870.38	1143.31
	ref.	PBE-QIDH	ωB97X-2					
SiH_4	324.95	319.35	323.16					
S_2	104.25	104.03	103.39					
SiO	193.06	185.17	192.15					
C_3H_4	705.06	706.96	699.97					
HCOCOH	633.99	631.31	630.31					
C_4H_8	1149.37	1157.00	1141.46					

Table S8: Barrier height energies (kcal mol^{-1}) 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
$H_3CH + OH \rightarrow [H_3CHOH]^{\ddagger}$	6.70	-16.76	-2.37	-5.24	2.45	6.00	-2.09	3.91
$[H_3CHOH]^{\ddagger} \rightarrow CH_3 + H_2O$	19.60	2.22	10.54	8.89	13.81	15.20	11.45	12.42
$H + HO \rightarrow [HHO]^{\ddagger}$	10.70	-1.97	1.42	3.60	8.12	9.41	3.37	6.92
$[HHO]^{\ddagger} \rightarrow H_2 + O$	13.10	-12.67	1.51	-1.35	8.38	10.01	5.52	7.28
$H + HSH \rightarrow [HHSH]^{\ddagger}$	3.60	-6.74	-2.12	-1.12	4.48	3.43	1.12	3.70
$[HHSH]^{\ddagger} \rightarrow H_2 + SH$	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
$H_3CH + OH \rightarrow [H_3CHOH]^{\ddagger}$	6.70	9.15	9.34	7.58	2.33	2.07	5.44	5.40
$[H_3CHOH]^{\ddagger} \rightarrow CH_3 + H_2O$	19.60	18.72	18.75	19.44	13.97	14.01	17.95	17.42
$H + HO \rightarrow [HHO]^{\ddagger}$	10.70	9.13	10.10	7.86	4.01	7.04	8.27	8.61
$[HHO]^{\ddagger} \rightarrow H_2 + O$	13.10	12.47	12.68	12.77	6.32	5.95	11.66	10.45
$H + HSH \rightarrow [HHSH]^{\ddagger}$	3.60	3.49	3.23	3.92	-0.48	1.18	4.60	3.95
$[HHSH]^{\ddagger} \rightarrow H_2 + SH$	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
$H_3CH + OH \rightarrow [H_3CHOH]^{\ddagger}$	6.70	6.00	5.84	5.86	5.36	4.87	5.81	4.95
$[H_3CHOH]^{\ddagger} \rightarrow CH_3 + H_2O$	19.60	15.20	18.58	16.61	17.73	17.56	19.29	15.64
$H + HO \rightarrow [HHO]^{\ddagger}$	10.70	9.41	9.85	10.19	9.87	10.27	10.05	10.57
$[HHO]^{\ddagger} \rightarrow H_2 + O$	13.10	10.01	11.03	10.98	11.58	11.55	16.13	11.00
$H + HSH \rightarrow [HHSH]^{\ddagger}$	3.60	3.43	4.30	3.49	4.41	5.45	5.79	6.94
$[HHSH]^{\ddagger} \rightarrow H_2 + SH$	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
$H_3CH + OH \rightarrow [H_3CHOH]^{\ddagger}$	6.70	4.42	3.72	1.50	7.77	4.88	26.65	4.39
$[H_3CHOH]^{\ddagger} \rightarrow CH_3 + H_2O$	19.60	15.45	15.23	14.13	19.31	18.74	28.81	17.03
$H + HO \rightarrow [HHO]^{\ddagger}$	10.70	9.73	8.78	9.77	10.00	8.74	17.36	8.03
$[HHO]^{\ddagger} \rightarrow H_2 + O$	13.10	10.15	9.80	7.13	13.07	10.24	32.84	10.01
$H + HSH \rightarrow [HHSH]^{\ddagger}$	3.60	5.60	4.17	4.53	4.24	2.62	11.91	2.04
$[HHSH]^{\ddagger} \rightarrow H_2 + SH$	17.30	17.59	16.80	13.27	18.08	16.43	27.17	16.62
	ref.	PBE-QIDH	ωB97X-2					
$H_3CH + OH \rightarrow [H_3CHOH]^{\ddagger}$	6.70	6.66	5.60					
$[H_3CHOH]^{\ddagger} \rightarrow CH_3 + H_2O$	19.60	19.22	18.34					
$H + HO \rightarrow [HHO]^{\ddagger}$	10.70	11.73	10.83					
$[HHO]^{\ddagger} \rightarrow H_2 + O$	13.10	12.57	12.66					
$H + HSH \rightarrow [HHSH]^{\ddagger}$	3.60	4.05	4.12					
$[HHSH]^{\ddagger} \rightarrow H_2 + SH$	17.30	15.04	17.14					

Table S9: Weak interaction energies (kcal mol^{-1}) 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$\cdots$water 0.90R_e	-4.66	-8.59	-3.95	-5.00	-3.81	-4.54	-4.95	-4.44
water$\cdots$water 1.00R_e	-4.95	-7.74	-4.40	-5.20	-4.24	-4.74	-4.88	-4.69
water$\cdots$water 1.50R_e	-2.11	-2.56	-1.93	-2.25	-2.06	-1.75	-1.96	-1.94
methane$\cdots$methane 0.90R_e	-0.34	-1.15	1.56	0.49	1.16	0.92	1.68	-0.15
methane$\cdots$methane 1.00R_e	-0.53	-0.82	0.66	-0.09	0.29	0.72	0.86	-0.50
methane$\cdots$methane 1.50R_e	-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$\cdots$water 0.90R_e	-4.66	-3.97	-3.78	-3.34	-4.45	-4.96	-4.97	-4.54
water$\cdots$water 1.00R_e	-4.95	-4.20	-4.37	-4.32	-4.77	-5.11	-5.31	-4.81
water$\cdots$water 1.50R_e	-2.11	-1.53	-1.88	-2.18	-2.03	-2.19	-2.30	-2.08
methane$\cdots$methane 0.90R_e	-0.34	0.16	0.07	-1.10	1.10	0.49	-0.03	-0.02
methane$\cdots$methane 1.00R_e	-0.53	0.20	0.18	-0.98	0.39	-0.04	-0.39	-0.26
methane$\cdots$methane 1.50R_e	-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$\cdots$water 0.90R_e	-4.66	-4.54	-4.72	-4.10	-4.97	-4.99	-5.23	-5.58
water$\cdots$water 1.00R_e	-4.95	-4.74	-5.12	-4.46	-5.20	-5.30	-5.18	-5.74
water$\cdots$water 1.50R_e	-2.11	-1.75	-2.27	-1.55	-2.23	-2.28	-2.39	-2.14
methane$\cdots$methane 0.90R_e	-0.34	0.92	-0.69	1.12	-0.39	-0.28	0.05	-0.63
methane$\cdots$methane 1.00R_e	-0.53	0.72	-0.71	0.96	-0.42	-0.49	-0.27	-0.39
methane$\cdots$methane 1.50R_e	-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$\cdots$water 0.90R_e	-4.66	-5.55	-4.89	-5.35	-4.17	-4.78	-3.02	-4.73
water$\cdots$water 1.00R_e	-4.95	-5.69	-5.10	-5.43	-4.69	-5.06	-3.88	-4.99
water$\cdots$water 1.50R_e	-2.11	-2.25	-2.21	-2.08	-1.99	-2.19	-2.09	-2.11
methane$\cdots$methane 0.90R_e	-0.34	-0.56	-0.45	0.62	-0.11	-0.23	1.32	0.51
methane$\cdots$methane 1.00R_e	-0.53	-0.54	-0.55	0.31	-0.07	-0.31	0.36	0.03
methane$\cdots$methane 1.50R_e	-0.06	-0.00	-0.07	0.01	-0.05	-0.02	0.00	-0.00
	ref.	PBE-QIDH	ωB97X-2	ωB97X-noD				
water$\cdots$water 0.90R_e	-4.66	-5.08	-5.14	-4.39				
water$\cdots$water 1.00R_e	-4.95	-5.18	-5.44	-4.65				
water$\cdots$water 1.50R_e	-2.11	-2.18	-2.34	-2.02				
methane$\cdots$methane 0.90R_e	-0.34	0.15	-0.58	0.76				
methane$\cdots$methane 1.00R_e	-0.53	-0.20	-0.72	0.21				
methane$\cdots$methane 1.50R_e	-0.06	-0.03	-0.04	0.00				

Table S10: Atomization energies (kcal mol^{-1}) 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_2	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
^2CH	83.80	92.21	85.49	84.53	83.16	79.10	80.12	82.63
$^3CH_2$	190.00	212.59	190.00	194.37	188.47	189.23	190.39	192.46
$^1CH_2$	180.70	198.57	179.88	178.69	178.25	172.75	174.93	179.01
$CH_3^\bullet$	306.60	339.13	307.15	309.93	305.11	303.24	304.76	307.05
CH_4	419.20	462.32	417.08	420.00	416.42	415.24	415.93	418.12
^3NH	83.50	95.14	89.35	88.30	83.36	80.37	77.39	82.22
$NH_2^\bullet$	181.50	207.55	189.36	188.36	181.35	178.44	173.05	180.17
NH_3	297.50	337.03	301.67	301.78	294.62	294.83	287.46	290.60
$OH^\bullet$	106.40	123.90	109.54	109.69	105.32	109.55	103.50	103.90
H_2O	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_2	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_2H_2	405.30	459.55	405.10	414.68	403.33	404.96	400.23	405.50
$H_2C{=}CH_2$	562.60	632.23	561.00	571.50	561.46	562.07	559.72	562.28
$H_3C{-}CH_3$	710.80	793.89	704.65	716.68	707.77	708.49	706.84	709.99
$CN^\bullet$	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
$HCO^\bullet$	278.70	332.41	287.12	295.04	280.39	289.84	278.74	280.21
$H_2C{=}O$	373.60	433.19	377.88	385.76	373.05	380.52	371.48	372.79
$CH_3{-}OH$	511.90	586.04	510.83	519.81	508.38	515.72	508.19	505.78
N_2	228.60	264.92	238.78	242.02	225.32	219.58	202.18	222.27
$H_2N{-}NH_2$	437.80	515.23	447.36	452.83	435.99	435.74	421.82	427.83
$NO^\bullet$	152.80	198.41	165.99	171.70	155.45	160.14	142.89	151.04
O_2	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_2	38.50	77.44	48.81	52.67	36.99	52.03	45.56	36.33
CO_2	389.10	472.24	399.96	416.14	393.46	414.40	390.36	397.00
$^1SiH_2$	151.30	166.03	151.98	147.87	151.12	151.27	150.62	154.90
$^3SiH_2$	131.20	147.03	130.61	131.73	130.37	134.65	132.33	135.78
$SiH_3^\bullet$	225.10	246.76	224.60	222.56	224.22	225.19	225.78	231.45
SiH_4	321.40	347.29	318.08	313.65	318.38	317.27	319.68	328.00
$PH_2^\bullet$	152.90	173.60	157.53	154.47	154.82	156.40	156.39	153.61
PH_3	241.80	269.49	242.44	239.05	240.48	243.43	244.09	240.62
H_2S	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_2	101.60	134.95	107.70	115.25	109.15	122.65	119.97	110.27
Cl_2	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
$ClO^\bullet$	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_3Cl	393.90	447.03	389.72	399.88	393.71	396.64	397.95	395.62
$H_3C{-}SH$	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_2	258.40	333.70	266.54	280.06	254.53	286.58	263.28	255.91
BF_3	469.90	547.86	468.67	481.43	467.54	480.55	483.16	464.55
BCl_3	322.70	381.67	311.54	335.24	326.21	340.06	343.34	335.99
AlF_3	426.50	482.41	421.70	427.54	420.08	429.87	437.93	417.41
$AlCl_3$	306.10	343.60	289.54	306.55	307.01	318.93	320.07	320.04
CF_4	476.30	598.18	476.84	503.37	478.71	503.68	496.36	472.20
CCl_4	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_2	277.70	343.37	284.87	301.31	287.21	305.80	301.53	294.39
COF_2	426.70	523.28	427.05	448.19	423.53	446.54	431.46	421.27
SiF_4	572.80	655.11	561.29	572.74	562.35	575.29	583.91	558.42
$SiCl_4$	383.30	443.12	357.97	386.25	382.37	402.54	404.75	399.51
N_2O	270.50	359.03	295.73	309.39	275.35	289.31	258.19	277.95
ClNO	191.20	264.81	213.26	224.24	194.82	213.81	192.87	199.03
NF_3	205.20	311.76	228.73	245.24	210.93	234.40	217.98	205.48

PF_3	363.90	442.62	367.24	376.02	361.15	381.98	378.82	353.08
O_3	147.10	239.05	169.80	183.71	140.36	179.36	145.47	143.04
F_2O	93.30	170.08	114.15	123.37	93.84	119.90	104.46	91.44
ClF_3	125.60	229.19	150.34	166.04	131.25	167.47	159.12	128.79
$F_2C{=}CF_2$	583.90	743.97	596.93	630.75	595.62	624.63	614.71	590.57
$Cl_2C{=}CCl_2$	466.80	589.13	456.03	500.87	474.57	497.58	494.82	483.83
CF_3CN	639.70	788.31	648.49	680.58	642.48	663.34	645.25	639.09
$CH{\equiv}C{-}CH_3$	704.20	801.33	701.60	720.79	703.77	706.84	700.55	707.21
$CH_2{=}C{=}CH_2$	702.40	804.69	704.63	723.84	705.71	710.12	703.90	708.02
C_3H_4	682.10	784.50	677.04	701.54	684.47	687.04	681.02	689.15
$CH_2{=}CHCH_3$	859.20	970.32	853.41	873.56	857.66	860.06	855.73	859.56
C_3H_6	851.90	968.30	842.43	868.17	852.90	854.66	850.36	856.75
C_3H_8	1004.60	1127.93	993.32	1014.86	1000.24	1002.86	998.97	1003.32
C_4H_6	1011.20	1150.48	1006.51	1034.53	1011.38	1015.81	1009.01	1013.47
C_4H_6	1002.80	1141.65	996.73	1025.54	1002.90	1006.98	999.51	1007.47
C_4H_6	989.50	1137.86	984.54	1018.44	995.47	1000.64	992.52	999.77
C_4H_{10}	1298.50	1461.93	1281.89	1312.97	1292.66	1296.56	1291.02	1296.67
C_4H_{10}	1300.30	1463.65	1282.26	1313.73	1293.11	1297.37	1291.56	1297.60
C_5H_8	1282.40	1474.06	1266.51	1315.40	1287.61	1293.96	1283.55	1294.24
C_6H_6	1366.00	1573.22	1357.14	1409.54	1373.29	1382.06	1370.32	1375.41
H_2CF_2	436.20	516.73	438.02	450.85	436.58	447.15	445.77	432.20
HCF_3	457.70	558.88	459.30	478.73	458.99	477.15	472.76	453.02
H_2CCl_2	369.60	433.53	362.44	380.42	370.55	379.79	380.17	373.24
$HCCl_3$	343.30	418.89	332.60	358.92	344.60	360.33	359.87	348.79
$H_3C{-}NH_2$	581.20	660.70	582.19	590.76	578.20	577.93	570.68	575.10
$CH_3{-}CN$	615.10	704.78	619.85	635.19	615.00	615.25	603.10	616.46
$CH_3{-}NO_2$	600.60	742.58	618.21	641.75	603.58	625.39	597.06	600.63
$CH_3{-}O{-}N{=}O$	598.30	735.21	615.02	636.53	598.21	617.60	590.75	597.60
$CH_3{-}SiH_3$	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
$HCOOCH_3$	784.20	921.18	787.57	811.20	783.61	800.18	783.38	783.20
CH_3CONH_2	867.10	1010.50	870.74	895.27	867.03	879.07	860.17	863.94
$CH_2{-}NH{-}CH_2$	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
$(CH_3)_2CH$	868.80	989.19	865.65	883.21	864.72	866.01	857.06	862.98
$CH_3{-}CH_2{-}NH_2$	875.70	996.89	872.87	890.94	872.52	874.43	864.82	870.12
$H_2C{=}C{=}O$	531.90	626.90	540.41	558.07	537.05	550.18	535.43	539.76
$CH_2{-}O{-}CH_2$	649.90	756.40	648.35	669.86	651.07	659.14	648.85	652.52
CH_3CHO	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_3CH_2OH	808.80	923.52	802.85	821.21	804.00	813.81	803.67	802.36
$CH_3{-}O{-}CH_3$	796.80	911.52	792.73	809.78	792.44	799.76	792.16	792.20
$CH_2{-}S{-}CH_2$	623.00	719.59	616.25	639.93	626.83	634.39	632.42	630.94
$(CH_3)_2SO$	854.10	992.22	847.62	874.44	850.90	871.71	858.59	851.50
$CH_3{-}CH_2{-}SH$	767.60	870.84	757.07	776.88	764.97	772.46	770.53	766.19
$CH_3{-}S{-}CH_3$	766.00	869.50	756.93	776.63	764.48	772.40	770.47	765.81
$H_2C{=}CHF$	571.30	663.47	573.87	589.87	573.45	580.93	577.28	572.35
$CH_3{-}CH_2{-}Cl$	690.10	783.45	680.77	700.39	688.44	693.75	692.56	691.31
$H_2C{=}CHCl$	538.60	624.54	538.79	557.49	543.72	549.78	547.43	546.03
$H_2C{=}CHCN$	763.30	878.86	767.76	790.68	763.17	765.89	750.88	764.76
$CH_3{-}CO{-}CH_3$	977.20	1120.35	972.76	999.92	975.46	986.95	973.92	977.19
CH_3COOH	802.20	939.28	802.65	828.04	800.82	820.38	800.44	798.83
CH_3COF	705.40	828.76	707.59	731.24	706.40	723.06	710.29	705.80
CH_3COCl	666.90	782.97	666.77	692.47	669.06	685.54	673.91	672.84
$CH_3CH_2CH_2Cl$	983.80	1117.39	969.36	998.51	980.89	987.52	984.64	984.67
$(CH_3)_2CH{-}OH$	1106.40	1261.78	1094.42	1122.59	1099.32	1110.60	1098.82	1099.03
$CH_3{-}CH_2{-}O{-}CH_3$	1093.30	1248.85	1084.63	1111.07	1088.00	1097.41	1087.51	1088.84
$(CH_3)_3N$	1158.60	1320.77	1150.42	1177.48	1152.64	1156.12	1144.85	1152.92
C_4H_4O	993.00	1164.94	989.91	1031.41	997.57	1014.63	996.98	997.52
C_4H_4S	962.10	1121.38	952.88	996.83	968.42	984.67	974.41	970.13
C_4H_4NH	1070.40	1249.85	1068.98	1111.03	1076.54	1086.83	1069.20	1074.17
C_5H_5N	1236.40	1440.09	1236.84	1285.24	1245.07	1252.90	1235.08	1244.50
$SH^\bullet$	86.90	99.55	87.75	87.98	87.38	90.08	89.97	86.91
$C_2H_3^\bullet$	444.00	507.08	446.61	457.50	445.94	447.47	444.72	448.85
$CH_3CO^\bullet$	580.90	676.54	586.31	603.52	583.16	594.73	581.87	583.61
$H_2COH^\bullet$	408.90	476.92	412.11	421.35	408.00	416.99	408.22	404.90
$CH_3O^\bullet$	400.50	463.72	404.46	412.45	400.86	405.32	399.74	400.88
$CH_3CH_2O^\bullet$	697.10	799.88	693.11	710.44	693.11	702.42	691.95	693.81
$CH_3S^\bullet$	380.60	435.59	379.87	389.27	382.64	386.61	385.73	382.46
$C_2H_5^\bullet$	602.20	677.03	599.82	611.85	601.47	602.00	600.55	604.31
$(CH_3)_2CH^\bullet$	898.80	1015.70	892.59	914.18	898.02	901.24	896.82	902.02

$NO_2^{\bullet}$	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_2	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
^2CH	83.80	86.23	83.44	85.47	85.40	82.86	84.68	84.36
$^3CH_2$	190.00	186.29	185.76	192.01	192.18	193.65	191.99	192.28
$^1CH_2$	180.70	183.16	183.33	180.78	180.79	176.22	182.56	182.62
$CH_3^{\bullet}$	306.60	303.27	306.02	306.24	310.12	308.43	309.90	307.68
CH_4	419.20	415.57	419.24	416.40	421.13	417.77	421.27	419.63
^3NH	83.50	85.49	82.12	84.56	87.92	85.08	84.28	82.41
$NH_2^{\bullet}$	181.50	186.08	186.58	182.89	187.82	182.93	183.04	181.10
NH_3	297.50	298.33	301.00	295.03	300.94	294.89	296.53	294.77
$OH^{\bullet}$	106.40	107.18	106.98	105.03	108.02	105.47	105.86	106.12
H_2O	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_2	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_2H_2	405.30	394.72	401.24	400.84	402.92	403.96	403.10	404.89
$H_2C{=}CH_2$	562.60	554.08	561.17	559.15	563.46	563.80	562.43	562.29
$H_3C{-}CH_3$	710.80	703.40	710.07	706.25	711.83	712.10	713.94	711.81
$CN^{\bullet}$	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
$HCO^{\bullet}$	278.70	274.41	273.89	278.32	280.08	280.03	279.74	279.82
$H_2C{=}O$	373.60	366.92	369.96	371.86	373.26	371.91	374.11	374.84
$CH_3{-}OH$	511.90	504.45	509.59	506.87	511.49	509.64	511.97	512.10
N_2	228.60	223.43	223.66	227.49	226.88	222.45	220.77	219.78
$H_2N{-}NH_2$	437.80	438.42	444.17	435.16	443.96	437.89	436.28	434.45
$NO^{\bullet}$	152.80	149.07	147.65	151.88	155.07	153.32	150.32	149.70
O_2	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_2	38.50	27.94	40.13	37.48	36.60	34.07	28.07	33.02
CO_2	389.10	386.74	384.47	393.90	386.92	390.41	395.73	396.68
$^1SiH_2$	151.30	153.53	154.80	155.04	153.81	147.35	153.60	157.83
$^3SiH_2$	131.20	134.16	138.86	140.47	133.28	132.43	132.03	133.62
$SiH_3^{\bullet}$	225.10	231.12	233.92	235.86	228.81	223.82	227.01	230.96
SiH_4	321.40	325.90	329.55	330.44	324.11	315.66	322.29	328.75
$PH_2^{\bullet}$	152.90	154.11	154.32	156.84	158.70	153.15	154.67	157.02
PH_3	241.80	241.53	241.90	244.09	244.85	237.45	240.44	244.62
H_2S	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_2	101.60	115.18	105.92	107.17	103.32	106.62	106.13	105.36
Cl_2	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
$ClO^{\bullet}$	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_3Cl	393.90	392.15	394.91	394.91	392.82	395.48	398.01	395.69
$H_3C{-}SH$	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_2	258.40	252.02	247.74	257.49	249.49	250.13	252.08	254.22
BF_3	469.90	458.82	477.02	470.84	464.49	466.15	470.07	474.11
BCl_3	322.70	330.82	339.52	337.45	313.64	329.13	328.74	328.04
AlF_3	426.50	404.17	425.43	422.09	417.03	413.32	424.77	421.30
$AlCl_3$	306.10	316.36	325.95	322.62	294.61	305.62	313.60	311.38
CF_4	476.30	467.92	481.26	486.65	468.35	478.33	480.43	483.29
CCl_4	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_2	277.70	293.85	288.85	290.34	276.71	283.74	285.15	284.72
COF_2	426.70	412.21	419.35	426.30	415.28	421.61	424.49	426.52
SiF_4	572.80	551.20	573.20	572.02	557.46	555.64	565.28	567.08
$SiCl_4$	383.30	388.29	403.77	404.85	363.99	382.93	390.66	390.17
N_2O	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_3	205.20	200.31	210.94	217.08	207.49	208.72	204.02	205.06
PF_3	363.90	343.11	358.35	364.55	358.74	355.72	358.52	365.52
O_3	147.10	127.60	128.38	141.95	137.68	135.00	132.60	133.48
F_2O	93.30	80.41	94.20	95.73	92.91	90.27	81.54	86.87

ClF_3	125.60	114.76	124.72	130.01	128.36	129.50	123.82	127.75
$F_2C{=}CF_2$	583.90	570.63	593.38	597.75	583.37	595.96	592.43	598.60
$Cl_2C{=}CCl_2$	466.80	473.27	472.88	484.41	452.51	480.44	474.85	474.35
CF_3CN	639.70	626.42	640.37	647.10	632.47	642.68	639.70	642.84
$CH{\equiv}C{-}CH_3$	704.20	691.80	701.75	699.90	702.44	707.44	704.84	706.00
$CH_2{=}C{=}CH_2$	702.40	693.98	704.55	702.48	704.58	709.31	703.74	705.11
C_3H_4	682.10	670.75	679.62	681.34	678.85	688.71	689.37	686.98
$CH_2{=}CHCH_3$	859.20	847.52	857.58	854.74	858.94	863.26	860.02	859.62
C_3H_6	851.90	840.06	851.23	850.14	849.95	859.56	860.27	856.59
C_3H_8	1004.60	993.11	1002.63	998.36	1003.74	1007.90	1008.03	1005.82
C_4H_6	1011.20	995.62	1009.32	1007.47	1009.98	1018.05	1009.52	1010.97
C_4H_6	1002.80	987.44	1000.77	997.54	1000.61	1009.60	1005.31	1005.84
C_4H_6	989.50	977.39	991.49	991.37	989.61	1003.16	999.18	996.84
C_4H_{10}	1298.50	1282.72	1295.19	1290.49	1295.57	1303.64	1302.04	1299.86
C_4H_{10}	1300.30	1284.04	1296.49	1292.23	1296.08	1304.44	1302.72	1301.32
C_5H_8	1282.40	1263.49	1281.63	1283.02	1276.98	1299.64	1297.66	1291.61
C_6H_6	1366.00	1346.32	1367.93	1367.28	1361.82	1385.70	1363.25	1367.33
H_2CF_2	436.20	424.53	436.34	436.99	434.79	436.34	438.84	438.77
HCF_3	457.70	446.38	459.61	462.76	453.13	458.61	460.87	461.83
H_2CCl_2	369.60	369.92	370.41	373.95	364.05	373.02	374.51	371.69
$HCCl_3$	343.30	346.50	344.01	351.40	332.45	348.04	348.15	345.84
$H_3C{-}NH_2$	581.20	577.41	583.90	577.35	584.31	581.27	581.61	579.69
$CH_3{-}CN$	615.10	607.12	613.56	613.59	615.31	616.81	614.72	614.09
$CH_3{-}NO_2$	600.60	591.05	593.16	602.05	601.76	604.13	601.41	599.69
$CH_3{-}O{-}N{=}O$	598.30	588.56	592.59	600.89	597.97	598.64	597.06	596.98
$CH_3{-}SiH_3$	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
$HCOOCH_3$	784.20	771.39	780.08	783.62	782.14	785.91	786.65	788.53
CH_3CONH_2	867.10	858.81	868.26	865.47	867.78	871.63	868.68	868.51
$CH_2{-}NH{-}CH_2$	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
$(CH_3)_2CH$	868.80	860.61	870.59	864.16	870.72	871.02	870.01	868.44
$CH_3{-}CH_2{-}NH_2$	875.70	868.93	878.22	871.39	878.12	878.94	877.52	875.36
$H_2C{=}C{=}O$	531.90	527.83	532.80	535.43	533.46	537.43	537.29	538.30
$CH_2{-}O{-}CH_2$	649.90	638.66	647.07	650.87	647.75	654.03	656.26	654.04
CH_3CHO	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_3CH_2OH	808.80	797.39	805.32	802.09	806.71	808.60	809.26	809.09
$CH_3{-}O{-}CH_3$	796.80	784.72	794.18	791.99	796.04	796.65	798.37	798.76
$CH_2{-}S{-}CH_2$	623.00	619.29	625.64	626.43	619.90	630.19	632.72	628.92
$(CH_3)_2SO$	854.10	846.58	851.12	853.80	848.55	855.16	854.14	853.30
$CH_3{-}CH_2{-}SH$	767.60	762.60	768.44	766.03	764.33	769.50	768.63	767.84
$CH_3{-}S{-}CH_3$	766.00	760.03	767.75	765.36	763.75	768.78	768.81	767.23
$H_2C{=}CHF$	571.30	560.43	572.43	571.73	572.15	575.22	573.17	574.18
$CH_3{-}CH_2{-}Cl$	690.10	684.25	689.73	689.20	687.03	693.51	694.36	691.86
$H_2C{=}CHCl$	538.60	537.14	542.63	543.79	539.78	546.75	544.38	543.51
$H_2C{=}CHCN$	763.30	749.31	759.52	760.46	760.90	765.89	758.66	759.76
$CH_3{-}CO{-}CH_3$	977.20	963.40	972.63	973.35	974.53	981.05	979.58	979.42
CH_3COOH	802.20	791.12	797.57	799.85	798.13	803.63	803.36	804.73
CH_3COF	705.40	692.91	702.23	705.95	702.22	708.10	708.65	709.17
CH_3COCl	666.90	662.52	665.49	670.51	662.88	671.86	672.30	671.62
$CH_3CH_2CH_2Cl$	983.80	973.77	982.25	981.28	978.88	989.28	988.36	985.87
$(CH_3)_2CH{-}OH$	1106.40	1090.69	1101.39	1098.16	1101.61	1107.56	1106.36	1106.69
$CH_3{-}CH_2{-}O{-}CH_3$	1093.30	1077.63	1089.91	1087.16	1091.16	1095.55	1095.56	1095.75
$(CH_3)_3N$	1158.60	1146.42	1159.82	1154.16	1158.60	1162.62	1160.08	1159.88
C_4H_4O	993.00	977.26	993.75	995.12	987.94	1005.57	992.64	995.62
C_4H_4S	962.10	953.59	966.20	967.89	954.46	976.31	961.94	962.60
C_4H_4NH	1070.40	1059.00	1076.62	1072.66	1069.43	1086.82	1070.49	1071.50
C_5H_5N	1236.40	1221.56	1241.87	1241.30	1235.73	1255.77	1233.88	1237.43
$SH^\bullet$	86.90	90.44	89.60	88.62	88.23	86.78	87.11	87.37
$C_2H_3^\bullet$	444.00	440.50	445.34	444.11	447.44	449.72	447.05	447.03
$CH_3CO^\bullet$	580.90	573.46	576.59	579.72	582.18	585.75	584.10	582.99
$H_2COH^\bullet$	408.90	402.61	406.21	405.65	410.73	410.52	410.35	409.62
$CH_3O^\bullet$	400.50	396.38	400.28	398.62	403.56	402.79	402.89	402.18
$CH_3CH_2O^\bullet$	697.10	685.87	692.70	690.29	695.42	698.39	696.71	695.70
$CH_3S^\bullet$	380.60	379.88	383.25	381.43	382.49	384.50	384.00	382.81
$C_2H_5^\bullet$	602.20	596.60	602.11	600.46	605.44	607.32	607.69	604.69
$(CH_3)_2CH^\bullet$	898.80	890.79	898.90	895.97	901.08	906.78	905.95	902.50
$NO_2^\bullet$	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_2	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
^2CH	83.80	83.77	81.89	83.36	83.01	82.48	84.73	83.48
$^3CH_2$	190.00	187.64	187.69	189.91	192.18	188.58	192.19	188.31
$^1CH_2$	180.70	179.33	177.77	178.70	178.63	178.51	180.94	178.94
$CH_3^\bullet$	306.60	305.63	305.39	306.98	305.93	306.73	308.70	306.06
CH_4	419.20	417.73	416.58	419.66	417.64	418.52	422.37	417.70
^3NH	83.50	84.34	81.81	85.41	83.02	82.99	85.15	84.14
$NH_2^\bullet$	181.50	182.96	182.15	184.48	180.49	181.29	181.22	182.56
NH_3	297.50	295.80	296.85	298.96	295.25	296.26	299.94	296.04
$OH^\bullet$	106.40	105.20	106.76	106.74	106.09	105.85	104.39	105.37
H_2O	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_2	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_2H_2	405.30	400.46	402.70	401.96	403.35	402.24	404.99	399.44
$H_2C{=}CH_2$	562.60	561.34	559.98	562.37	561.05	562.26	566.57	559.87
$H_3C{-}CH_3$	710.80	710.40	707.20	712.21	709.50	711.02	716.40	710.78
$CN^\bullet$	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
$HCO^\bullet$	278.70	276.26	277.92	281.52	277.52	276.23	273.38	278.10
$H_2C{=}O$	373.60	370.07	372.89	374.93	372.08	370.84	371.68	371.39
$CH_3{-}OH$	511.90	508.04	511.44	512.42	511.49	511.69	516.50	509.49
N_2	228.60	224.87	224.40	226.14	223.26	221.66	223.51	226.42
$H_2N{-}NH_2$	437.80	438.02	440.43	442.30	436.40	437.02	444.45	439.42
$NO^\bullet$	152.80	152.35	153.53	154.00	151.46	149.76	149.23	156.19
O_2	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_2	38.50	29.21	38.29	31.64	32.25	28.95	29.35	37.36
CO_2	389.10	385.05	390.76	393.21	388.48	385.48	372.83	388.08
$^1SiH_2$	151.30	151.25	152.64	153.14	153.32	150.93	150.54	152.53
$^3SiH_2$	131.20	129.12	134.61	131.03	134.58	127.45	135.05	131.23
$SiH_3^\bullet$	225.10	224.44	229.57	226.82	227.47	221.87	225.67	227.89
SiH_4	321.40	320.36	324.67	323.24	320.76	316.59	316.36	324.56
$PH_2^\bullet$	152.90	154.68	154.66	155.86	156.62	155.84	159.35	155.37
PH_3	241.80	241.13	241.61	243.24	242.57	241.71	245.67	241.41
H_2S	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_2	101.60	104.85	103.49	103.70	104.79	108.49	104.34	100.20
Cl_2	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
$ClO^\bullet$	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_3Cl	393.90	394.39	393.67	396.49	394.45	395.22	399.52	394.04
$H_3C{-}SH$	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_2	258.40	243.79	254.04	253.44	248.61	247.99	236.56	248.42
BF_3	469.90	460.41	480.07	473.62	474.05	479.04	475.41	468.06
BCl_3	322.70	325.31	331.67	331.49	326.95	326.45	322.35	324.43
AlF_3	426.50	412.47	432.22	420.97	425.20	433.13	435.89	430.67
$AlCl_3$	306.10	306.44	315.54	312.82	310.90	310.97	306.21	310.51
CF_4	476.30	469.63	488.50	477.99	480.39	482.37	479.91	481.05
CCl_4	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_2	277.70	279.70	282.99	280.69	280.22	281.48	272.95	271.11
COF_2	426.70	413.92	427.18	422.30	421.07	420.37	413.59	421.93
SiF_4	572.80	553.40	581.49	567.11	574.97	585.05	587.29	571.36
$SiCl_4$	383.30	382.21	392.91	392.59	387.61	386.47	382.83	385.32
N_2O	270.50	265.86	269.54	267.12	263.17	259.67	246.33	268.66
ClNO	191.20	185.50	189.13	189.14	184.78	182.11	172.17	185.77
NF_3	205.20	200.59	214.39	204.47	204.11	203.32	201.19	214.15
PF_3	363.90	352.23	370.82	364.45	366.58	373.25	376.29	364.19
O_3	147.10	122.70	135.90	129.09	124.27	118.69	101.18	133.73
F_2O	93.30	82.18	95.87	86.56	87.02	83.39	82.24	93.87
ClF_3	125.60	114.93	130.10	121.74	123.03	127.24	125.42	128.68
$F_2C{=}CF_2$	583.90	581.61	605.20	591.07	592.95	593.88	590.17	593.78
$Cl_2C{=}CCl_2$	466.80	469.78	476.27	469.77	473.16	472.50	472.21	469.54

CF_3CN	639.70	632.54	647.79	641.15	640.32	639.83	635.68	642.04
$CH{\equiv}C{-}CH_3$	704.20	701.73	701.84	703.06	703.62	702.95	706.41	700.73
$CH_2{=}C{=}CH_2$	702.40	702.97	702.57	703.91	703.34	703.69	706.52	700.30
C_3H_4	682.10	682.59	682.06	680.85	683.51	681.92	684.15	683.26
$CH_2{=}CHCH_3$	859.20	858.72	855.75	859.74	857.91	859.70	864.85	857.86
C_3H_6	851.90	854.45	851.62	853.82	854.11	854.41	859.26	856.40
C_3H_8	1004.60	1004.39	999.78	1006.31	1003.28	1005.53	1012.57	1005.68
C_4H_6	1011.20	1010.54	1007.47	1010.71	1009.36	1011.52	1015.70	1007.16
C_4H_6	1002.80	1001.74	999.74	1002.84	1002.68	1002.41	1006.71	1000.78
C_4H_6	989.50	994.68	992.21	993.43	994.01	993.99	997.25	995.04
C_4H_{10}	1298.50	1298.34	1292.40	1300.41	1297.08	1300.04	1308.74	1300.57
C_4H_{10}	1300.30	1299.06	1293.86	1301.41	1298.44	1301.50	1310.42	1301.79
C_5H_8	1282.40	1288.88	1284.92	1285.81	1288.27	1287.69	1292.40	1292.86
C_6H_6	1366.00	1370.90	1365.70	1368.94	1367.48	1371.57	1370.82	1364.41
H_2CF_2	436.20	432.22	441.25	437.85	437.48	439.99	443.74	438.16
HCF_3	457.70	452.16	466.06	459.35	460.09	462.55	463.60	460.94
H_2CCl_2	369.60	370.32	370.75	372.43	370.96	371.53	375.46	369.94
$HCCl_3$	343.30	343.41	345.91	345.52	345.13	345.41	348.69	343.39
$H_3C{-}NH_2$	581.20	580.59	580.34	583.99	579.70	580.85	588.05	581.19
$CH_3{-}CN$	615.10	613.68	613.03	617.61	613.48	612.65	615.24	613.67
$CH_3{-}NO_2$	600.60	595.84	601.41	600.02	596.22	594.88	590.36	602.72
$CH_3{-}O{-}N{=}O$	598.30	592.18	600.20	597.94	594.44	591.47	589.66	599.34
$CH_3{-}SiH_3$	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
$HCOOCH_3$	784.20	779.88	787.36	789.11	785.93	784.77	786.84	783.98
CH_3CONH_2	867.10	865.70	868.58	873.08	866.64	867.39	869.00	868.95
$CH_2{-}NH{-}CH_2$	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
$(CH_3)_2CH$	868.80	868.56	867.71	872.40	867.98	869.31	879.99	869.98
$CH_3{-}CH_2{-}NH_2$	875.70	876.38	874.74	879.94	875.24	877.14	885.79	877.87
$H_2C{=}C{=}O$	531.90	531.11	534.59	536.53	533.55	531.97	527.82	531.72
$CH_2{-}O{-}CH_2$	649.90	649.44	652.49	652.55	652.26	651.15	653.12	651.97
CH_3CHO	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_3CH_2OH	808.80	805.15	806.98	809.61	808.20	809.13	814.91	807.47
$CH_3{-}O{-}CH_3$	796.80	793.52	796.91	798.96	797.52	797.77	806.30	795.67
$CH_2{-}S{-}CH_2$	623.00	626.84	625.37	627.27	627.15	627.83	631.31	626.30
$(CH_3)_2SO$	854.10	849.91	851.88	853.61	851.50	854.92	857.56	852.48
$CH_3{-}CH_2{-}SH$	767.60	767.62	766.26	768.29	767.24	769.98	777.05	767.85
$CH_3{-}S{-}CH_3$	766.00	766.77	765.33	768.16	766.75	769.47	777.78	766.86
$H_2C{=}CHF$	571.30	569.82	574.55	573.31	572.51	574.04	576.97	571.93
$CH_3{-}CH_2{-}Cl$	690.10	690.54	688.36	692.80	690.28	691.84	697.45	690.94
$H_2C{=}CHCl$	538.60	542.39	542.26	543.44	542.64	543.40	546.65	540.96
$H_2C{=}CHCN$	763.30	759.81	759.22	762.81	759.17	758.51	759.87	757.70
$CH_3{-}CO{-}CH_3$	977.20	974.99	974.77	980.23	976.03	976.54	977.78	978.01
CH_3COOH	802.20	797.10	802.88	805.10	802.04	801.33	799.75	801.21
CH_3COF	705.40	701.13	707.43	708.18	705.14	705.65	703.09	707.09
CH_3COCl	666.90	665.35	667.52	671.23	667.22	666.56	663.81	667.02
$CH_3CH_2CH_2Cl$	983.80	984.50	980.97	986.96	984.11	986.41	993.78	985.83
$(CH_3)_2CH{-}OH$	1106.40	1102.19	1103.25	1107.04	1105.54	1107.29	1114.37	1105.92
$CH_3{-}CH_2{-}O{-}CH_3$	1093.30	1090.60	1092.42	1096.13	1094.19	1095.16	1104.60	1093.61
$(CH_3)_3N$	1158.60	1158.26	1157.88	1162.89	1158.85	1160.49	1174.90	1161.08
C_4H_4O	993.00	992.72	998.01	997.95	995.36	995.66	997.21	991.65
C_4H_4S	962.10	965.14	964.84	963.16	963.49	967.05	967.61	960.18
C_4H_4NH	1070.40	1074.38	1075.55	1078.41	1073.10	1075.17	1080.53	1072.06
C_5H_5N	1236.40	1242.45	1239.65	1243.24	1238.54	1241.28	1242.64	1236.79
$SH^\bullet$	86.90	87.39	88.27	86.92	87.41	88.29	89.38	86.99
$C_2H_3^\bullet$	444.00	444.11	443.74	444.89	444.77	444.69	445.90	443.30
$CH_3CO^\bullet$	580.90	579.87	579.91	585.21	580.19	579.92	577.97	582.15
$H_2COH^\bullet$	408.90	406.00	410.06	410.20	409.08	409.38	410.87	408.18
$CH_3O^\bullet$	400.50	400.64	401.09	403.31	400.47	400.61	400.86	401.02
$CH_3CH_2O^\bullet$	697.10	696.95	693.55	697.25	693.97	694.86	696.58	695.68
$CH_3S^\bullet$	380.60	383.15	382.01	383.74	382.53	384.59	387.82	382.93
$C_2H_5^\bullet$	602.20	602.72	600.43	603.75	601.83	603.33	605.27	603.51
$(CH_3)_2CH^\bullet$	898.80	900.27	896.34	901.13	898.68	900.80	903.17	901.67
$NO_2^\bullet$	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_2	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
^2CH	83.80	83.12	83.05	80.56	83.49	83.22	56.81	83.73

$^3CH_2$	190.00	189.97	190.75	190.35	188.53	188.38	155.09	190.61
$^1CH_2$	180.70	178.71	178.71	174.95	180.60	180.21	126.76	178.91
$CH_3^\bullet$	306.60	306.85	307.27	304.99	303.53	307.74	243.00	307.92
CH_4	419.20	418.61	419.19	415.50	415.95	420.94	328.23	419.09
^3NH	83.50	83.94	83.98	81.13	82.45	83.81	51.16	85.03
$NH_2^\bullet$	181.50	182.69	182.93	178.34	182.17	186.83	117.45	184.26
NH_3	297.50	296.57	297.13	291.99	297.17	304.42	200.59	298.19
$OH^\bullet$	106.40	106.02	106.53	106.25	107.14	107.84	68.04	106.73
H_2O	232.20	228.70	229.82	229.22	230.98	234.77	155.06	230.49
HF	140.80	137.96	138.51	139.13	139.54	142.91	96.14	139.50
Li_2	24.40	21.35	20.12	16.25	39.49	23.14	3.98	20.80
LiF	137.50	136.45	133.40	134.99	139.39	138.82	89.81	136.99
C_2H_2	405.30	400.48	400.74	399.37	396.76	402.31	292.57	404.41
$H_2C{=}CH_2$	562.60	561.22	561.78	559.45	556.05	562.10	428.35	562.11
$H_3C{-}CH_3$	710.80	711.53	711.87	707.92	704.76	712.73	551.40	710.03
$CN^\bullet$	180.90	174.04	174.13	170.93	172.03	176.50	90.75	179.43
HCN	312.60	308.59	308.30	302.92	306.03	313.09	196.23	313.96
CO	259.30	255.72	255.53	252.71	254.54	257.82	171.97	257.93
$HCO^\bullet$	278.70	278.29	278.75	278.04	274.25	278.92	181.20	280.45
$H_2C{=}O$	373.60	371.92	372.45	371.53	369.57	373.59	256.24	373.45
$CH_3{-}OH$	511.90	510.55	511.18	510.40	508.88	514.86	368.83	510.53
N_2	228.60	224.20	222.58	212.05	220.27	229.92	109.32	229.03
$H_2N{-}NH_2$	437.80	439.24	439.22	432.17	438.28	450.55	267.26	439.25
$NO^\bullet$	152.80	154.40	153.28	148.33	147.37	156.32	54.11	154.78
O_2	120.50	122.32	122.12	119.39	112.26	117.34	27.50	122.31
$HO{-}OH$	268.70	264.36	265.34	266.43	267.88	269.85	132.28	265.57
F_2	38.50	35.64	35.06	37.94	37.56	35.46	-38.16	35.84
CO_2	389.10	388.14	388.91	390.39	384.26	389.20	243.34	390.71
$^1SiH_2$	151.30	153.27	153.22	150.12	152.61	153.99	110.65	152.14
$^3SiH_2$	131.20	132.33	132.75	133.37	129.96	133.86	106.66	132.04
$SiH_3^\bullet$	225.10	228.42	228.19	226.53	227.24	229.09	180.62	227.13
SiH_4	321.40	324.66	324.08	320.29	324.98	324.83	256.78	322.61
$PH_2^\bullet$	152.90	156.98	157.44	154.22	148.09	155.77	108.98	155.30
PH_3	241.80	243.58	244.40	240.48	236.05	242.64	172.83	241.47
H_2S	182.40	182.42	183.37	182.89	184.05	183.89	129.65	181.23
HCl	106.30	105.68	106.27	106.51	107.89	107.52	76.98	105.38
S_2	101.60	102.92	104.94	111.61	107.67	104.01	50.78	103.54
Cl_2	58.00	57.38	58.81	63.63	60.92	60.12	18.77	56.35
NaCl	98.00	101.44	99.01	98.49	104.38	101.47	69.81	94.76
SiO	192.30	186.86	186.49	187.73	184.39	187.06	108.46	191.64
CS	171.30	165.60	166.97	167.97	169.40	165.72	96.75	169.53
SO	125.10	124.86	125.89	128.24	124.42	125.14	52.17	126.75
$ClO^\bullet$	64.40	64.56	65.45	69.04	65.33	65.17	5.82	63.68
ClF	61.50	60.98	60.99	64.93	62.49	63.68	6.99	60.49
CH_3Cl	393.90	394.66	394.82	395.53	392.38	396.28	296.69	392.92
$H_3C{-}SH$	473.00	474.11	474.59	474.68	471.32	475.27	350.97	471.31
HOCl	164.40	162.47	163.49	166.52	165.82	166.95	77.27	162.93
SO_2	258.40	250.02	251.64	256.20	249.51	250.64	99.51	255.74
BF_3	469.90	466.82	464.85	476.56	473.11	471.24	361.62	469.18
BCl_3	322.70	324.40	323.52	336.07	331.56	318.32	244.38	320.38
AlF_3	426.50	424.97	419.64	433.34	427.04	439.93	320.99	425.02
$AlCl_3$	306.10	309.59	307.70	319.59	317.43	311.33	244.27	303.63
CF_4	476.30	477.90	474.59	485.42	477.22	480.71	312.83	473.12
CCl_4	312.80	311.75	309.72	323.67	313.29	310.44	179.36	305.44
$O{=}C{=}S$	333.30	332.78	334.72	340.02	333.77	333.44	204.57	336.35
CS_2	277.70	274.50	278.06	288.38	282.31	274.71	163.91	280.83
COF_2	426.70	420.35	419.11	425.34	417.26	421.94	263.08	418.49
SiF_4	572.80	566.85	561.26	577.28	569.31	581.81	429.25	567.60
$SiCl_4$	383.30	385.06	383.28	399.36	390.25	382.06	284.56	376.39
N_2O	270.50	267.02	267.22	262.06	260.81	272.81	76.84	275.54
ClNO	191.20	186.25	188.22	186.89	186.37	188.61	39.71	192.49
NF_3	205.20	209.32	206.17	207.64	206.10	213.08	35.21	205.13
PF_3	363.90	363.26	360.29	368.10	354.04	367.13	234.30	361.74
O_3	147.10	132.73	134.43	134.99	127.86	131.14	-66.33	145.66
F_2O	93.30	91.53	90.55	94.32	92.53	92.51	-43.57	90.83
ClF_3	125.60	126.89	125.88	138.07	125.01	132.94	-23.30	127.43
$F_2C{=}CF_2$	583.90	591.11	588.50	602.48	586.99	592.78	373.85	585.84
$Cl_2C{=}CCl_2$	466.80	468.67	466.65	484.02	468.43	466.52	289.49	462.47
CF_3CN	639.70	638.50	634.89	640.81	632.84	640.77	396.62	639.00
$CH{\equiv}C{-}CH_3$	704.20	701.73	701.66	701.04	694.38	702.52	523.47	703.66
$CH_2{=}C{=}CH_2$	702.40	701.97	702.70	702.97	696.23	702.38	522.62	702.97

C_3H_4	682.10	682.20	680.55	681.89	673.38	683.80	497.20	679.25
$CH_2{=}CHCH_3$	859.20	859.02	859.27	856.90	849.92	858.85	655.24	857.93
C_3H_6	851.90	855.28	853.65	853.39	843.94	855.84	645.64	849.81
C_3H_8	1004.60	1006.16	1006.34	1001.69	995.23	1006.28	775.44	1002.62
C_4H_6	1011.20	1009.01	1009.65	1009.72	998.82	1007.39	761.92	1009.62
C_4H_6	1002.80	1001.70	1001.33	1001.37	990.73	1001.44	753.05	1001.74
C_4H_6	989.50	994.38	993.00	994.83	981.61	993.56	739.75	989.59
C_4H_{10}	1298.50	1300.77	1300.87	1295.43	1285.67	1299.88	999.41	1295.20
C_4H_{10}	1300.30	1301.85	1301.91	1296.11	1286.85	1301.15	999.67	1296.20
C_5H_8	1282.40	1289.72	1286.44	1289.50	1270.21	1288.40	959.37	1278.84
C_6H_6	1366.00	1366.49	1367.08	1373.88	1351.27	1361.72	1025.17	1366.21
H_2CF_2	436.20	436.84	435.50	439.88	433.97	440.11	309.31	435.51
HCF_3	457.70	458.64	456.27	464.02	456.51	461.63	312.10	455.84
H_2CCl_2	369.60	370.20	369.81	375.00	368.63	370.85	262.37	366.67
$HCCl_3$	343.30	343.18	342.04	351.67	342.81	342.72	223.74	338.15
$H_3C{-}NH_2$	581.20	581.64	581.92	576.52	578.27	588.03	416.54	581.28
$CH_3{-}CN$	615.10	613.34	612.71	608.14	606.82	616.80	431.23	616.51
$CH_3{-}NO_2$	600.60	601.58	600.99	599.33	590.20	605.50	337.84	602.12
$CH_3{-}O{-}N{=}O$	598.30	597.77	596.68	593.25	589.43	601.19	338.85	597.98
$CH_3{-}SiH_3$	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
$HCOOCH_3$	784.20	784.58	784.35	786.10	777.92	786.94	545.97	783.66
CH_3CONH_2	867.10	869.13	868.78	867.42	860.98	874.35	606.42	867.06
$CH_2{-}NH{-}CH_2$	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
$(CH_3)_2CH$	868.80	870.25	870.24	864.22	863.06	875.23	634.99	867.96
$CH_3{-}CH_2{-}NH_2$	875.70	878.08	878.14	872.11	870.39	883.25	642.26	875.70
$H_2C{=}C{=}O$	531.90	532.53	533.29	534.67	528.24	534.08	369.36	534.00
$CH_2{-}O{-}CH_2$	649.90	651.31	650.47	651.58	644.50	653.48	459.75	648.12
CH_3CHO	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_3CH_2OH	808.80	808.30	808.44	807.37	802.33	811.36	596.13	806.31
$CH_3{-}O{-}CH_3$	796.80	796.61	796.69	795.37	791.11	799.25	585.81	794.92
$CH_2{-}S{-}CH_2$	623.00	626.21	625.52	629.78	619.95	628.05	453.10	621.52
$(CH_3)_2SO$	854.10	853.62	853.82	856.97	846.65	854.51	600.88	850.30
$CH_3{-}CH_2{-}SH$	767.60	769.04	769.12	768.85	762.06	769.12	575.23	764.39
$CH_3{-}S{-}CH_3$	766.00	768.04	768.13	768.45	761.12	768.87	573.68	763.63
$H_2C{=}CHF$	571.30	572.17	571.86	573.87	567.03	573.56	418.16	571.72
$CH_3{-}CH_2{-}Cl$	690.10	691.37	691.15	691.55	684.92	691.85	522.88	687.81
$H_2C{=}CHCl$	538.60	541.87	541.98	544.51	537.70	541.96	398.54	540.70
$H_2C{=}CHCN$	763.30	758.00	757.75	755.24	750.10	759.62	532.07	762.80
$CH_3{-}CO{-}CH_3$	977.20	978.21	977.79	976.83	966.63	977.80	721.00	975.17
CH_3COOH	802.20	801.81	801.60	803.79	795.12	804.16	562.20	799.96
CH_3COF	705.40	706.20	705.10	708.22	698.16	707.15	498.60	704.05
CH_3COCl	666.90	667.39	667.45	671.22	661.45	667.21	469.25	665.48
$CH_3CH_2CH_2Cl$	983.80	985.98	985.66	985.31	975.32	985.48	746.88	980.44
$(CH_3)_2CH{-}OH$	1106.40	1106.37	1106.18	1104.22	1096.03	1108.42	822.82	1102.24
$CH_3{-}CH_2{-}O{-}CH_3$	1093.30	1094.31	1094.02	1092.28	1084.51	1095.76	813.05	1090.69
$(CH_3)_3N$	1158.60	1161.02	1160.67	1153.54	1150.16	1164.93	854.48	1156.87
C_4H_4O	993.00	992.91	993.01	1000.04	984.02	992.24	709.61	991.63
C_4H_4S	962.10	961.75	961.97	972.22	953.49	958.61	696.02	960.18
C_4H_4NH	1070.40	1072.97	1073.02	1076.57	1062.77	1075.95	765.99	1071.44
C_5H_5N	1236.40	1238.10	1238.27	1242.51	1225.43	1236.86	891.82	1238.72
$SH^\bullet$	86.90	87.92	88.40	87.94	87.67	88.35	61.06	87.07
$C_2H_3{}^\bullet$	444.00	444.74	445.15	444.74	439.90	444.98	337.61	445.13
$CH_3CO^\bullet$	580.90	582.31	582.21	582.21	573.46	582.41	415.11	582.20
$H_2COH^\bullet$	408.90	409.18	409.66	410.29	406.10	412.27	289.42	409.03
$CH_3O^\bullet$	400.50	401.86	401.95	401.95	398.73	401.84	291.55	400.10
$CH_3CH_2O^\bullet$	697.10	696.29	698.33	695.64	688.81	695.22	516.01	692.44
$CH_3S^\bullet$	380.60	383.87	383.84	384.28	379.35	384.28	284.88	381.08
$C_2H_5{}^\bullet$	602.20	604.27	604.28	602.21	597.01	604.23	468.71	602.87
$(CH_3)_2CH^\bullet$	898.80	902.33	902.11	899.86	891.19	901.44	695.04	898.63
$NO_2{}^\bullet$	227.50	228.63	228.80	226.72	218.16	229.36	49.98	232.38

	ref.	PBE-QIDH	ωB97X-2
H_2	109.20	105.10	107.79
LiH	57.80	52.80	55.83
BeH	49.80	55.31	55.00
^2CH	83.80	81.59	81.93
$^3CH_2$	190.00	192.62	189.81
$^1CH_2$	180.70	175.74	176.95
$CH_3{}^\bullet$	306.60	307.69	305.67

CH_4	419.20	418.15	416.94
^3NH	83.50	81.85	82.32
$NH_2^\bullet$	181.50	179.36	180.65
NH_3	297.50	292.96	294.79
$OH^\bullet$	106.40	104.13	105.96
H_2O	232.20	227.01	229.99
HF	140.80	137.25	139.46
Li_2	24.40	19.06	21.26
LiF	137.50	132.16	136.50
C_2H_2	405.30	403.48	401.38
$H_2C{=}CH_2$	562.60	562.63	558.56
$H_3C{-}CH_3$	710.80	712.62	707.50
$CN^\bullet$	180.90	172.75	173.59
HCN	312.60	307.93	310.60
CO	259.30	254.57	257.80
$HCO^\bullet$	278.70	276.87	278.23
$H_2C{=}O$	373.60	370.18	371.52
$CH_3{-}OH$	511.90	509.19	509.00
N_2	228.60	219.39	226.49
$H_2N{-}NH_2$	437.80	432.02	433.75
$NO^\bullet$	152.80	147.77	152.57
O_2	120.50	115.55	122.46
$HO{-}OH$	268.70	258.20	265.65
F_2	38.50	28.24	36.82
CO_2	389.10	387.47	389.06
$^1SiH_2$	151.30	148.27	151.35
$^3SiH_2$	131.20	132.91	133.65
$SiH_3^\bullet$	225.10	225.52	227.73
SiH_4	321.40	319.30	323.16
$PH_2^\bullet$	152.90	151.47	153.32
PH_3	241.80	236.87	239.93
H_2S	182.40	180.21	181.59
HCl	106.30	105.64	105.88
S_2	101.60	103.42	103.18
Cl_2	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
$ClO^\bullet$	64.40	59.77	62.13
ClF	61.50	57.43	61.34
CH_3Cl	393.90	395.81	392.77
$H_3C{-}SH$	473.00	473.49	471.33
HOCl	164.40	159.87	163.70
SO_2	258.40	248.49	257.39
BF_3	469.90	469.33	469.08
BCl_3	322.70	332.37	325.39
AlF_3	426.50	421.77	428.16
$AlCl_3$	306.10	314.27	311.29
CF_4	476.30	476.90	474.07
CCl_4	312.80	320.28	313.33
$O{=}C{=}S$	333.30	334.94	335.01
CS_2	277.70	281.60	279.03
COF_2	426.70	418.06	417.91
SiF_4	572.80	565.91	570.70
$SiCl_4$	383.30	392.77	387.11
N_2O	270.50	263.20	270.79
ClNO	191.20	181.48	189.40
NF_3	205.20	195.94	204.27
PF_3	363.90	356.15	362.43
O_3	147.10	128.02	146.34
F_2O	93.30	79.02	91.83
ClF_3	125.60	118.28	128.36
$F_2C{=}CF_2$	583.90	588.74	584.23
$Cl_2C{=}CCl_2$	466.80	480.12	468.53
CF_3CN	639.70	638.37	637.21
$CH{\equiv}C{-}CH_3$	704.20	706.51	699.87
$CH_2{=}C{=}CH_2$	702.40	705.05	697.43
C_3H_4	682.10	686.04	676.33
$CH_2{=}CHCH_3$	859.20	862.22	854.07
C_3H_6	851.90	858.92	847.91

C_3H_8	1004.60	1008.96	1000.12
C_4H_6	1011.20	1015.25	1003.87
C_4H_6	1002.80	1008.39	997.28
C_4H_6	989.50	999.97	985.75
C_4H_{10}	1298.50	1305.32	1292.76
C_4H_{10}	1300.30	1306.57	1294.20
C_5H_8	1282.40	1297.88	1277.10
C_6H_6	1366.00	1383.07	1360.63
H_2CF_2	436.20	435.22	434.67
HCF_3	457.70	457.25	455.85
H_2CCl_2	369.60	373.38	368.74
$HCCl_3$	343.30	348.82	342.86
H_3C-NH_2	581.20	579.02	577.22
CH_3-CN	615.10	614.24	612.22
CH_3-NO_2	600.60	595.09	598.69
$CH_3-O-N=O$	598.30	589.52	595.34
CH_3-SiH_3	626.10	625.52	625.53
$HCOOH$	500.70	497.29	498.27
$HCOOCH_3$	784.20	783.34	781.62
CH_3CONH_2	867.10	867.14	862.24
$CH_2-NH-CH_2$	719.00	721.94	714.84
$NCCN$	502.30	496.21	498.72
$(CH_3)_2CH$	868.80	868.93	863.62
$CH_3-CH_2-NH_2$	875.70	877.11	871.58
$H_2C=C=O$	531.90	533.10	530.29
CH_2-O-CH_2	649.90	651.72	647.04
CH_3CHO	676.20	675.75	672.84
$O=CH-CH=O$	633.40	630.04	630.24
CH_3CH_2OH	808.80	808.58	804.62
CH_3-O-CH_3	796.80	796.05	792.82
CH_2-S-CH_2	623.00	629.69	622.06
$(CH_3)_2SO$	854.10	854.48	850.72
CH_3-CH_2-SH	767.60	770.35	764.48
CH_3-S-CH_3	766.00	769.27	763.67
$H_2C=CHF$	571.30	572.51	568.62
CH_3-CH_2-Cl	690.10	694.38	687.59
$H_2C=CHCl$	538.60	545.31	539.13
$H_2C=CHCN$	763.30	761.57	756.74
$CH_3-CO-CH_3$	977.20	979.41	972.50
CH_3COOH	802.20	801.28	798.09
CH_3COF	705.40	705.39	702.31
CH_3COCl	666.90	669.50	664.72
$CH_3CH_2CH_2Cl$	983.80	990.80	980.30
$(CH_3)_2CH-OH$	1106.40	1108.39	1100.86
$CH_3-CH_2-O-CH_3$	1093.30	1095.47	1088.48
$(CH_3)_3N$	1158.60	1161.42	1152.86
C_4H_4O	993.00	1001.97	988.40
C_4H_4S	962.10	975.01	959.09
C_4H_4NH	1070.40	1082.02	1065.71
C_5H_5N	1236.40	1250.02	1231.56
$SH^\bullet$	86.90	86.13	86.83
$C_2H_3^\bullet$	444.00	446.14	440.70
$CH_3CO^\bullet$	580.90	582.07	579.26
$H_2COH^\bullet$	408.90	407.97	406.93
$CH_3O^\bullet$	400.50	398.81	397.20
$CH_3CH_2O^\bullet$	697.10	694.82	689.38
$CH_3S^\bullet$	380.60	383.15	380.23
$C_2H_5^\bullet$	602.20	605.92	599.84
$(CH_3)_2CH^\bullet$	898.80	905.22	895.17
$NO_2^\bullet$	227.50	221.03	229.07

Table S11: Barrier height energies (kcal mol^{-1}) 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
$H + N_2O \rightarrow [HON_2]^{\ddagger}$	-17.13	-2.82	-8.76	-10.19	-18.46	-13.33	-11.24	-19.37
$[HON_2]^{\ddagger} \rightarrow OH + N_2$	-82.47	-32.15	-61.61	-52.52	-72.52	-52.75	-58.30	-67.08
$H + ClH \rightarrow [HClH]^{\ddagger}$	-18.00	-2.26	-9.96	-9.80	-18.27	-11.87	-12.69	-17.80
$[HClH]^{\ddagger} \rightarrow HCl + H$	-18.00	-2.26	-9.96	-9.80	-18.27	-11.87	-12.69	-17.80
$CH_3 + FCl \rightarrow [ClFCH_3]^{\ddagger}$	-6.75	10.46	6.04	5.41	-1.26	1.49	4.78	3.62
$[ClFCH_3]^{\ddagger} \rightarrow FCH_3 + Cl$	-60.00	-37.59	-41.65	-41.48	-53.74	-44.44	-43.39	-47.52
$Cl^- \cdots CH_3Cl \rightarrow [ClCH_3Cl]^{-\ddagger}$	-13.41	-6.37	-5.31	-6.71	-10.83	-7.64	-8.21	-10.23
$[ClCH_3Cl]^{-\ddagger} \rightarrow ClCH_3 \cdots Cl^-$	-13.41	-6.37	-5.31	-6.71	-10.83	-7.64	-8.21	-10.23
$F^- \cdots CH_3Cl \rightarrow [FCH_3Cl]^{-\ddagger}$	-3.44	1.70	2.42	1.44	-0.89	0.41	0.61	-0.45
$[FCH_3Cl]^{-\ddagger} \rightarrow FCH_3 \cdots Cl^-$	-29.42	-21.84	-21.31	-21.75	-28.83	-22.13	-22.76	-28.07
$HO^- \cdots CH_3F \rightarrow [HOCH_3F]^{-\ddagger}$	2.44	17.48	13.11	13.77	6.10	14.73	12.64	7.04
$[HOCH_3F]^{-\ddagger} \rightarrow HOCH_3 \cdots F^-$	-17.66	-4.02	-7.17	-7.34	-15.62	-11.73	-9.90	-13.43
$H + N_2 \rightarrow [HN_2]^{\ddagger}$	-14.36	2.25	-5.27	-5.23	-12.32	-6.62	-6.67	-10.99
$[HN_2]^{\ddagger} \rightarrow HN_2$	-10.61	-9.32	-8.40	-8.99	-12.82	-11.51	-12.08	-10.69
$H + C_2H_4 \rightarrow [HCH_2CH_2]^{\ddagger}$	-1.72	5.44	0.68	0.12	-4.29	-1.61	-1.30	-3.43
$[HCH_2CH_2]^{\ddagger} \rightarrow CH_3CH_2$	-41.75	-39.34	-38.20	-40.27	-44.27	-41.51	-42.08	-45.39
$HCN \rightarrow [HCN]^{\ddagger}$	-48.07	-44.93	-46.88	-45.65	-46.82	-46.29	-46.28	-48.21
$[HCN]^{\ddagger} \rightarrow HNC$	-32.82	-30.82	-31.88	-30.68	-33.05	-33.74	-33.58	-33.27
$HO + CH_4 \rightarrow [HOCH_4]^{\ddagger}$	-6.70	16.76	2.37	5.24	-2.45	3.52	2.09	-3.91
$[HOCH_4]^{\ddagger} \rightarrow CH_3 + H_2O$	-19.60	-2.22	-10.54	-8.89	-13.81	-12.77	-11.45	-12.42
$H + OH \rightarrow [HHO]^{\ddagger}$	-10.70	1.97	-1.42	-3.60	-8.12	-5.66	-3.37	-6.92
$[HHO]^{\ddagger} \rightarrow O + H_2$	-13.10	12.67	-1.51	1.34	-8.38	-0.75	-5.52	-7.28
$H + H_2S \rightarrow [HH_2S]^{\ddagger}$	-3.60	6.74	2.12	1.12	-4.48	0.01	-1.12	-3.70
$[HH_2S]^{\ddagger} \rightarrow HS + H_2$	-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
$H + N_2O \rightarrow [HON_2]^{\ddagger}$	-17.13	-16.46	-16.66	-17.98	-11.59	-14.14	-18.89	-18.59
$[HON_2]^{\ddagger} \rightarrow OH + N_2$	-82.47	-73.57	-80.19	-72.53	-72.92	-69.05	-69.99	-72.43
$H + ClH \rightarrow [HClH]^{\ddagger}$	-18.00	-15.05	-16.08	-17.65	-12.57	-13.53	-18.36	-17.44
$[HClH]^{\ddagger} \rightarrow HCl + H$	-18.00	-15.05	-16.08	-17.65	-12.57	-13.53	-18.36	-17.44
$CH_3 + FCl \rightarrow [ClFCH_3]^{\ddagger}$	-6.75	-0.93	-0.97	-1.39	0.56	-1.98	-0.92	-0.88
$[ClFCH_3]^{\ddagger} \rightarrow FCH_3 + Cl$	-60.00	-54.25	-54.27	-51.10	-50.81	-53.29	-55.93	-54.64
$Cl^- \cdots CH_3Cl \rightarrow [ClCH_3Cl]^{-\ddagger}$	-13.41	-12.46	-12.14	-12.90	-8.86	-10.92	-14.08	-11.16
$[ClCH_3Cl]^{-\ddagger} \rightarrow ClCH_3 \cdots Cl^-$	-13.41	-12.46	-12.14	-12.90	-8.86	-10.92	-14.08	-11.16
$F^- \cdots CH_3Cl \rightarrow [FCH_3Cl]^{-\ddagger}$	-3.44	0.62	-0.70	-1.41	0.33	-1.04	-2.91	-1.42
$[FCH_3Cl]^{-\ddagger} \rightarrow FCH_3 \cdots Cl^-$	-29.42	-36.74	-33.94	-33.16	-26.83	-28.58	-30.22	-29.17
$HO^- \cdots CH_3F \rightarrow [HOCH_3F]^{-\ddagger}$	2.44	1.51	3.19	4.67	8.63	7.50	4.35	4.89
$[HOCH_3F]^{-\ddagger} \rightarrow HOCH_3 \cdots F^-$	-17.66	-15.05	-17.57	-14.99	-12.64	-14.66	-17.38	-16.61
$H + N_2 \rightarrow [HN_2]^{\ddagger}$	-14.36	-9.75	-10.74	-12.05	-7.56	-8.60	-11.78	-11.68
$[HN_2]^{\ddagger} \rightarrow HN_2$	-10.61	-10.74	-11.43	-9.81	-10.79	-11.57	-12.58	-11.39
$H + C_2H_4 \rightarrow [HCH_2CH_2]^{\ddagger}$	-1.72	-2.56	-2.25	-2.40	0.15	-0.70	-2.91	-2.82
$[HCH_2CH_2]^{\ddagger} \rightarrow CH_3CH_2$	-41.75	-44.95	-43.11	-43.75	-41.81	-44.19	-48.17	-45.14
$HCN \rightarrow [HCN]^{\ddagger}$	-48.07	-43.51	-44.34	-43.84	-47.49	-46.39	-45.87	-47.21
$[HCN]^{\ddagger} \rightarrow HNC$	-32.82	-32.39	-35.25	-32.20	-33.54	-32.71	-32.88	-34.19
$HO + CH_4 \rightarrow [HOCH_4]^{\ddagger}$	-6.70	-9.15	-9.34	-7.58	-2.33	-2.07	-5.44	-5.40
$[HOCH_4]^{\ddagger} \rightarrow CH_3 + H_2O$	-19.60	-18.72	-18.75	-19.44	-13.97	-14.01	-17.95	-17.42
$H + OH \rightarrow [HHO]^{\ddagger}$	-10.70	-9.13	-10.10	-7.86	-4.01	-7.04	-8.27	-8.61
$[HHO]^{\ddagger} \rightarrow O + H_2$	-13.10	-12.47	-12.68	-12.77	-6.32	-5.95	-11.66	-10.45
$H + H_2S \rightarrow [HH_2S]^{\ddagger}$	-3.60	-3.49	-3.23	-3.92	0.48	-1.18	-4.60	-3.95
$[HH_2S]^{\ddagger} \rightarrow HS + H_2$	-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
$H + N_2O \rightarrow [HON_2]^{\ddagger}$	-17.13	-17.74	-15.90	-17.17	-17.41	-19.07	-16.60	-21.01
$[HON_2]^{\ddagger} \rightarrow OH + N_2$	-82.47	-80.19	-75.96	-82.00	-81.62	-84.97	-94.81	-82.35
$H + ClH \rightarrow [HClH]^{\ddagger}$	-18.00	-17.73	-18.50	-17.04	-18.25	-19.94	-20.00	-23.11
$[HClH]^{\ddagger} \rightarrow HCl + H$	-18.00	-17.73	-18.50	-17.04	-18.25	-19.94	-20.00	-23.11
$CH_3 + FCl \rightarrow [ClFCH_3]^{\ddagger}$	-6.75	-4.24	-4.47	-3.48	-5.72	-4.80	-11.42	-5.74
$[ClFCH_3]^{\ddagger} \rightarrow FCH_3 + Cl$	-60.00	-59.46	-56.81	-58.29	-58.92	-59.24	-64.38	-59.71
$Cl^- \cdots CH_3Cl \rightarrow [ClCH_3Cl]^{-\ddagger}$	-13.41	-13.52	-12.55	-13.43	-13.51	-11.61	-11.94	-17.47
$[ClCH_3Cl]^{-\ddagger} \rightarrow ClCH_3 \cdots Cl^-$	-13.41	-13.52	-12.55	-13.43	-13.51	-11.61	-11.94	-17.47
$F^- \cdots CH_3Cl \rightarrow [FCH_3Cl]^{-\ddagger}$	-3.44	-2.64	-1.80	-2.88	-3.28	-1.93	-2.55	-4.83
$[FCH_3Cl]^{-\ddagger} \rightarrow FCH_3 \cdots Cl^-$	-29.42	-31.29	-32.17	-31.61	-32.85	-30.86	-31.67	-31.30
$HO^- \cdots CH_3F \rightarrow [HOCH_3F]^{-\ddagger}$	2.44	3.85	5.65	3.26	5.12	6.76	8.20	6.00
$[HOCH_3F]^{-\ddagger} \rightarrow HOCH_3 \cdots F^-$	-17.66	-17.82	-14.74	-18.55	-16.30	-14.54	-13.23	-16.23
$H + N_2 \rightarrow [HN_2]^{\ddagger}$	-14.36	-12.57	-12.19	-13.27	-13.78	-14.72	-16.91	-15.69
$[HN_2]^{\ddagger} \rightarrow HN_2$	-10.61	-12.31	-12.18	-12.76	-10.98	-12.83	-13.10	-15.05

$H + C_2H_4 \rightarrow [HCH_2CH_2]^{\ddagger}$	-1.72	-1.89	-2.33	-2.96	-2.79	-3.71	-3.26	-4.95
$[HCH_2CH_2]^{\ddagger} \rightarrow CH_3CH_2$	-41.75	-43.24	-42.78	-44.32	-43.50	-44.74	-41.89	-48.58
$HCN \rightarrow [HCN]^{\ddagger}$	-48.07	-46.01	-45.43	-46.20	-46.05	-46.62	-46.06	-45.98
$[HCN]^{\ddagger} \rightarrow HNC$	-32.82	-32.91	-33.88	-34.74	-33.21	-33.43	-34.82	-33.02
$HO + CH_4 \rightarrow [HOCH_4]^{\ddagger}$	-6.70	-6.00	-5.84	-5.86	-5.36	-4.87	-5.81	-4.95
$[HOCH_4]^{\ddagger} \rightarrow CH_3 + H_2O$	-19.60	-15.20	-18.58	-16.61	-17.73	-17.56	-19.29	-15.64
$H + OH \rightarrow [HHO]^{\ddagger}$	-10.70	-9.41	-9.85	-10.19	-9.87	-10.27	-10.05	-10.57
$[HHO]^{\ddagger} \rightarrow O + H_2$	-13.10	-10.01	-11.03	-10.98	-11.58	-11.55	-16.13	-11.00
$H + H_2S \rightarrow [HH_2S]^{\ddagger}$	-3.60	-3.43	-4.30	-3.49	-4.41	-5.45	-5.79	-6.93
$[HH_2S]^{\ddagger} \rightarrow HS + H_2$	-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
$H + N_2O \rightarrow [HON_2]^{\ddagger}$	-17.13	-19.57	-17.92	-17.22	-17.55	-17.55	-27.89	-16.79
$[HON_2]^{\ddagger} \rightarrow OH + N_2$	-82.47	-81.01	-78.35	-72.14	-82.41	-80.86	-124.03	-76.96
$H + ClH \rightarrow [HClH]^{\ddagger}$	-18.00	-20.80	-18.34	-17.46	-18.03	-17.20	-31.46	-15.83
$[HClH]^{\ddagger} \rightarrow HCl + H$	-18.00	-20.80	-18.34	-17.46	-18.03	-17.20	-31.46	-15.83
$CH_3 + FCl \rightarrow [ClFCH_3]^{\ddagger}$	-6.75	-5.10	-4.13	-0.81	-3.20	-7.40	-16.65	-3.66
$[ClFCH_3]^{\ddagger} \rightarrow FCH_3 + Cl$	-60.00	-58.35	-56.67	-52.28	-55.43	-59.91	-78.72	-56.36
$Cl^- \cdots CH_3Cl \rightarrow [ClCH_3Cl]^{-\ddagger}$	-13.41	-15.75	-13.95	-11.34	-13.19	-15.47	-16.42	-10.59
$[ClCH_3Cl]^{-\ddagger} \rightarrow ClCH_3 \cdots Cl^-$	-13.41	-15.75	-13.95	-11.34	-13.19	-15.47	-16.42	-10.59
$F^- \cdots CH_3Cl \rightarrow [FCH_3Cl]^{-\ddagger}$	-3.44	-3.62	-2.44	-1.51	-1.95	-4.17	-3.76	-0.72
$[FCH_3Cl]^{-\ddagger} \rightarrow FCH_3 \cdots Cl^-$	-29.42	-31.45	-31.03	-27.78	-33.64	-29.98	-41.57	-27.81
$HO^- \cdots CH_3F \rightarrow [HOCH_3F]^{-\ddagger}$	2.44	5.77	5.23	8.18	3.57	5.17	-5.39	8.29
$[HOCH_3F]^{-\ddagger} \rightarrow HOCH_3 \cdots F^-$	-17.66	-16.15	-16.78	-15.18	-17.56	-17.66	-27.45	-12.90
$H + N_2 \rightarrow [HN_2]^{\ddagger}$	-14.36	-14.19	-12.56	-11.29	-12.43	-12.27	-22.94	-12.38
$[HN_2]^{\ddagger} \rightarrow HN_2$	-10.61	-14.27	-13.34	-14.68	-12.02	-11.67	-13.59	-10.54
$H + C_2H_4 \rightarrow [HCH_2CH_2]^{\ddagger}$	-1.72	-4.10	-3.07	-4.00	-1.37	-1.73	-4.05	-1.84
$[HCH_2CH_2]^{\ddagger} \rightarrow CH_3CH_2$	-41.75	-47.12	-45.53	-46.69	-42.27	-43.84	-44.26	-42.59
$HCN \rightarrow [HCN]^{\ddagger}$	-48.07	-46.40	-46.54	-47.32	-44.92	-45.34	-47.47	-48.75
$[HCN]^{\ddagger} \rightarrow HNC$	-32.82	-33.35	-33.49	-34.95	-34.11	-33.64	-37.68	-33.39
$HO + CH_4 \rightarrow [HOCH_4]^{\ddagger}$	-6.70	-4.42	-3.72	-1.50	-7.77	-4.88	-26.65	-4.39
$[HOCH_4]^{\ddagger} \rightarrow CH_3 + H_2O$	-19.60	-15.45	-15.23	-14.13	-19.31	-18.74	-28.81	-17.03
$H + OH \rightarrow [HHO]^{\ddagger}$	-10.70	-9.73	-8.78	-9.77	-10.00	-8.74	-17.36	-8.03
$[HHO]^{\ddagger} \rightarrow O + H_2$	-13.10	-10.15	-9.80	-7.13	-13.07	-10.24	-32.84	-10.01
$H + H_2S \rightarrow [HH_2S]^{\ddagger}$	-3.60	-5.60	-4.17	-4.53	-4.24	-2.62	-11.91	-2.04
$[HH_2S]^{\ddagger} \rightarrow HS + H_2$	-17.30	-17.59	-16.80	-13.27	-18.08	-16.43	-27.17	-16.62
	ref.	PBE-QIDH	ωB97X-2					
$H + N_2O \rightarrow [HON_2]^{\ddagger}$	-17.13	-20.89	-20.42					
$[HON_2]^{\ddagger} \rightarrow OH + N_2$	-82.47	-80.28	-82.18					
$H + ClH \rightarrow [HClH]^{\ddagger}$	-18.00	-18.14	-19.01					
$[HClH]^{\ddagger} \rightarrow HCl + H$	-18.00	-18.14	-19.01					
$CH_3 + FCl \rightarrow [ClFCH_3]^{\ddagger}$	-6.75	-9.14	-7.71					
$[ClFCH_3]^{\ddagger} \rightarrow FCH_3 + Cl$	-60.00	-63.65	-60.21					
$Cl^- \cdots CH_3Cl \rightarrow [ClCH_3Cl]^{-\ddagger}$	-13.41	-13.68	-12.61					
$[ClCH_3Cl]^{-\ddagger} \rightarrow ClCH_3 \cdots Cl^-$	-13.41	-13.68	-12.61					
$F^- \cdots CH_3Cl \rightarrow [FCH_3Cl]^{-\ddagger}$	-3.44	-2.79	-1.91					
$[FCH_3Cl]^{-\ddagger} \rightarrow FCH_3 \cdots Cl^-$	-29.42	-31.44	-28.64					
$HO^- \cdots CH_3F \rightarrow [HOCH_3F]^{-\ddagger}$	2.44	5.17	8.47					
$[HOCH_3F]^{-\ddagger} \rightarrow HOCH_3 \cdots F^-$	-17.66	-17.15	-12.70					
$H + N_2 \rightarrow [HN_2]^{\ddagger}$	-14.36	-14.81	-16.09					
$[HN_2]^{\ddagger} \rightarrow HN_2$	-10.61	-12.20	-10.98					
$H + C_2H_4 \rightarrow [HCH_2CH_2]^{\ddagger}$	-1.72	-2.91	-3.39					
$[HCH_2CH_2]^{\ddagger} \rightarrow CH_3CH_2$	-41.75	-46.14	-44.69					
$HCN \rightarrow [HCN]^{\ddagger}$	-48.07	-48.44	-48.48					
$[HCN]^{\ddagger} \rightarrow HNC$	-32.82	-33.72	-32.75					
$HO + CH_4 \rightarrow [HOCH_4]^{\ddagger}$	-6.70	-6.66	-5.60					
$[HOCH_4]^{\ddagger} \rightarrow CH_3 + H_2O$	-19.60	-19.22	-18.34					
$H + OH \rightarrow [HHO]^{\ddagger}$	-10.70	-11.73	-10.83					
$[HHO]^{\ddagger} \rightarrow O + H_2$	-13.10	-12.57	-12.66					
$H + H_2S \rightarrow [HH_2S]^{\ddagger}$	-3.60	-4.05	-4.12					
$[HH_2S]^{\ddagger} \rightarrow HS + H_2$	-17.30	-15.04	-17.14					

Table S12: Weak interaction energies (kcal mol^{-1}) 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
$(NH_3)_2$	3.15	5.29	2.30	3.23	2.29	2.40	2.35	2.77
$(HF)_2$	4.57	7.39	4.38	4.96	3.90	4.04	4.81	4.41
$(H_2O)_2$	4.97	8.07	4.50	5.32	4.23	4.02	4.92	4.72
$NH_3\cdots H_2O$	6.41	10.19	5.92	7.02	5.68	5.03	6.34	6.18
$(HCONH_2)_2$	14.94	21.27	12.10	14.27	11.97	9.75	13.39	14.29
$(HCOOH)_2$	16.15	25.13	13.84	16.34	13.94	10.37	16.45	16.37
$C_2H_4\cdots F_2$	1.06	4.37	2.44	2.89	0.74	4.45	2.46	1.38
$NH_3\cdots F_2$	1.81	7.21	4.70	5.12	1.73	5.85	4.52	3.02
$C_2H_2\cdots ClF$	3.81	10.18	4.29	6.08	3.25	3.07	4.70	5.30
$HCN\cdots ClF$	4.86	9.70	4.63	5.78	3.51	3.29	4.69	5.13
$NH_3\cdots Cl_2$	4.88	11.66	6.37	7.80	4.62	5.08	6.35	6.63
$H_2O\cdots ClF$	5.36	11.32	6.07	7.30	4.62	4.50	6.25	6.50
$NH_3\cdots ClF$	10.62	23.36	14.41	16.84	11.64	13.77	15.57	13.54
$(H_2S)_2$	1.66	3.37	0.67	1.74	0.90	1.70	0.69	1.30
$(HCl)_2$	2.01	3.88	1.08	2.04	1.12	1.55	1.15	1.68
$HCl\cdots H_2S$	3.35	6.55	2.71	4.06	2.73	3.07	2.97	3.42
$CH_3Cl\cdots HCl$	3.55	6.44	1.88	3.36	1.90	2.32	2.13	3.29
$HCN\cdots CH_3SH$	3.59	5.83	2.16	3.50	2.47	4.08	2.31	3.40
$CH_3SH\cdots HCl$	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_2	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
$CH_4\cdots Ne$	0.22	0.40	-0.21	0.17	-0.04	1.67	-0.21	0.23
$(CH_4)_2$	0.51	0.94	-0.82	0.02	-0.44	3.07	-1.03	0.43
$(C_2H_2)_2$	1.34	2.09	0.09	0.98	0.48	2.25	-0.05	0.91
$(C_2H_4)_2$	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
$(NH_3)_2$	3.15	2.45	2.38	2.57	2.56	3.04	3.18	2.91
$(HF)_2$	4.57	3.47	4.04	4.25	4.64	4.79	5.06	4.33
$(H_2O)_2$	4.97	4.15	4.35	4.25	4.83	5.17	5.33	4.85
$NH_3\cdots H_2O$	6.41	5.31	5.40	5.17	6.19	6.73	6.61	6.34
$(HCONH_2)_2$	14.94	12.91	12.78	12.08	13.06	14.22	13.40	14.02
$(HCOOH)_2$	16.15	14.60	15.24	13.69	15.14	16.53	15.38	16.13
$C_2H_4\cdots F_2$	1.06	0.65	0.95	1.91	1.27	1.23	1.67	0.65
$NH_3\cdots F_2$	1.81	1.48	1.89	2.65	2.64	2.32	2.64	1.63
$C_2H_2\cdots ClF$	3.81	4.66	4.41	4.82	3.70	4.58	3.98	4.69
$HCN\cdots ClF$	4.86	3.90	3.95	4.19	4.43	4.79	4.65	5.12
$NH_3\cdots Cl_2$	4.88	6.07	5.21	5.16	5.33	5.80	5.07	5.65
$H_2O\cdots ClF$	5.36	5.64	5.63	5.67	5.58	5.93	5.66	5.94
$NH_3\cdots ClF$	10.62	10.62	11.01	10.39	12.57	13.52	10.80	11.91
$(H_2S)_2$	1.66	1.15	0.94	1.31	0.85	1.48	1.59	1.36
$(HCl)_2$	2.01	1.44	1.25	1.60	1.25	1.78	1.95	1.64
$HCl\cdots H_2S$	3.35	2.85	2.55	2.67	2.78	3.57	3.53	3.28
$CH_3Cl\cdots HCl$	3.55	2.72	2.66	3.21	2.17	2.99	3.18	3.27
$HCN\cdots CH_3SH$	3.59	2.87	2.80	3.32	2.55	3.36	3.37	3.44
$CH_3SH\cdots HCl$	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_2	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
$CH_4\cdots Ne$	0.22	-0.58	-0.21	0.25	-0.10	0.10	0.23	0.13
$(CH_4)_2$	0.51	-0.12	-0.13	1.11	-0.50	-0.03	0.38	0.20
$(C_2H_2)_2$	1.34	0.97	0.86	1.67	0.41	0.95	1.20	0.97
$(C_2H_4)_2$	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
$(NH_3)_2$	3.15	2.60	3.07	2.28	3.06	3.06	2.75	3.65
$(HF)_2$	4.57	4.42	4.86	4.27	4.94	5.08	4.70	5.32
$(H_2O)_2$	4.97	4.77	5.18	4.50	5.26	5.34	5.30	5.82
$NH_3\cdots H_2O$	6.41	6.15	6.42	5.83	6.57	6.59	6.78	7.27
$(HCONH_2)_2$	14.94	13.89	14.07	13.25	14.54	14.81	15.07	15.62
$(HCOOH)_2$	16.15	15.87	16.58	15.58	16.78	17.05	18.31	17.66
$C_2H_4\cdots F_2$	1.06	0.14	1.05	-0.25	0.90	0.96	0.64	1.00
$NH_3\cdots F_2$	1.81	1.04	1.48	0.78	1.41	1.39	0.47	1.85
$C_2H_2\cdots ClF$	3.81	3.57	4.43	3.39	4.54	4.71	4.38	4.48
$HCN\cdots ClF$	4.86	4.16	4.65	4.04	4.86	4.86	4.28	5.40

$NH_3\cdots Cl_2$	4.88	4.57	4.71	4.28	4.98	4.99	4.45	4.86
$H_2O\cdots ClF$	5.36	5.21	5.56	4.97	5.87	5.94	5.67	6.27
$NH_3\cdots ClF$	10.62	10.55	10.14	10.73	10.35	11.38	10.78	10.44
$(H_2S)_2$	1.66	1.00	1.66	0.60	1.40	1.42	1.06	1.98
$(HCl)_2$	2.01	1.35	1.93	0.99	1.73	1.74	1.23	2.29
$HCl\cdots H_2S$	3.35	2.90	3.29	2.49	3.16	3.14	2.78	3.83
$CH_3Cl\cdots HCl$	3.55	2.47	3.56	2.24	3.38	3.31	2.96	3.94
$HCN\cdots CH_3SH$	3.59	2.73	3.55	2.43	3.57	3.63	3.67	4.01
$CH_3SH\cdots HCl$	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_2	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
$CH_4\cdots Ne$	0.22	-0.35	0.23	-0.73	0.26	0.22	0.24	0.04
$(CH_4)_2$	0.51	-0.74	0.78	-0.98	0.44	0.49	0.23	0.50
$(C_2H_2)_2$	1.34	0.48	1.47	0.22	1.26	1.34	1.10	1.51
$(C_2H_4)_2$	1.42	-0.19	2.07	-0.28	1.44	1.36	1.00	1.79
	ref.	ωB97X	ωB97XD	N12-SX	MN12-SX	M11	HF	B2-PLYP
$(NH_3)_2$	3.15	3.63	3.25	3.01	2.68	2.82	1.57	2.85
$(HF)_2$	4.57	5.21	4.46	5.19	4.30	4.62	3.72	4.74
$(H_2O)_2$	4.97	5.76	5.15	5.49	4.70	5.14	3.70	5.04
$NH_3\cdots H_2O$	6.41	7.22	6.76	6.87	5.72	6.29	4.37	6.38
$(HCONH_2)_2$	14.94	15.42	14.89	14.74	13.29	14.48	10.02	13.93
$(HCOOH)_2$	16.15	17.48	16.85	17.46	15.29	16.79	12.07	15.72
$C_2H_4\cdots F_2$	1.06	0.94	0.64	1.23	0.82	0.52	-1.17	1.11
$NH_3\cdots F_2$	1.81	1.76	1.27	2.38	1.50	0.94	-1.14	2.11
$C_2H_2\cdots ClF$	3.81	4.41	3.70	4.25	3.93	3.55	-0.61	3.84
$HCN\cdots ClF$	4.86	5.29	4.21	4.81	4.03	4.18	1.77	4.86
$NH_3\cdots Cl_2$	4.88	5.15	4.88	5.52	4.76	4.03	0.67	5.16
$H_2O\cdots ClF$	5.36	6.22	5.31	5.91	5.41	5.31	2.41	5.60
$NH_3\cdots ClF$	10.62	11.02	11.10	13.32	10.04	9.46	2.39	12.18
$(H_2S)_2$	1.66	1.98	1.57	1.27	1.07	1.09	-0.13	1.19
$(HCl)_2$	2.01	2.27	1.75	1.66	1.39	1.38	0.17	1.58
$HCl\cdots H_2S$	3.35	3.81	3.36	3.34	2.55	2.72	0.75	3.04
$CH_3Cl\cdots HCl$	3.55	3.82	3.24	2.89	2.66	3.01	0.43	2.80
$HCN\cdots CH_3SH$	3.59	3.96	3.73	3.18	2.97	3.41	1.59	3.06
$CH_3SH\cdots HCl$	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_2	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
$CH_4\cdots Ne$	0.22	0.14	0.15	-0.13	-0.11	0.10	-0.11	0.00
$(CH_4)_2$	0.51	0.60	0.57	-0.34	0.11	0.33	-0.53	-0.10
$(C_2H_2)_2$	1.34	1.56	1.38	0.71	1.11	1.11	0.28	0.83
$(C_2H_4)_2$	1.42	1.67	1.68	0.19	0.97	1.39	-0.87	0.35
	ref.	PBE-QIDH	ωB97X-2					
$(NH_3)_2$	3.15	3.09	3.48					
$(HF)_2$	4.57	4.72	5.03					
$(H_2O)_2$	4.97	5.20	5.51					
$NH_3\cdots H_2O$	6.41	6.67	6.91					
$(HCONH_2)_2$	14.94	14.80	15.06					
$(HCOOH)_2$	16.15	16.96	16.55					
$C_2H_4\cdots F_2$	1.06	0.82	1.54					
$NH_3\cdots F_2$	1.81	1.39	2.21					
$C_2H_2\cdots ClF$	3.81	4.15	4.68					
$HCN\cdots ClF$	4.86	4.90	5.54					
$NH_3\cdots Cl_2$	4.88	4.98	5.43					
$H_2O\cdots ClF$	5.36	5.50	6.09					
$NH_3\cdots ClF$	10.62	11.88	11.95					
$(H_2S)_2$	1.66	1.55	1.93					
$(HCl)_2$	2.01	1.85	2.25					
$HCl\cdots H_2S$	3.35	3.47	3.71					
$CH_3Cl\cdots HCl$	3.55	3.27	3.88					
$HCN\cdots CH_3SH$	3.59	3.58	4.02					
$CH_3SH\cdots HCl$	4.16	4.94	5.29					
HeNe	0.04	0.02	0.07					
HeAr	0.06	0.02	0.09					
Ne_2	0.08	0.03	0.13					
NeAr	0.13	0.04	0.19					
$CH_4\cdots Ne$	0.22	0.07	0.27					
$(CH_4)_2$	0.51	0.16	0.74					

$(C_2H_2)_2$	1.34	1.17	1.66
$(C_2H_4)_2$	1.42	0.88	1.82

Table S13: Density value (a.u.) at the considered critical points for the SiH_4 system. All the computations are 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	ωB97	ωB97X	ωB97X-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	ωB97X-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_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)	0.201548	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	ωB97	ωB97X	ωB97X-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	ωB97X-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	ωB97	ωB97X	ωB97X-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	ωB97X-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_3H_4 system. All the computations are 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	ωB97	ωB97X	ωB97X-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	ωB97X-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	ωB97	ωB97X	ωB97X-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	ωB97X-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_4H_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)	0.090090	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
(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_4H_8 system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97X-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	ωB97X-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 $[H_3CHOH]^{\ddagger}$ 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	ωB97	ωB97X	ωB97X-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	ωB97X-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]‡ system. All the computations are 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	ωB97	ωB97X	ωB97X-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	ωB97X-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 [HHSH]‡ system. All the computations are 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	ωB97	ωB97X	ωB97X-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	ωB97X-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$\cdots$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$\cdots$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$\cdots$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$\cdots$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	ωB97	ωB97X	ωB97X-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	ωB97X-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$\cdots$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	ωB97	ωB97X	ωB97X-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	ωB97X-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$\cdots$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	ωB97	ωB97X	ωB97X-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	ωB97X-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_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)	0.274997	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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}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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $^3CH_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $^1CH_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3^{\bullet}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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}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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $NH_2^{\bullet}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.345392	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $OH^{\bullet}$ 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)	0.363327	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2O system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.012144	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2H_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)	0.411162	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2C{=}CH_2$ 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)	0.355264	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3C-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)	0.249783	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CN^{\bullet}$ 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)	0.477528	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $HCO^{\bullet}$ 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)	0.435352	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2C{=}O$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.657507	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2N{-}NH_2$ 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)	0.306996	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $NO^{\bullet}$ 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)	0.620755	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.493712	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.277927	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.454306	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $^1SiH_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $^3SiH_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $SiH_3^{\bullet}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $PH_2^{\bullet}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.166619	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2S system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.191759	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.159956	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $ClO^{\bullet}$ 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)	0.261892	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 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)	0.209068	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3Cl system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3C-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.288441	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.214240	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.163000	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $AlCl_3$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.251829	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.459999	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $SiCl_4$ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2O system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.168995	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.425838	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2O system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.235780	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $F_2C{=}CF_2$ 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)	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $Cl_2C{=}CCl_2$ 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)	0.346181	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	0.459257	0.214970	0.230215	0.219830	0.220530	0.218729		

Table S101: Density value (a.u.) at the considered critical points for the CF_3CN system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 CH≡C−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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2=C=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)	0.359546	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3H_4 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2=$CHCH_3$ 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)	0.354838	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3H_6 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3H_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)	0.251951	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		0.276998	0.282534	0.280109	0.279790	0.275294	0.282236	0.279547
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	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	ωB97X-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		0.281331	0.287761	0.283050	0.281998	0.280663		

Table S108: Density value (a.u.) at the considered critical points for the C_4H_6 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4H_6 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4H_6 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4H_{10} system. All the computations are 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)	0.280532	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	ωB97	ωB97X	ωB97XD	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)	0.280532	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	ωB97X-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)	0.280532	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_4H_{10} system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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
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		0.283257	0.288859	0.286460	0.285409	0.281038	0.288814	0.286093
(3,-1)	0.286992		0.283257	0.288859	0.286460	0.285409	0.281038	0.288814	0.286093
(3,-1)	0.286992		0.283257	0.288859	0.286460	0.285409	0.281038	0.288814	0.286093
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	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
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	ωB97X-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		0.288873	0.294598	0.289385	0.288404	0.287059		
(3,-1)	0.286992		0.288873	0.294598	0.289385	0.288404	0.287059		
(3,-1)	0.286992		0.288873	0.294598	0.289385	0.288404	0.287059		

Table S114: Density value (a.u.) at the considered critical points for the C_6H_6 system. All the computations are 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	0.319695	0.316706	0.310844	0.315471	0.319592	0.315631
(3,-1)	0.318278	0.299606	0.316207	0.319695	0.316706	0.310844	0.315471	0.319592	0.315631
(3,-1)	0.318279	0.299606	0.316207	0.319695	0.316706	0.310844	0.315471	0.319592	0.315631
(3,-1)	0.318279		0.316207	0.319695	0.316706	0.310844	0.315471	0.319592	0.315631
(3,-1)	0.318279		0.316207	0.319695	0.316706	0.310844	0.315471	0.319592	0.315631
(3,-1)	0.318278		0.316207	0.319695	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2CF_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)	0.263983	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.318158	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2CCl_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)	0.199370	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $HCCl_3$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_3C{-}NH_2$ 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)	0.270904	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3{-}NO_2$ 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)	0.256867	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3-O-N=O$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3-SiH_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)	0.122118	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $HCOOCH_3$ 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)	0.423989	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3CONH_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)	0.414002	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_2-NH-CH_2$ 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)	0.212967	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(CH_3)_2CH$ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3-CH_2-NH_2$ 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)	0.252014	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2C{=}C{=}O$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2-O-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)	0.217247	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3CHO system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3CH_2OH system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3-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)	0.263785	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_2{-}S{-}CH_2$ 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)	0.152890	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(CH_3)_2SO$ system. All the computations are 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	0.276551	0.284443	0.281629

Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3-CH_2-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3-S-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)	0.188103	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2C{=}CHF$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3-CH_2-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2C{=}CHCl$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2C{=}CHCN$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3-CO-CH_3$ 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)	0.408790	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3COOH system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3COF system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3COCl system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3CH_2CH_2Cl$ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(CH_3)_2CH-OH$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3-CH_2-O-CH_3$ 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)	0.261276	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(CH_3)_3N$ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4H_4O system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4H_4S system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4H_4NH system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_5H_5N system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $SH^{\bullet}$ 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)	0.220930	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3CO^{\bullet}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2COH^{\bullet}$ 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)	0.284074	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3O^{\bullet}$ 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)	0.287445	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3CH_2O^{\bullet}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3S^{\bullet}$ 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)	0.190936	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $C_2H_5^{\bullet}$ 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)	0.266401	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(CH_3)_2CH^{\bullet}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $NO_2^{\bullet}$ 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)	0.515186	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[HON_2]^{\ddagger}$ 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)	0.486165	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 [HClH]‡ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[ClFCH_3]^{\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[ClCH_3Cl]^{-\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[FCH_3Cl]^{-\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[HOCH_3F]^{-\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[HN_2]^{\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[HCH_2CH_2]^{\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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]‡ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[HOCH_4]^{\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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]‡ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[HH_2S]^{\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(NH_3)_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(HF)_2$ 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)	0.017459	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(H_2O)_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $NH_3 \cdots H_2O$ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(HCONH_2)_2$ 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)	0.022387	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(HCOOH)_2$ 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)	0.001283	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $C_2H_4 \cdots F_2$ 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)	0.001749	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $NH_3 \cdots F_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $C_2H_2\cdots ClF$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$\cdots$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $NH_3 \cdots Cl_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2O\cdots ClF$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $NH_3 \cdots ClF$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(H_2S)_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(HCl)_2$ 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)	0.022874	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$\cdots$H$_2$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3Cl\cdots HCl$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$_3$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3SH\cdots HCl$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.001245	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_4 \cdots Ne$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(CH_4)_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(C_2H_2)_2$ 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)	0.011983	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	-0.308550	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3H_4 system. All the computations 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4H_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)	0.337807	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
(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	ωB97	ωB97X	ωB97XD	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
(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	ωB97X-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 $[H_3CHOH]^{\ddagger}$ 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)	-0.041461	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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]‡ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 [HHSH]‡ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$\cdots$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$\cdots$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$\cdots$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$\cdots$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$\cdots$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$\cdots$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	-1.372582	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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}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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $^3CH_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $^1CH_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3^{\bullet}$ 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)	-1.184642	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4 system. All the computations 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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}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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $NH_2^{\bullet}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	-1.793615		

Table S231: Laplacian of the density value (a.u.) at the considered critical points for the NH_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)	-1.827132	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$^{\bullet}$ 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)	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2O system. All the computations 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.007788	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2H_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)	-1.264093	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2C{=}CH_2$ 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
(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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_3C{-}CH_3$ 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)	-0.650899	-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
(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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CN^{\bullet}$ 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)	0.907235	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$^{\bullet}$ 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)	0.336865	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2C{=}O$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2N{-}NH_2$ 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)	-0.562680	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$^{\bullet}$ 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)	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	-0.638847	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.515059	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.002370	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $^1SiH_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $^3SiH_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $SiH_3^{\bullet}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $PH_2^{\bullet}$ 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)	-0.102742	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	-0.092390	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2S system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	-0.683195		

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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	-0.267723	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	-0.078345	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$^{\bullet}$ 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)	-0.380319	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 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)	-0.196364	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3Cl system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3C-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.834585	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	1.242942	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	-0.014863	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $AlCl_3$ 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)	0.378431	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4 system. All the computations are 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
(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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.350892	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	-0.142225	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4 system. All the computations 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $SiCl_4$ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2O system. All the computations 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.795680	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	-0.257655	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2O system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	-0.326868	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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
(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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $Cl_2C{=}CCl_2$ 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)	-1.066921	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3CN system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 CH≡C−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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 CH_2=C=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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	-1.147688		
(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_3H_4 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2=$CHCH_3$ 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)	-1.152266	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	-1.086573

Table S298: Laplacian of the density value (a.u.) at the considered critical points for the C_3H_6 system. All the computations are 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
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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3H_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)	-0.658259	-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
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	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	ωB97X-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	-1.097556		
(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		-1.106123	-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_4H_6 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4H_6 system. All the computations 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
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
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	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
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	ωB97X-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_4H_6 system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4H_{10} system. All the computations are 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)	-1.107283	-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	ωB97	ωB97X	ωB97XD	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)	-1.107283	-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	ωB97X-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)	-1.107283	-0.946174	-1.106660	-1.155325	-1.091945	-1.081341	-1.089957
(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_4H_{10} system. All the computations 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	-0.663787
(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 S305: Laplacian of the 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)	-0.585623	-0.483865	-0.523686	-0.501509	-0.542345	-0.467797	-0.490284	-0.497599	-0.590933
(3,-1)	-0.585623	-0.483865	-0.523686	-0.501509	-0.542345	-0.467797	-0.490284	-0.497599	-0.590933
(3,+1)	0.091923	0.126082	0.138171	0.122111	0.094933	0.150743	0.175331	0.112149	0.071337
(3,-1)	-0.459433	-0.365262	-0.402880	-0.384391	-0.423968	-0.346673	-0.366925	-0.379613	-0.474374
(3,-1)	-0.585623	-0.483865	-0.523686	-0.501509	-0.542345	-0.467797	-0.490284	-0.497599	-0.590933
(3,-1)	-0.585623	-0.483865	-0.523686	-0.501509	-0.542345	-0.467797	-0.490284	-0.497599	-0.590933
(3,+1)	0.091923	0.126082	0.138171	0.122111	0.094933	0.150743	0.175331	0.112149	0.071337
(3,-1)	-0.459433	-0.365262	-0.402880	-0.384391	-0.423968	-0.346673	-0.366925	-0.379613	-0.474374
(3,-1)	-1.165569	-1.067781	-1.109991	-1.075023	-1.121244	-0.970000	-1.084802	-1.002686	-0.901185
(3,-1)	-1.165569	-1.067781	-1.109991	-1.075023	-1.121244	-0.970000	-1.084802	-1.002686	-0.901185
(3,-1)	-1.165569	-1.067781	-1.109991	-1.075023	-1.121244	-0.970000	-1.084802	-1.002686	-0.901185
(3,-1)	-1.165569	-1.067781	-1.109991	-1.075023	-1.121244	-0.970000	-1.084802	-1.002686	-0.901185
(3,-1)	-1.165569	-1.067781	-1.109991	-1.075023	-1.121244	-0.970000	-1.084802	-1.002686	-0.901185
(3,-1)	-1.165569	-1.067781	-1.109991	-1.075023	-1.121244	-0.970000	-1.084802	-1.002686	-0.901185
(3,-1)	-1.165569	-1.067781	-1.109991	-1.075023	-1.121244	-0.970000	-1.084802	-1.002686	-0.901185
(3,-1)	-1.165569	-1.067781	-1.109991	-1.075023	-1.121244	-0.970000	-1.084802	-1.002686	-0.901185
Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,-1)	-0.585623	0.150585	-0.571726	-0.547657	-0.533168	-0.408936	-0.451945	-0.566033	-0.527264
(3,-1)	-0.585623	-0.916304	-0.571726	-0.547657	-0.533168	-0.408936	-0.451945	-0.566033	-0.527264
(3,+1)	0.091923	-0.916304	0.059454	0.125323	0.107956	0.123895	0.075538	0.090202	0.120150
(3,-1)	-0.459433	-0.916304	-0.459452	-0.424070	-0.412495	-0.295901	-0.337926	-0.443822	-0.412387
(3,-1)	-0.585623	-0.916304	-0.571726	-0.547657	-0.533168	-0.408936	-0.451945	-0.566033	-0.527264
(3,-1)	-0.585623	-0.916304	-0.571726	-0.547657	-0.533168	-0.408936	-0.451945	-0.566033	-0.527264
(3,+1)	0.091923	-0.916304	0.059454	0.125323	0.107956	0.123895	0.075538	0.090202	0.120150
(3,-1)	-0.459433	-1.055615	-0.459452	-0.424070	-0.412495	-0.295901	-0.337926	-0.443822	-0.412387
(3,-1)	-1.165569	-1.055615	-1.074435	-1.131917	-1.104300	-1.069713	-0.976304	-1.131089	-1.092350
(3,-1)	-1.165569	-1.055615	-1.074435	-1.131917	-1.104300	-1.069713	-0.976304	-1.131089	-1.092350
(3,-1)	-1.165569	-1.055615	-1.074435	-1.131917	-1.104300	-1.069713	-0.976304	-1.131089	-1.092350
(3,-1)	-1.165569	-1.055615	-1.074435	-1.131917	-1.104300	-1.069713	-0.976304	-1.131089	-1.092350
(3,-1)	-1.165569	-1.055615	-1.074435	-1.131917	-1.104300	-1.069713	-0.976304	-1.131089	-1.092350
(3,-1)	-1.165569		-1.074435	-1.131917	-1.104300	-1.069713	-0.976304	-1.131089	-1.092350
(3,-1)	-1.165569		-1.074435	-1.131917	-1.104300	-1.069713	-0.976304	-1.131089	-1.092350
(3,-1)	-1.165569		-1.074435	-1.131917	-1.104300	-1.069713	-0.976304	-1.131089	-1.092350
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	N12-SX
(3,-1)	-0.585623	-0.486382	-0.519528	-0.575080	-0.585828	-0.536507	-0.539438	-0.534548	-0.510473
(3,-1)	-0.585623	-0.486382	-0.519528	-0.575080	-0.585828	-0.536507	-0.539438	-0.534548	-0.510473
(3,+1)	0.091923	0.387839	0.096777	0.112967	0.118959	0.104104	0.101437	0.121672	0.118939
(3,-1)	-0.459433	-0.362026	-0.396556	-0.448239	-0.460627	-0.420740	-0.419419	-0.408309	-0.392755
(3,-1)	-0.585623	-0.486382	-0.519528	-0.575080	-0.585828	-0.536507	-0.539438	-0.534548	-0.510473
(3,-1)	-0.585623	-0.486382	-0.519528	-0.575080	-0.585828	-0.536507	-0.539438	-0.534548	-0.510473
(3,+1)	0.091923	0.387839	0.096777	0.112967	0.118959	0.104104	0.101437	0.121672	0.118939
(3,-1)	-0.459433	-0.362026	-0.396556	-0.448239	-0.460627	-0.420740	-0.419419	-0.408309	-0.392755
(3,-1)	-1.165569	-1.060348	-1.195159	-1.287724	-1.476081	-1.117134	-1.115453	-1.103829	-1.078464
(3,-1)	-1.165569	-1.060348	-1.195159	-1.287724	-1.476081	-1.117134	-1.115453	-1.103829	-1.078464
(3,-1)	-1.165569	-1.060348	-1.195159	-1.287724	-1.476081	-1.117134	-1.115453	-1.103829	-1.078464
(3,-1)	-1.165569	-1.060348	-1.195159	-1.287724	-1.476081	-1.117134	-1.115453	-1.103829	-1.078464
(3,-1)	-1.165569	-1.060348	-1.195159	-1.287724	-1.476081	-1.117134	-1.115453	-1.103829	-1.078464
(3,-1)	-1.165569	-1.060348	-1.195159	-1.287724	-1.476081	-1.117134	-1.115453	-1.103829	-1.078464
(3,-1)	-1.165569	-1.060348	-1.195159	-1.287724	-1.476081	-1.117134	-1.115453	-1.103829	-1.078464
Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	ωB97X-2		
(3,-1)	-0.585623	0.151150	-0.508689	-0.655363	-0.553519	-0.553958	-0.562222		
(3,-1)	-0.585623	-0.937266	-0.508689	-0.655363	-0.553519	-0.553958	-0.562222		
(3,+1)	0.091923	-0.937266	0.153632	0.081053	0.115565	0.098202	0.067077		
(3,-1)	-0.459433	-0.937266	-0.381966	-0.520770	-0.430667	-0.432326	-0.442926		
(3,-1)	-0.585623	-0.937266	-0.508689	-0.655363	-0.553519	-0.553958	-0.562222		
(3,-1)	-0.585623	-0.937266	-0.508689	-0.655363	-0.553519	-0.553958	-0.562221		
(3,+1)	0.091923	-0.937266	0.153632	0.081053	0.115565	0.098202	0.067077		
(3,-1)	-0.459433	-1.019269	-0.381966	-0.520770	-0.430667	-0.432326	-0.442926		
(3,-1)	-1.165569	-1.019269	-1.189385	-1.214280	-1.147626	-1.138321	-1.146769		
(3,-1)	-1.165569	-1.019269	-1.189385	-1.214280	-1.147626	-1.138321	-1.146768		
(3,-1)	-1.165569	-1.019269	-1.189385	-1.214280	-1.147626	-1.138321	-1.146769		
(3,-1)	-1.165569	-1.019269	-1.189385	-1.214280	-1.147626	-1.138321	-1.146768		
(3,-1)	-1.165569	-1.019269	-1.189385	-1.214280	-1.147626	-1.138321	-1.146769		
(3,-1)	-1.165569		-1.189385	-1.214280	-1.147626	-1.138321	-1.146769		
(3,-1)	-1.165569		-1.189385	-1.214280	-1.147626	-1.138321	-1.146769		
(3,-1)	-1.165569		-1.189385	-1.214280	-1.147626	-1.138321	-1.146769		

Table S306: Laplacian of the density value (a.u.) at the considered critical points for the C_6H_6 system. All the computations are done at the def2-QZVP level of theory.

Type	CCSD	SVWN5	BLYP	PBE	B97-2	SOGGA11	N12	M06-L	M11-L
(3,+1)	0.149852	0.149219	0.147102	0.149723	0.151346	0.146062	0.149865	0.152933	0.151128
(3,-1)	-1.017517	-0.880725	-0.938938	-0.902459	-0.957321	-0.873747	-0.891863	-0.949473	-0.987998
(3,-1)	-1.017517	-0.880725	-0.938938	-0.902459	-0.957321	-0.873747	-0.891863	-0.949473	-0.987998
(3,-1)	-1.017517	-0.880725	-0.938938	-0.902459	-0.957321	-0.873747	-0.891863	-0.949473	-0.987998
(3,-1)	-1.017517	-0.880725	-0.938938	-0.902459	-0.957321	-0.873747	-0.891863	-0.949473	-0.987998
(3,-1)	-1.017517	-0.880725	-0.938938	-0.902459	-0.957321	-0.873747	-0.891863	-0.949473	-0.987998
(3,-1)	-1.017517	-0.880725	-0.938938	-0.902459	-0.957321	-0.873747	-0.891863	-0.949473	-0.987998
(3,-1)	-1.193286	-1.092886	-1.134649	-1.099257	-1.147829	-0.990504	-1.111575	-1.011249	-0.914351
(3,-1)	-1.193285	-1.092886	-1.134649	-1.099257	-1.147829	-0.990504	-1.111575	-1.011249	-0.914351
(3,-1)	-1.193285	-1.092886	-1.134649	-1.099257	-1.147829	-0.990504	-1.111575	-1.011249	-0.914351
(3,-1)	-1.193286	-1.092886	-1.134649	-1.099257	-1.147829	-0.990504	-1.111575	-1.011249	-0.914351
(3,-1)	-1.193285	-1.092886	-1.134649	-1.099257	-1.147829	-0.990504	-1.111575	-1.011249	-0.914351
(3,-1)	-1.193285	-1.092886	-1.134649	-1.099257	-1.147829	-0.990504	-1.111575	-1.011249	-0.914351

Type	CCSD	MN12-L	MN15-L	B3LYP	PBE0	M05	M06	SOGGA11-X	MN15
(3,+1)	0.149852	0.032375	0.155497	0.148775	0.151581	0.159587	0.150222	0.154677	0.143552
(3,-1)	-1.017517	0.032375	-0.937975	-0.969219	-0.944014	-0.892268	-0.929020	-0.982442	-0.915684
(3,-1)	-1.017517	-1.186368	-0.937975	-0.969219	-0.944014	-0.892268	-0.929020	-0.982442	-0.915684
(3,-1)	-1.017517	-1.186368	-0.937975	-0.969219	-0.944014	-0.892268	-0.929020	-0.982442	-0.915684
(3,-1)	-1.017517		-0.937975	-0.969219	-0.944014	-0.892268	-0.929020	-0.982442	-0.915684
(3,-1)	-1.017517		-0.937975	-0.969219	-0.944014	-0.892268	-0.929020	-0.982442	-0.915684
(3,-1)	-1.017517		-0.937975	-0.969219	-0.944014	-0.892268	-0.929020	-0.982442	-0.915684
(3,-1)	-1.193286		-1.109342	-1.158898	-1.131300	-1.087783	-0.986373	-1.159926	-1.125072
(3,-1)	-1.193285		-1.109342	-1.158898	-1.131300	-1.087783	-0.986373	-1.159926	-1.125072
(3,-1)	-1.193285		-1.109342	-1.158898	-1.131300	-1.087783	-0.986373	-1.159926	-1.125072
(3,-1)	-1.193286		-1.109342	-1.158898	-1.131300	-1.087783	-0.986373	-1.159926	-1.125072
(3,-1)	-1.193285		-1.109342	-1.158898	-1.131300	-1.087783	-0.986373	-1.159926	-1.125072
(3,-1)	-1.193285		-1.109342	-1.158898	-1.131300	-1.087783	-0.986373	-1.159926	-1.125072

Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	N12-SX
(3,+1)	0.149852	0.156779	0.156840	0.152590	0.155150	0.153524	0.152592	0.152583	0.151480
(3,-1)	-1.017517	-0.852586	-0.994140	-1.046126	-1.039393	-0.917293	-0.938672	-0.945898	-0.910064
(3,-1)	-1.017517	-0.852586	-0.994140	-1.046126	-1.039393	-0.917293	-0.938672	-0.945898	-0.910064
(3,-1)	-1.017517	-0.852586	-0.994140	-1.046126	-1.039393	-0.917293	-0.938672	-0.945898	-0.910064
(3,-1)	-1.017517	-0.852586	-0.994140	-1.046126	-1.039393	-0.917293	-0.938672	-0.945898	-0.910064
(3,-1)	-1.017517	-0.852586	-0.994140	-1.046126	-1.039393	-0.917293	-0.938672	-0.945898	-0.910064
(3,-1)	-1.017517	-0.852586	-0.994140	-1.046126	-1.039393	-0.917293	-0.938672	-0.945898	-0.910064
(3,-1)	-1.193286	-1.086164	-1.221032	-1.316055	-1.501055	-1.144927	-1.143338	-1.131824	-1.105405
(3,-1)	-1.193285	-1.086164	-1.221032	-1.316055	-1.501055	-1.144927	-1.143338	-1.131824	-1.105405
(3,-1)	-1.193285	-1.086164	-1.221032	-1.316055	-1.501055	-1.144927	-1.143338	-1.131824	-1.105405
(3,-1)	-1.193286	-1.086164	-1.221032	-1.316055	-1.501055	-1.144927	-1.143338	-1.131824	-1.105405
(3,-1)	-1.193285	-1.086164	-1.221032	-1.316055	-1.501055	-1.144927	-1.143338	-1.131824	-1.105405
(3,-1)	-1.193285	-1.086164	-1.221032	-1.316055	-1.501055	-1.144927	-1.143338	-1.131824	-1.105405

Type	CCSD	MN12-SX	M11	HF	B2-PLYP	PBE-QIDH	ωB97X-2
(3,+1)	0.149852	-0.028893	0.158469	0.154041	0.150212	0.153008	0.149886
(3,-1)	-1.017517	-0.028893	-0.996355	-1.109078	-0.979356	-0.974991	-0.995958
(3,-1)	-1.017517	-1.124244	-0.996355	-1.109078	-0.979356	-0.974991	-0.996058
(3,-1)	-1.017517	-1.124244	-0.996355	-1.109078	-0.979356	-0.974991	-0.995958
(3,-1)	-1.017517		-0.996355	-1.109078	-0.979356	-0.974991	-0.995958
(3,-1)	-1.017517		-0.996355	-1.109078	-0.979356	-0.974991	-0.995958
(3,-1)	-1.017517		-0.996355	-1.109078	-0.979356	-0.974991	-0.996058
(3,-1)	-1.193286		-1.226304	-1.248663	-1.172399	-1.163956	-1.171567
(3,-1)	-1.193285		-1.226304	-1.248663	-1.172399	-1.163956	-1.171440
(3,-1)	-1.193285		-1.226304	-1.248663	-1.172399	-1.163956	-1.171440
(3,-1)	-1.193286		-1.226304	-1.248663	-1.172399	-1.163956	-1.171566
(3,-1)	-1.193285		-1.226304	-1.248663	-1.172399	-1.163956	-1.171439
(3,-1)	-1.193285		-1.226304	-1.248663	-1.172399	-1.163956	-1.171440

Table S307: Laplacian of the density value (a.u.) at the considered critical points for the H_2CF_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)	-0.230160	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 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
(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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_2CCl_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)	-0.337168	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $HCCl_3$ 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
(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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_3C{-}NH_2$ 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)	-0.787542	-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		-1.084379	-1.132625	-1.102217	-1.063719	-0.967129	-1.129761	-1.097494
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	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	ωB97X-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		-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_3-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3{-}NO_2$ 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)	-0.762730	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3-O-N=O$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3-SiH_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)	0.219152	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $HCOOCH_3$ 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)	-0.314615	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3CONH_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)	-0.471506	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_2{-}NH{-}CH_2$ 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)	0.161124	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	-1.172912

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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(CH_3)_2CH$ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	-1.137263

Table S322: Laplacian of the density value (a.u.) at the considered critical points for the $CH_3-CH_2-NH_2$ 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)	-0.692663	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2C{=}C{=}O$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	-0.648933	-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_2-O-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)	0.236579	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3CHO system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3CH_2OH system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3-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)	-0.618383	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_2{-}S{-}CH_2$ 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)	0.090173	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(CH_3)_2SO$ system. All the computations are 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	-1.074108	-1.042270	-0.947770	-1.101033	-1.065420

Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	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	ωB97X-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	-1.188696	-1.116548	-1.106708	-1.114338

Table S331: Laplacian of the density value (a.u.) at the considered critical points for the CH_3-CH_2-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3-S-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)	-0.369759	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	-1.122859		

Table S333: Laplacian of the density value (a.u.) at the considered critical points for the $H_2C{=}CHF$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3-CH_2-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2C{=}CHCl$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2C{=}CHCN$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3-CO-CH_3$ 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)	-0.259132	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3COOH system. All the computations are 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		-1.032770	-1.092818	-1.062571	-1.026856	-0.937375	-1.087517	-1.052329
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	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	ωB97X-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		-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_3COF system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_3COCl system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3CH_2CH_2Cl$ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(CH_3)_2CH-OH$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3-CH_2-O-CH_3$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(CH_3)_3N$ system. All the computations are 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		-1.079071	-1.127013	-1.097307	-1.058641	-0.964323	-1.124107	-1.091129
(3,-1)	-1.158826		-1.079071	-1.127013	-1.097307	-1.058641	-0.964323	-1.124107	-1.091129
Type	CCSD	BMK	M06-2X	M05-2X	M06-HF	ωB97	ωB97X	ωB97XD	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)	-1.080995	-0.986308	-1.100953	-1.189495	-1.363604	-1.035928	-1.033120	-1.020913	-0.999289
(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	ωB97X-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		-1.168835	-1.212122	-1.142263	-1.131114	-1.140881		
(3,-1)	-1.158826		-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_4H_4O system. All the computations are 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	-0.843988	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_4H_4S system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	-1.175652		

Table S347: Laplacian of the density value (a.u.) at the considered critical points for the C_4H_4NH system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_5H_5N system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	-1.217540
(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 $SH^{\bullet}$ 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)	-0.674617	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3CO^{\bullet}$ 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)	-0.659186	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2COH^{\bullet}$ 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)	-0.420914	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3O^{\bullet}$ 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)	-0.683464	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3CH_2O^{\bullet}$ 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)	-0.646651	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3S^{\bullet}$ 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)	-0.352568	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $C_2H_5^{\bullet}$ 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)	-0.729342	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(CH_3)_2CH^{\bullet}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $NO_2^{\bullet}$ 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)	-1.262060	-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[HON_2]^{\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 [HClH]‡ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[ClFCH_3]^{\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[ClCH_3Cl]^{-\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[FCH_3Cl]^{-\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[HOCH_3F]^{-\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[HN_2]^{\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[HCH_2CH_2]^{\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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]‡ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[HOCH_4]^{\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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]‡ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $[HH_2S]^{\ddagger}$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(NH_3)_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(HF)_2$ 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)	0.047762	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(H_2O)_2$ 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)	0.072320	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $NH_3 \cdots H_2O$ system. All the computations are 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(HCONH_2)_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(HCOOH)_2$ 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)	0.008545	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $C_2H_4\cdots F_2$ 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)	0.009522	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $NH_3 \cdots F_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $C_2H_2\cdots ClF$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$\cdots$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)	0.136280	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $NH_3 \cdots Cl_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $H_2O\cdots ClF$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $NH_3 \cdots ClF$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(H_2S)_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(HCl)_2$ 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)	0.094481	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$_2$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3Cl\cdots HCl$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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$_3$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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_3SH\cdots HCl$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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_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)	0.006704	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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $CH_4 \cdots Ne$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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 $(CH_4)_2$ 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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-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	ωB97	ωB97X	ωB97XD	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	ωB97X-2		
(3,-1)	0.045892	0.048915	0.050145	0.047648	0.044372	0.044582	0.044346		