

## Supplementary material

### Thermodynamic stability versus kinetic lability of ZnS<sub>4</sub> core

Delphine Picot, Gilles Ohanessian, Gilles Frison

Laboratoire des Mécanismes Réactionnels,

Département de Chimie, Ecole Polytechnique and CNRS,

91128 Palaiseau Cedex, France.

Fax: + 00 33 (0)1 69 33 48 03

gilles.frison@polytechnique.org

a) Zn-S bond length in systems **1a** and **2a** as a function of the method of calculation.

Method for geometry optimisation	Zn-S bond length (Å)
<b>1a</b>	
B3LYP/BS1	2.432
B3LYP/BS1+	2.434
B3LYP/BS1*	2.434
B3LYP/def2-SVP	2.434
RI-B3LYP/def2-SVP	2.434
B3LYP/BS2	2.437
B3LYP/BS4	2.433
B3LYP/def2-TZVPP	2.434
RI-B3LYP-D/def2-SVP	2.418
BLYP/BS1	2.457
BP86/BS1	2.419
BP86/def2-SVP	2.419
RI-BP86/def2-SVP	2.419
MARIJ-BP86/def2-SVP	2.419
SVWN/BS2	2.334
MP2/BS1	2.389
<b>2a</b>	
B3LYP/BS1	2.295
B3LYP/BS1+	2.298
B3LYP/BS1*	2.295
RI-B3LYP/def2-SVP	2.299
B3LYP/BS4	2.293
B3LYP/def2-TZVPP	2.297
RI-B3LYP-D/def2-SVP	2.290
BLYP/BS1	2.312
BP86/BS1	2.285
MARIJ-BP86/def2-SVP	2.287
MP2/BS1	2.258
SVWN/BS2	2.222

BS1 : combination of the 6-31G(d,p) basis set for the C, S, and H atoms and the contracted Wachters basis [14s9p5d1f/9s5p3d1f] for the Zn atom.

BS1+ : BS1 basis set augmented by one set of diffuse functions on all atoms except H

BS1\* : BS1 basis set augmented by a second set of polarization functions on all atoms except H

BS2 : combination of the 6-311++G(d,p) basis set for the C, S, and H atoms and the contracted Wachters basis [15s11p6d1f/10s7p4d1f] for the Zn atom.

BS3 : combination of the 6-311+G(2d,2p) basis set for the C, S, and H atoms and the contracted Wachters basis [15s11p6d2f/10s7p4d2f] for the Zn atom.

BS4 : combination of the Aug-cc-pVTZ basis set for the C, S, and H atoms and the contracted Wachters basis [15s11p6d3f/10s7p4d3f] for the Zn atom.

b) Zn-S binding energy  $E_0$  in system **1a** as a function of the method of calculation.

Calculation level for energy calculation	$E_0$ (in kJ/mol)
B3LYP/BS1//B3LYP/BS1	-162
RI-B3LYP/def2-SVP//RI-B3LYP/def2-SVP	-132
RI-B3LYP-D/def2-SVP//RI-B3LYP-D/def2-SVP	-108
MARIJ-BP86/def2-SVP//MARIJ-BP86/def2-SVP	-134
SVWN/BS2//SVWN/BS2	-134
BLYP/BS3//BLYP/BS1	-201
BP86/BS3//BP86/BS1	-191
B3LYP/BS3//B3LYP/BS1	-189
B3LYP/BS3//B3LYP/BS1+	-190
B3LYP/BS3//B3LYP/BS1*	-192
B3LYP/BS3//MP2/BS1	-195
B3LYP/BS3//SVWN/BS2	-209
B3LYP/BS4//B3LYP/BS4	-182
B3LYP/def2-TZVPP//MARIJ-BP86/def2-SVP	-185
B3LYP/def2-TZVPP//B3LYP/def2-TZVPP	-180
B3LYP-D/def2-TZVPP//MARIJ-BP86/def2-SVP	-159
MP2/BS1//MP2/BS1	-145
MP2/BS3//SVWN/BS2	-150
MP2/BS3//B3LYP/BS1	-142
MP2/BS3//MP2/BS1	-145
RI-MP2/def2-TZVPP//MARIJ-BP86/def2-SVP	-140
RI-CC2/def2-TZVPP//MARIJ-BP86/def2-SVP	-140

c) Absolute electronic energies and ZPE, thermal and solvation corrections to enthalpies and Gibbs free energies for all the molecules depicted in Scheme 1 and related transition states.

System	Electronic Energy <sup>a,b</sup>	ZPE correction	Correction to $H_{\text{gaz}}^{\text{b,c}}$	Correction to $G_{\text{gaz}}^{\text{b,d}}$	Electronic Energy <sup>b,e</sup>	Electronic Energy <sup>b,f</sup>	Electronic Energy <sup>b,g</sup>	Electronic Energy <sup>b,h</sup>	Correction to $G^{\text{78.4b,i}}$
1a	-3531.495939	0.147588	0.165042	0.097812	-3531.653406	-3531.680283	-3529.595573	-3529.628485	-0.272263
TS1-2a	-3531.473411	0.146833	0.163835	0.096245	-3531.638617	-3531.660771	-3529.568820	-3529.601417	-0.270879
2a	-3093.557067	0.111015	0.123153	0.067993	-3093.657935	-3093.673568	-3091.944287	-3091.973694	-0.084294
3a	-437.989745	0.033796	0.037539	0.009842	-438.065824	-438.067256	-437.704607	-437.708046	-0.117471
4a	-3319.639401	0.181898	0.200182	0.128691	-3319.827397	-3319.856662	-3317.825873	-3317.867396	-0.102232
5a	-2881.570008	0.146331	0.160495	0.099505	-2881.703091	-2881.722406	-2880.046973	-2880.084327	-0.025194
6a	-226.073313	0.069216	0.073239	0.042101	-226.175002	-226.178752	-225.873690	-225.885033	-0.016309
1b	-4926.626892	0.779778	0.831251	0.675305	-4927.261272	-4927.424650	-4923.310520	-4923.416422	-0.216261
TS1-2b	-4926.608060	0.779086	0.830047	0.673570	-4927.247233	-4927.410499			-0.215767
2b	-4139.871232	0.586396	0.625275	0.498864	-4140.332501	-4140.455023	-4137.205279	-4137.286802	-0.072010
3b	-786.800870	0.192639	0.204429	0.152536	-786.987563	-787.017216	-786.146234	-786.168032	-0.092339
4b	-4405.241355	0.684221	0.729228	0.587530	-4405.805388	-4405.956308	-4402.348179	-4402.444954	-0.081285
6b	-265.354361	0.096071	0.101683	0.066211	-265.469281	-265.477037	-265.109436	-265.122614	-0.013825
1c	-4519.310092	0.418218	0.452588	0.336871	-4519.861050	-4519.935970			-0.271317
TS1-2c	-4519.286060	0.418273	0.451917	0.336166	-4519.845272	-4519.915883			-0.267294
2c	-3834.387904	0.315812	0.341295	0.250089	-3834.782485	-3834.837109			-0.100246
3c	-684.961847	0.102669	0.110192	0.069584	-685.130831	-685.142475			-0.108492
1d	-4298.043385	0.354401	0.382719	0.281409	-4298.475797	-4298.538682	-4295.382185	-4295.458577	-0.237159
TS1-2d	-4298.014760	0.354207	0.381965	0.279615	-4298.455999	-4298.514263	-4295.352658	-4295.427647	-0.234171
2d	-3668.430280	0.267747	0.288905	0.207370	-3668.737835	-3668.783320	-3666.248417	-3666.308449	-0.075902
3d	-629.647437	0.086812	0.092748	0.056096	-629.786401	-629.795185	-629.163566	-629.178323	-0.099022
1e	-4666.853822	0.350491	0.386132	0.266580	-4667.486621	-4667.558310			-0.197148
TS1-2e	-4666.816582	0.349995	0.385130	0.263632	-4667.459613	-4667.524645			-0.199384
2e	-3945.006843	0.263829	0.290645	0.194455	-3945.464943	-3945.514270			-0.070013
3e	-721.856212	0.086011	0.093719	0.052533	-722.043392	-722.054091			-0.086991
1f	-5404.316619	0.338421	0.389343	0.233174	-5405.342797	-5405.435695			-0.177318
TS1-2f	-5404.271622	0.337741	0.388147	0.231079	-5405.307057	-5405.392606			-0.185318
2f	-4498.073133	0.254398	0.292740	0.168990	-4498.826192	-4498.890730			-0.078328
3f	-906.234192	0.083230	0.094686	0.044348	-906.518458	-906.533860			-0.075986

<sup>a</sup> Electronic energy at the MARIJ-BP86/def2-SVP level

<sup>b</sup> Values are given in a.u.

<sup>c</sup> Thermal correction to gas phase enthalpy computed at the MARIJ-BP86/def2-SVP level

<sup>d</sup> Thermal correction to gas phase Gibbs free energy computed at the MARIJ-BP86/def2-SVP level

<sup>e</sup> Electronic energy at the B3LYP/def2-TZVPP//MARIJ-BP86/def2-SVP level

<sup>f</sup> Electronic energy at the B3LYP-D/def2-TZVPP//MARIJ-BP86/def2-SVP level

<sup>g</sup> Electronic energy at the RI-MP2/def2-TZVPP//MARIJ-BP86/def2-SVP level

<sup>h</sup> Electronic energy at the RI-CC2/def2-TZVPP//MARIJ-BP86/def2-SVP level

<sup>i</sup> Solvation correction to Gibbs free energy in water computed at the B3LYP/def2-TZVPP//MARIJ-BP86/def2-SVP level

d) Solvation corrections to Gibbs free energies for **1-3a**, **2-6b** and **1-3d** at different values of dielectric constant.

System	Correction to $G^{46.7a,b}$	Correction to $G^{36.6a,c}$	Correction to $G^{4a,d}$
<b>1a</b>	-0.268626	-0.266164	-0.183594
<b>TS1-2a</b>	-0.267237	-0.264772	-0.182292
<b>2a</b>	-0.083145	-0.082368	-0.056482
<b>3a</b>	-0.115877	-0.114799	-0.078841
<b>1b</b>		-0.210929	
<b>TS1-2b</b>		-0.210471	
<b>2b</b>		-0.070188	
<b>3b</b>		-0.090085	
<b>4b</b>		-0.079150	
<b>6b</b>		-0.013434	
<b>1d</b>	-0.233725		
<b>TS1-2d</b>	-0.230804		
<b>2d</b>	-0.074798		
<b>3d</b>	-0.090690		

<sup>a</sup> Values are given in a.u.

<sup>b</sup> Solvation correction to Gibbs free energy in DMSO computed at the B3LYP/def2-TZVPP//MARIJ-BP86/def2-SVP level

<sup>c</sup> Solvation correction to Gibbs free energy in acetonitrile computed at the B3LYP/def2-TZVPP//MARIJ-BP86/def2-SVP level

<sup>d</sup> Solvation correction to Gibbs free energy in a buried protein site computed at the B3LYP/def2-TZVPP//MARIJ-BP86/def2-SVP level

e) Cartesian coordinates of the optimized geometries for all the molecules depicted in Scheme 1 and related transition states at the MARIJ-BP86/def2-SVP level of theory.

**1a**

```
Zn  0.0000052 -0.0000048 -0.0000006
S   1.4193988 -1.4267953  1.3422400
S  -1.4193853  1.4267815  1.3422533
S   1.4267875  1.4193945 -1.3422463
S  -1.4268053 -1.4193751 -1.3422468
C   2.2036043  2.2010242  0.1345778
H   1.4297984  2.6894817  0.7678751
H   2.6995771  1.4312683  0.7669208
H   2.9613635  2.9655392 -0.1643111
C   2.2011231 -2.2035109 -0.1345876
H   2.9655390 -2.9613710  0.1642985
H   1.4313917 -2.6993531 -0.7670637
H   2.6897092 -1.4296775 -0.7677514
C  -2.2036182 -2.2010091  0.1345775
H  -2.6995267 -1.4311911  0.7668932
H  -2.9614077 -2.9654942 -0.1643109
H  -1.4298733 -2.6895311  0.7679015
C  -2.2011205  2.2035029 -0.1345653
H  -2.6897073  1.4296707 -0.7677299
H  -2.9655366  2.9613595  0.1643293
H  -1.4313934  2.6993498 -0.7670428
```

**TS1-2a**

```
C   3.9824982 -0.2529776  0.2927246
S   2.7552298 -0.5194704  1.6290793
Zn  -0.7481503  0.1886400 -0.4004821
S   0.4950569  1.7679132 -1.5320157
C   1.1283961  2.6253222 -0.0193484
S  -1.0096150 -2.0369720 -1.0033290
```

C	0.7776052	-2.5040524	-1.0763212
S	-2.3843747	0.9596532	1.0817525
C	-2.6775456	-0.5867851	2.0411735
H	3.5136113	0.1890084	-0.6177167
H	4.8130589	0.4443434	0.5861395
H	4.4904813	-1.1963100	-0.0426717
H	1.8082034	3.4526801	-0.3262537
H	0.2959530	3.0551115	0.5787301
H	1.6876118	1.9035773	0.6232799
H	-2.2760600	-1.4630807	1.4864956
H	-2.1769105	-0.5506766	3.0350455
H	-3.7671837	-0.7449798	2.2189568
H	0.8618277	-3.6137267	-1.1306056
H	1.2657690	-2.0741660	-1.9773709
H	1.3314401	-2.1312680	-0.1804265

#### 2a

Zn	0.0007433	0.0011128	-0.0013220
S	-0.8532978	2.1226290	0.0219083
S	2.2631384	-0.3235856	-0.0038788
S	-1.4083664	-1.7996222	-0.0202471
C	0.7220836	3.0782546	-0.0311148
H	0.4912758	4.1631936	0.0389427
H	1.3956186	2.8127679	0.8100781
H	1.2832132	2.9056165	-0.9732204
C	-3.0249685	-0.9157007	0.0133343
H	-3.1150842	-0.1877327	-0.8200874
H	-3.8473861	-1.6571907	-0.0824689
H	-3.1740982	-0.3578768	0.9617767
C	2.2968717	-2.1660071	0.0276736
H	1.8239016	-2.6046018	-0.8760666
H	3.3526302	-2.5113280	0.0665478
H	1.7664797	-2.5754565	0.9128861

#### 3a

C	0.0000000	-0.0000346	-1.2112426
H	0.0000000	1.0260276	-1.6780715
H	0.8886915	-0.5128232	-1.6781893
H	-0.8886915	-0.5128232	-1.6781893
S	-0.0000000	0.0000010	0.6119945

#### 4a

Zn	-0.0248988	0.0531296	-0.4441957
S	-0.8510957	1.8899343	-1.6186005
S	-1.2784896	-1.9268057	-0.5371697
S	2.3513672	-0.1299652	-0.3974050
C	2.5315807	-1.9520285	-0.6263362
H	3.0703879	-2.4138424	0.2304997
H	1.5316306	-2.4297856	-0.7166282
H	3.1148913	-2.1742469	-1.5467156
C	0.4723587	2.0632906	-2.8908722
H	0.1615039	1.6211427	-3.8632891
H	0.6971532	3.1382387	-3.0685658
H	1.4046830	1.5566295	-2.5633730
C	-2.0298518	-1.7017379	-2.2043568
H	-1.4386014	-2.2140092	-2.9953001
H	-3.0562903	-2.1301348	-2.2233725
H	-2.0852922	-0.6201572	-2.4558668
N	-0.3025160	0.3705614	1.7299908
C	0.7581095	0.3647446	2.5253948

C	-1.4164174	0.4040441	2.5373257
H	1.7893138	0.2911952	2.1326205
C	-1.0251000	0.4267941	3.8653258
H	-2.4238609	0.3803201	2.1067933
H	-1.5893980	0.4480844	4.8036182
N	0.3638710	0.4010324	3.8349934
H	0.9834551	0.3916839	4.6450229

### 5a

Zn	-0.0229214	0.0451067	-0.5225585
S	-2.0743246	-0.2839677	-1.3120913
S	2.1697423	0.3625043	-0.8582287
C	2.4897903	-0.5742910	-2.4146310
H	2.2570048	-1.6524256	-2.3102320
H	1.9124404	-0.1629804	-3.2659800
H	3.5680784	-0.4741694	-2.6497617
C	-1.9594363	0.3344036	-3.0465539
H	-1.2604261	-0.2726579	-3.6550319
H	-2.9688551	0.2507816	-3.4959464
H	-1.6481732	1.3964897	-3.0928985
N	-0.1565790	0.0156536	1.5692390
C	0.8943617	-0.2300312	2.3493759
C	-1.2442506	0.2169480	2.3965208
H	1.9103120	-0.4229067	1.9785298
C	-0.8387928	0.0919026	3.7120125
H	-2.2357460	0.4360609	1.9845138
H	-1.3809041	0.1765257	4.6586356
N	0.5171363	-0.1908549	3.6560336
H	1.1319760	-0.3444107	4.4569971

### 6a

N	-0.4842063	0.0000500	-1.0262041
C	-1.1027463	-0.0000543	0.2012944
N	-0.2237631	0.0000510	1.1908459
C	1.0130753	-0.0000344	0.5814101
C	0.8805697	0.0000007	-0.7997034
H	-2.1958924	-0.0001012	0.3059695
H	1.9425341	-0.0000664	1.1651013
H	1.6085631	-0.0000315	-1.6174523
H	-0.9417885	-0.0001556	-1.9389117

### 1b

C	-1.8195286	2.8363103	-3.5034648
C	-1.8809299	2.2713073	-2.1848538
C	-2.4780293	3.0170611	-1.1174520
C	-2.9694844	4.3226011	-1.3695197
C	-2.8901500	4.8585455	-2.6685060
C	-2.3314606	4.1356701	-3.7389883
S	-1.2806834	0.6095672	-1.9883417
Zn	-0.0330513	-0.0000992	-0.0013008
S	1.2041032	2.0016706	0.5760706
C	1.8647218	2.2309627	2.2099103
C	2.4583250	1.1731007	2.9723243
C	3.0012053	1.4556983	4.2510731
C	2.9736225	2.7736224	4.7447731
C	2.4168877	3.8337180	4.0052461
C	1.8548762	3.5688740	2.7324789
S	-1.2719026	-0.6054413	1.9924323
C	-1.8791572	-2.2641941	2.1924494
C	-2.4847581	-3.0076308	1.1282044

C	-2.9811757	-4.3107233	1.3832538
C	-2.8984287	-4.8463779	2.6821396
C	-2.3312812	-4.1256444	3.7496163
C	-1.8142784	-2.8288715	3.5110348
S	1.1924803	-2.0072646	-0.5854263
C	1.8534343	-2.2381574	-2.2188299
C	2.4463289	-1.1814698	-2.9834603
C	2.9889399	-1.4661801	-4.2618586
C	2.9616047	-2.7849602	-4.7532808
C	2.4053865	-3.8438924	-4.0117054
C	1.8436653	-3.5770017	-2.7392540
C	-2.5761093	-2.4004024	-0.2451905
C	-3.5999532	-5.1511994	0.2829686
H	-3.2884564	-5.8632451	2.8692648
C	-2.2857532	-4.7695096	5.1232513
C	-1.1922727	-2.0221682	4.6268666
C	2.4751920	0.2143549	-2.4233424
C	3.6006654	-0.3778416	-5.1230500
H	3.3888058	-2.9951992	-5.7504455
C	2.4214119	-5.2400439	-4.6068212
C	1.2328619	-4.6836673	-1.9117423
C	2.4876488	-0.2216902	2.4096116
C	3.6134645	0.3660238	5.1101884
H	3.4009500	2.9821868	5.7422397
C	2.4327947	5.2288460	4.6027640
C	1.2436997	4.6767710	1.9068656
C	-2.5657622	2.4093044	0.2559586
C	-3.5791751	5.1654444	-0.2659811
H	-3.2761282	5.8773908	-2.8532214
C	-2.2891960	4.7801562	-5.1124532
C	-1.2065422	2.0272204	-4.6225551
H	3.1634409	0.8867173	-2.9709752
H	1.4570714	0.6663325	-2.4500828
H	2.7554388	0.2113760	-1.3505283
H	3.9613848	-0.7946065	-6.0866840
H	2.8735237	0.4292266	-5.3576715
H	4.4664011	0.1162440	-4.6294476
H	1.1969652	-5.6515081	-2.4496922
H	1.7922317	-4.8281894	-0.9616155
H	0.2079915	-4.4064925	-1.5876006
H	2.9833328	-5.9660946	-3.9782400
H	1.3993501	-5.6614620	-4.7331003
H	2.8995568	-5.2319186	-5.6083870
H	-1.1461888	2.5898510	-5.5749416
H	-0.1913987	1.6786172	-4.3394728
H	-1.7802381	1.0915149	-4.8000176
H	-3.2772952	2.9389700	0.9187759
H	-2.8516338	1.3396029	0.2016263
H	-1.5665134	2.4141262	0.7482073
H	-3.8904142	6.1576145	-0.6545534
H	-4.4771318	4.6879157	0.1845662
H	-2.8670238	5.3401814	0.5690406
H	-1.2524803	4.8834676	-5.5029652
H	-2.8539927	4.1990086	-5.8748845
H	-2.7308567	5.7978643	-5.0797997
H	-3.2945149	-2.9262535	-0.9036404
H	-2.8551622	-1.3289548	-0.1902259
H	-1.5796268	-2.4116714	-0.7429515
H	-1.1295080	-2.5849704	5.5789963
H	-0.1771855	-1.6777719	4.3384972

H	-1.7610897	-1.0840369	4.8072165
H	-3.9139230	-6.1417683	0.6734260
H	-4.4978300	-4.6697423	-0.1635641
H	-2.8925686	-5.3295166	-0.5553364
H	-1.2477515	-4.8775284	5.5090684
H	-2.8442962	-4.1852532	5.8879124
H	-2.7323859	-5.7851243	5.0932701
H	3.1782180	-0.8941040	2.9542926
H	1.4702291	-0.6750833	2.4382021
H	2.7650114	-0.2160961	1.3360790
H	1.2071929	5.6436112	2.4465606
H	1.8032882	4.8234137	0.9571906
H	0.2190794	4.3996465	1.5819568
H	2.9945129	5.9560848	3.9753794
H	1.4106664	5.6498456	4.7298759
H	2.9109651	5.2190406	5.6043004
H	3.9741537	0.7811495	6.0745355
H	2.8866263	-0.4417176	5.3433821
H	4.4793294	-0.1268229	4.6155656

### TS1-2b

C	2.8776007	2.9209999	2.0713298
C	2.2863910	1.6798182	1.6699800
C	2.3492416	0.5371174	2.5266137
C	2.9656644	0.6656617	3.7991675
C	3.5353830	1.8943586	4.1781639
C	3.5130140	3.0198974	3.3346591
S	1.5746917	1.5986057	0.0308104
Zn	-0.6019866	0.7949680	0.1449659
S	-1.8320699	1.0821829	-1.8492752
C	-1.5172254	2.7054595	-2.5157723
C	-1.3126398	2.8096122	-3.9306562
C	-1.1331793	4.0852335	-4.5205059
C	-1.1434503	5.2295674	-3.7010859
C	-1.3430728	5.1504348	-2.3108243
C	-1.5510440	3.8850314	-1.7063490
C	-1.2889545	1.5521307	-4.7675067
C	-0.9169243	4.2547905	-6.0125278
C	-1.3254165	6.4245747	-1.4895399
C	-1.7995249	3.7764250	-0.2235187
C	1.7724436	-0.7877403	2.1010138
C	3.0202583	-0.5047473	4.7589819
C	4.1665169	4.3048901	3.8073309
C	2.8223176	4.1093098	1.1385280
S	-1.7906436	0.8716079	2.1734341
C	-2.1497179	-0.7663686	2.7881142
C	-2.6705200	-1.7906005	1.9415309
C	-2.8592224	-3.0922846	2.4731350
C	-2.6297272	-3.3212267	3.8407793
C	-2.1910408	-2.3030458	4.7086021
C	-1.9280337	-1.0140802	4.1808403
C	-2.9873690	-1.5146167	0.4963369
C	-3.2512458	-4.2369634	1.5660766
C	-1.9847583	-2.6269954	6.1764784
C	-1.4076638	0.1005196	5.0598346
S	0.1620207	-2.8865985	-0.5885429
C	0.8945610	-3.6168557	-2.0052143
C	0.9873968	-5.0527928	-2.1120711
C	1.5606468	-5.6498304	-3.2597797
C	2.0565437	-4.8310485	-4.2939864



C	1.9997544	-3.4236391	-4.2124259
C	1.4240026	-2.8085942	-3.0756948
C	0.4567096	-5.8935545	-0.9766308
C	1.3483570	-1.3097011	-2.9441876
C	2.5639576	-2.6083620	-5.3624872
C	1.6543363	-7.1574236	-3.4158311
H	-2.7870268	-4.3369999	4.2449857
H	2.5012277	-5.3019159	-5.1896694
H	4.0168355	1.9768865	5.1688869
H	-0.9868030	6.2201684	-4.1637886
H	1.7627675	-0.7741011	-3.8209370
H	0.3007396	-0.9752285	-2.7798190
H	1.8813414	-0.9601878	-2.0331655
H	2.9557996	-3.2735924	-6.1610788
H	1.8017799	-1.9451916	-5.8279149
H	3.3983337	-1.9447598	-5.0447127
H	0.7832948	-6.9525714	-1.0309996
H	0.7658884	-5.4476061	-0.0071341
H	-0.6567647	-5.8736308	-0.9446786
H	2.2737716	-7.6329525	-2.6217957
H	0.6598614	-7.6551134	-3.3706509
H	2.1125448	-7.4241975	-4.3919190
H	-0.9823106	1.7413398	-5.8145114
H	-0.6069822	0.8011665	-4.3179940
H	-2.2855149	1.0588549	-4.7812975
H	-2.1886706	4.7168096	0.2139060
H	-2.5127755	2.9553400	-0.0046438
H	-0.8583433	3.5261502	0.3193588
H	-1.1323018	7.3073399	-2.1335869
H	-2.2885275	6.6024156	-0.9613959
H	-0.5393618	6.4039234	-0.7037729
H	-0.0049659	3.7283614	-6.3702323
H	-1.7646762	3.8573851	-6.6131299
H	-0.8011469	5.3274752	-6.2719491
H	-3.8515528	-2.1149305	0.1436782
H	-3.2097719	-0.4412439	0.3385021
H	-2.1279646	-1.7911672	-0.1655783
H	-1.1502874	-0.2468608	6.0792975
H	-0.5155079	0.5735615	4.5989377
H	-2.1508516	0.9233841	5.1548668
H	-3.3048251	-5.1932215	2.1262188
H	-4.2371714	-4.0739565	1.0764784
H	-2.5018263	-4.3471471	0.7513635
H	-0.9317870	-2.4752327	6.5018484
H	-2.6137863	-1.9989512	6.8458698
H	-2.2409706	-3.6869285	6.3812340
H	2.3242440	-1.6455216	2.5338002
H	0.7138645	-0.8913010	2.4280775
H	1.7613679	-0.9089196	1.0003404
H	3.1380153	5.0511577	1.6287535
H	3.4674294	3.9542027	0.2454477
H	1.7985524	4.2334059	0.7297755
H	4.9847430	4.6403971	3.1322858
H	3.4465614	5.1507412	3.8709294
H	4.6055423	4.1713480	4.8177927
H	3.5026886	-0.2130387	5.7150197
H	2.0065989	-0.8935558	4.9931553
H	3.5906271	-1.3635150	4.3413266

2b

Zn	0.6942108	-0.9119202	-0.1637477
S	0.8106081	1.3017079	0.4176988
S	2.6837852	-2.0214836	-0.5219238
S	-0.8975647	-2.5411281	-0.4949912
C	-0.8421680	2.0019062	0.5045273
C	-1.7879421	1.5129026	1.4568831
C	-3.0676723	2.1188528	1.5395376
C	-3.3630242	3.2150651	0.7081930
C	-2.4368215	3.7240869	-0.2170271
C	-1.1631585	3.1109621	-0.3364011
C	3.9966510	-0.8669761	-0.1104390
C	4.2244787	-0.4942063	1.2508962
C	5.2987332	0.3770683	1.5649147
C	6.1409815	0.8315216	0.5342363
C	5.9436946	0.4623455	-0.8067712
C	4.8583522	-0.3863229	-1.1436255
C	-2.5612344	-1.8738133	-0.5334519
C	-2.9171554	-0.8632360	-1.4790996
C	-4.2543788	-0.3942049	-1.5263606
C	-5.2130673	-0.9628556	-0.6679402
C	-4.8872886	-1.9744232	0.2513201
C	-3.5478241	-2.4329163	0.3361715
H	-4.3560764	3.6906742	0.7845658
H	6.9794353	1.5038729	0.7864861
H	-6.2547594	-0.6015650	-0.7186736
C	6.8812513	0.9774332	-1.8768734
H	7.3761580	0.1504646	-2.4314858
H	6.3474067	1.5831316	-2.6421309
H	7.6773618	1.6145329	-1.4411890
C	5.5530703	0.8373609	2.9854368
H	4.6779989	1.3739328	3.4106802
H	5.7659401	-0.0106466	3.6725972
H	6.4215936	1.5253582	3.0288628
C	4.6390561	-0.7589096	-2.5915351
H	3.6816922	-1.3020490	-2.7040686
H	4.6237594	0.1396169	-3.2456465
H	5.4527126	-1.4151202	-2.9748523
C	3.3133919	-1.0049290	2.3405614
H	2.3979950	-0.3740005	2.4099347
H	2.9653671	-2.0292647	2.1005645
H	3.7996283	-1.0023611	3.3358721
C	-2.8017252	4.9180162	-1.0720520
H	-3.8227427	5.2814463	-0.8384110
H	-2.0988682	5.7669315	-0.9244948
H	-2.7711223	4.6803404	-2.1580159
C	-4.1305175	1.6098521	2.4911307
H	-4.4116610	0.5599620	2.2619082
H	-3.7968030	1.6324262	3.5511226
H	-5.0500296	2.2248227	2.4189000
C	-0.1769818	3.6564900	-1.3430515
H	0.1968960	4.6615836	-1.0444739
H	0.6972625	2.9844240	-1.4300302
H	-0.6402936	3.7775737	-2.3456664
C	-1.4184299	0.3598914	2.3567470
H	-2.1527994	0.2050255	3.1687384
H	-1.3471949	-0.5905794	1.7818341
H	-0.4146539	0.5227063	2.8009395
C	-5.9648565	-2.5647266	1.1350822
H	-6.9515211	-2.1054661	0.9239659
H	-6.0662161	-3.6629612	0.9926793

H	-5.7499122	-2.4137453	2.2159541
C	-4.6754792	0.7105675	-2.4731321
H	-4.1183362	1.6507882	-2.2755826
H	-4.4962091	0.4462646	-3.5378642
H	-5.7561091	0.9336673	-2.3635073
C	-1.8696920	-0.3028562	-2.4088855
H	-1.1959884	0.4032361	-1.8725118
H	-1.2211208	-1.1162157	-2.7929261
H	-2.3107766	0.2464341	-3.2621521
C	-3.2004427	-3.5136564	1.3343564
H	-3.6024483	-4.5037955	1.0215028
H	-2.1023137	-3.6145379	1.4255002
H	-3.6293947	-3.3002300	2.3364780

### 3b

C	1.2968254	-1.2380191	0.0007011
C	-0.1168764	-1.2343120	0.0049801
C	-0.8611651	0.0093336	0.0009492
C	-0.0899778	1.2365184	-0.0007496
C	1.3234713	1.2096677	-0.0001681
C	2.0091824	-0.0217694	-0.0010382
S	-2.6098141	0.0279593	-0.0032250
C	-0.8623862	-2.5497891	0.0087171
C	-0.8060760	2.5683051	-0.0008990
C	2.1151283	2.5020265	0.0030758
H	3.1139204	-0.0338944	-0.0034673
C	2.0606477	-2.5471223	-0.0070788
H	-0.5063273	3.2099224	-0.8613858
H	-1.8978114	2.3686910	-0.0523997
H	-0.5932704	3.1606260	0.9197922
H	3.2079228	2.3058370	0.0050752
H	1.8888280	3.1363945	-0.8833534
H	1.8850676	3.1337061	0.8903818
H	3.1572700	-2.3740634	-0.0142969
H	1.8257268	-3.1772538	0.8801849
H	1.8129135	-3.1731762	-0.8936812
H	-0.5443028	-3.2143038	0.8444492
H	-1.9470118	-2.3273283	0.1012821
H	-0.7000959	-3.1280878	-0.9311535

### 4b

N	1.3430798	2.2798552	2.4792071
C	0.5610053	1.6553385	1.5531496
N	1.2334214	0.6833197	0.9396222
C	2.5015883	0.6708541	1.4899306
C	2.5865324	1.6589794	2.4534499
Zn	0.2346130	-0.4099803	-0.6166679
S	-1.4211870	-1.0386656	1.0045544
C	-2.9851276	-1.7064330	0.4756641
C	-3.2050137	-2.2594488	-0.8246068
C	-4.4898576	-2.7608505	-1.1554407
C	-5.5172555	-2.7253708	-0.1950683
C	-5.3171021	-2.2056556	1.0967177
C	-4.0446489	-1.6883199	1.4416874
C	0.9314676	3.3785228	3.3354790
S	-0.1680548	1.2513702	-2.2795983
C	-0.6336029	2.6946559	-1.3366807
C	-1.9703849	2.8447344	-0.8477099
C	-2.2951453	3.9704060	-0.0472732
C	-1.3058225	4.9398135	0.2120856

C	-0.0012706	4.8421885	-0.3104512
C	0.3435929	3.7126991	-1.0964331
S	1.5651529	-2.0667275	-1.6455951
C	3.0349720	-2.0531703	-0.6311621
C	4.1883429	-1.3427150	-1.0881452
C	5.3677084	-1.3525430	-0.2994794
C	5.3712435	-2.0643181	0.9159566
C	4.2486374	-2.7787354	1.3781680
C	3.0642194	-2.7842459	0.5970633
C	-3.0024956	1.7951901	-1.1744755
C	-3.6844272	4.1612101	0.5288037
H	-1.5698759	5.8173322	0.8282654
C	0.9925471	5.9508552	-0.0185495
C	1.7328555	3.5535441	-1.6679572
C	4.1170833	-0.5844727	-2.3928684
C	6.6244108	-0.6192202	-0.7266892
H	6.2903916	-2.0646256	1.5274188
C	4.3410669	-3.5195994	2.6978681
C	1.8296475	-3.5316191	1.0385850
C	-2.0776165	-2.3095301	-1.8225886
C	-4.7894016	-3.3391863	-2.5247164
H	-6.5123081	-3.1206222	-0.4635236
C	-6.4742436	-2.2134329	2.0772706
C	-3.7831950	-1.1158221	2.8151674
H	-0.4808746	1.9318895	1.3518314
H	3.2654665	-0.0418238	1.1592418
H	3.4052061	1.9715673	3.1093209
H	1.7066228	4.1700640	3.3429230
H	-0.0030380	3.8126121	2.9340987
H	0.7587115	3.0358242	4.3770851
H	1.9903036	-4.1155142	1.9647731
H	0.9737592	-2.8398709	1.2015818
H	1.4865814	-4.2155107	0.2341843
H	5.3437974	-3.3899754	3.1540595
H	3.5904487	-3.1607129	3.4343484
H	4.1689032	-4.6111443	2.5791319
H	7.4306961	-0.7504092	0.0234682
H	7.0140670	-0.9859910	-1.7007179
H	6.4570474	0.4731660	-0.8458432
H	5.0255468	0.0165152	-2.5887243
H	3.9636706	-1.2797243	-3.2459378
H	3.2279050	0.0797923	-2.4084733
H	-2.3259359	-2.9134549	-2.7151440
H	-1.8033029	-1.2902408	-2.1781759
H	-1.1574451	-2.7316628	-1.3669728
H	-4.6802562	-1.1362101	3.4627047
H	-2.9652783	-1.6678596	3.3270383
H	-3.4165804	-0.0692588	2.7422959
H	-5.8486820	-3.6603791	-2.5920771
H	-4.6101662	-2.6054004	-3.3395294
H	-4.1588978	-4.2251764	-2.7561231
H	-7.3790486	-2.6526571	1.6104978
H	-6.2533347	-2.8084666	2.9904747
H	-6.7453649	-1.1921030	2.4234929
H	-4.0377249	2.1396695	-0.9898166
H	-2.9003347	1.4809962	-2.2328693
H	-2.8329391	0.8760645	-0.5727733
H	-3.7289568	5.0701838	1.1627915
H	-4.4540102	4.2744996	-0.2657157
H	-4.0033925	3.2989333	1.1517359

H	2.3469614	4.4679929	-1.5584128
H	2.2673271	2.7104853	-1.1798780
H	1.6816825	3.2740993	-2.7398803
H	1.9164884	5.5770339	0.4730686
H	1.3222745	6.4725974	-0.9435029
H	0.5446634	6.7164945	0.6475763

**6b**

C	0.8727355	-0.1101423	-0.7830851
N	-0.4831135	0.0421164	-1.0258826
C	-1.0839616	0.1858595	0.2055273
N	-0.2125152	0.1375366	1.2000567
C	1.0119012	-0.0466373	0.5963674
H	-2.1702634	0.3240494	0.3012698
H	1.9381329	-0.1231020	1.1807424
H	1.5945194	-0.2447961	-1.5961553
C	-1.1388810	0.0410559	-2.3221622
H	-0.7165177	0.8264452	-2.9814254
H	-1.0320096	-0.9409099	-2.8272956
H	-2.2166660	0.2469852	-2.1828354

**1c**

C	-3.1022822	2.8970646	-2.1197042
C	-2.3935313	2.0535382	-1.2193555
C	-2.7541060	2.1538627	0.1529589
C	-3.7553400	3.0346095	0.5837985
C	-4.4555485	3.8637765	-0.3207704
C	-4.1049140	3.7783691	-1.6854853
S	-1.1714249	0.9410695	-1.8434347
Zn	0.0584234	-0.0000129	0.0000169
S	1.2859087	1.8408354	0.9439869
C	2.4396823	1.2069484	2.1239733
C	2.8519610	-0.1530359	2.1803267
C	3.7757046	-0.5980483	3.1355981
C	4.3437137	0.2807408	4.0850841
C	3.9533938	1.6361361	4.0321100
C	3.0238560	2.0833005	3.0797334
S	-1.1714307	-0.9410693	1.8434765
C	-2.3935663	-2.0535040	1.2193926
C	-2.7541484	-2.1538276	-0.1529188
C	-3.7554066	-3.0345524	-0.5837479
C	-4.4556320	-3.8636969	0.3208280
C	-4.1049893	-3.7782908	1.6855413
C	-3.1023335	-2.8970085	2.1197501
S	1.2858917	-1.8408755	-0.9439442
C	2.4396071	-1.2069917	-2.1239902
C	2.8520275	0.1529540	-2.1802445
C	3.7757087	0.5979696	-3.1355748
C	4.3435195	-0.2807806	-4.0852156
C	3.9530715	-1.6361422	-4.0323314
C	3.0235918	-2.0833076	-3.0798990
H	-2.2479264	-1.5020806	-0.8850465
H	-4.0067617	-3.0737067	-1.6590422
N	-5.4391933	-4.7955878	-0.1338448
H	-4.6262609	-4.4184917	2.4210285
H	-2.8486376	-2.8454758	3.1914801
H	2.4329169	0.8666551	-1.4502568
H	4.0639052	1.6645816	-3.1453063
N	5.3199619	0.1722709	-5.0253166
H	4.3815874	-2.3531155	-4.7566856

H	2.7221335	-3.1436573	-3.0676734
H	2.4326863	-0.8667694	1.4504649
H	4.0637979	-1.6646877	3.1454037
N	5.3202174	-0.1723155	5.0251197
H	4.3820603	2.3531383	4.7563465
H	2.7225036	3.1436791	3.0674354
H	-2.2478974	1.5020987	0.8850813
H	-4.0066885	3.0737627	1.6590942
N	-5.4390849	4.7956889	0.1339121
H	-4.6261743	4.4185866	-2.4209662
H	-2.8485912	2.8455315	-3.1914355
H	5.2363625	0.3352634	5.9139184
H	5.1893289	-1.1700754	5.2286122
H	5.2359500	-0.3352073	-5.9141580
H	5.1891541	1.1700655	-5.2286898
H	-6.1966499	-4.8959750	0.5523123
H	-5.8609194	-4.4747382	-1.0130811
H	-6.1965284	4.8961183	-0.5522531
H	-5.8608338	4.4748313	1.0131346

### TS1-2c

C	-4.1959739	1.3457844	2.3833887
C	-3.2335853	0.4689697	1.8123119
C	-3.7262456	-0.7520333	1.2811074
C	-5.0918305	-1.0671992	1.3195528
C	-6.0408702	-0.1881102	1.8862794
C	-5.5616679	1.0269682	2.4229978
S	-1.5316290	0.9609265	1.8232471
Zn	-0.2391464	-0.7049051	0.8289246
S	-0.9417435	-2.2814305	-0.7088270
C	-1.7887868	-1.3401023	-1.9655407
C	-1.3429487	-0.0695967	-2.4060032
C	-2.0170587	0.6171590	-3.4237450
C	-3.1571417	0.0722908	-4.0555499
C	-3.5953910	-1.2022209	-3.6340044
C	-2.9262542	-1.8889386	-2.6071556
S	1.5472391	-1.1497473	2.2246846
C	2.7372403	-2.0291442	1.2365919
C	3.0863665	-1.6271507	-0.0784551
C	4.0664532	-2.3419515	-0.7799351
C	4.7247294	-3.4510347	-0.2156287
C	4.3892266	-3.8609799	1.0938742
C	3.4014951	-3.1455793	1.8025817
S	1.9265579	1.4989795	-2.0727811
C	2.4062036	2.9480532	-1.2224832
C	2.8534340	4.1186242	-1.9146292
C	3.2397197	5.2932858	-1.2498229
C	3.1999628	5.3828984	0.1589469
C	2.7664066	4.2385844	0.8669803
C	2.3844772	3.0643419	0.2039208
H	2.8844819	4.0768507	-3.0162664
H	3.5803125	6.1674917	-1.8368375
H	2.7209197	4.2721694	1.9713762
H	2.0443058	2.1944609	0.7874527
H	3.1205241	-3.4638360	2.8212795
H	5.4988929	-3.9978972	-0.7815374
H	4.3259258	-2.0131994	-1.7999656
H	2.6090870	-0.7448037	-0.5446648
H	-3.2932133	-2.8759219	-2.2818095
H	-4.4799072	-1.6595933	-4.1125136

H	-1.6267153	1.6026208	-3.7314638
H	-0.4417489	0.4006725	-1.9657897
H	-3.8486008	2.3054106	2.7994082
H	-3.0182281	-1.4560216	0.8108541
H	-5.4319512	-2.0236006	0.8843126
H	-6.2745640	1.7389249	2.8768145
N	-3.8083568	0.7566607	-5.1195880
H	-4.8229141	0.6047365	-5.1034425
H	-3.6346097	1.7662619	-5.0700168
N	3.6378376	6.5666221	0.8438453
H	3.3518719	7.4055145	0.3221493
H	3.1815399	6.6249932	1.7628944
N	5.0673716	-4.9508043	1.7069546
H	4.4932489	-5.3840259	2.4380381
H	5.3192979	-5.6716127	1.0223535
N	-7.4208943	-0.5378046	1.9641315
H	-8.0201337	0.2923098	1.8918226
H	-7.6808130	-1.1781725	1.2055967

### 2c

C	-3.7165435	-2.6218428	0.8151055
C	-2.5790796	-1.9098460	0.3571780
C	-2.7040075	-1.2283846	-0.8782226
C	-3.8993476	-1.2580425	-1.6102804
C	-5.0300390	-1.9689573	-1.1488793
C	-4.9119678	-2.6527695	0.0826055
S	-1.1041863	-1.9371066	1.3548475
Zn	0.5522588	-0.7567585	0.2551735
S	2.5058074	-1.8780379	0.6620209
C	3.9163452	-0.8953751	0.1992191
C	3.8720965	0.4792011	-0.1390558
C	5.0346585	1.1842968	-0.4811400
C	6.3010989	0.5574123	-0.4986564
C	6.3537707	-0.8130107	-0.1573320
C	5.1900340	-1.5188926	0.1805521
S	0.3496104	1.1431442	-1.0389678
C	-0.9262249	2.1519396	-0.3052266
C	-1.6807715	1.7932871	0.8369484
C	-2.6677812	2.6446325	1.3519614
C	-2.9506000	3.8934224	0.7547575
C	-2.1979922	4.2577320	-0.3846810
C	-1.2111100	3.4058415	-0.9003766
H	-1.5040679	0.8179333	1.3216127
H	-3.2387578	2.3256989	2.2406113
N	-3.9069114	4.7716530	1.3123713
H	-2.3888210	5.2279803	-0.8752983
H	-0.6418291	3.7121070	-1.7926999
H	2.9009711	1.0006471	-0.1542674
H	4.9548677	2.2532712	-0.7440467
N	7.4774338	1.2880359	-0.7878715
H	7.3259109	-1.3361683	-0.1586020
H	5.2585433	-2.5890858	0.4337110
H	-1.8490206	-0.6497738	-1.2647993
H	-3.9556566	-0.7087880	-2.5655522
N	-6.2140476	-2.0444273	-1.9192244
H	-5.7739414	-3.2214853	0.4725553
H	-3.6536068	-3.1606475	1.7739872
H	-7.0538847	-2.1725309	-1.3469524
H	-6.3406550	-1.2323725	-2.5305446
H	-4.3398952	5.3865301	0.6171977

H	-4.6370924	4.2821893	1.8377364
H	8.2155059	0.7065760	-1.1958298
H	7.3029002	2.0911327	-1.3991909

### 3c

C	1.1600872	-1.2048361	0.0020453
C	-0.2424099	-1.2040647	0.0040273
C	-1.0255386	-0.0000065	0.0035586
C	-0.2423760	1.2040724	0.0038144
C	1.1601075	1.2051087	0.0028133
C	1.8996737	0.0001799	-0.0011232
S	-2.7618208	-0.0000703	-0.0049684
H	-0.7908762	-2.1608686	0.0003284
H	-0.7910333	2.1607888	0.0001530
H	1.7036811	2.1693222	0.0054849
N	3.3333931	0.0006468	0.0590701
H	1.7037645	-2.1690773	0.0032318
H	3.7100220	-0.8299129	-0.4150764
H	3.7111897	0.8175882	-0.4372701

### 1d

Zn	-0.0011883	-0.0002796	0.0004995
S	-1.2266605	-1.0965024	1.7568872
S	1.2230800	-1.7570286	-1.0956634
S	1.2231509	1.7559502	1.0975515
S	-1.2254842	1.0968161	-1.7561410
C	-2.4154217	-2.1874787	1.0514586
C	-2.7847766	-2.1791722	-0.3242548
C	-3.7501965	-3.0672309	-0.8185763
C	-4.3920686	-3.9966656	0.0248454
C	-4.0419988	-4.0149637	1.3890202
C	-3.0751888	-3.1322930	1.8918408
C	2.4133818	-1.0521684	-2.1853345
C	2.7815775	0.3238933	-2.1785892
C	3.7479712	0.8175431	-3.0659419
C	4.3913648	-0.0266330	-3.9936571
C	4.0424010	-1.3911232	-4.0104075
C	3.0750229	-1.8934016	-3.1280324
C	2.4155888	1.0511744	2.1849927
C	2.7845270	-0.3246648	2.1768639
C	3.7524851	-0.8183203	3.0625226
C	4.3967572	0.0255958	3.9898536
C	4.0469458	1.3898605	4.0080645
C	3.0781367	1.8921717	3.1273041
C	-2.4136304	2.1885035	-1.0507723
C	-2.7842676	2.1792888	0.3245875
C	-3.7492543	3.0678810	0.8187984
C	-4.3893943	3.9987476	-0.0243590
C	-4.0380017	4.0179546	-1.3881806
C	-3.0716252	3.1347556	-1.8909100
H	-2.3075565	-1.4471739	-0.9965467
H	-4.0083961	-3.0275941	-1.8908333
H	-5.1495149	-4.6923441	-0.3732657
H	-4.5278167	-4.7326301	2.0741224
H	-2.8028849	-3.1559725	2.9597898
H	2.3028414	0.9968239	-1.4481687
H	4.0052988	1.8900473	-3.0275167
H	5.1493733	0.3710561	-4.6889646
H	4.5295810	-2.0768867	-4.7265101
H	2.8035571	-2.9615884	-3.1505496



H	2.3052505	-0.9974721	1.4466404
H	4.0104207	-1.8906406	3.0229767
H	5.1559459	-0.3721332	4.6838519
H	4.5346820	2.0754256	4.7239803
H	2.8060700	2.9601837	3.1509049
H	-2.3083400	1.4462544	0.9966823
H	-4.0084587	3.0275568	1.8907901
H	-5.1464790	4.6948527	0.3736884
H	-4.5224494	4.7367442	-2.0730788
H	-2.7982590	3.1591665	-2.9585680

**TS1-2d**

C	-4.3640966	1.1980715	2.5147351
C	-3.4066797	0.3743034	1.8551770
C	-3.8768985	-0.8419102	1.2881960
C	-5.2274453	-1.2073817	1.3854030
C	-6.1621955	-0.3859546	2.0447719
C	-5.7118733	0.8239992	2.6071149
S	-1.7301330	0.9261031	1.8121057
Zn	-0.3904985	-0.7282562	0.8582586
S	-1.0136658	-2.2695172	-0.7462086
C	-1.8182563	-1.3201411	-2.0173028
C	-1.4144110	-0.0079578	-2.3717882
C	-2.0508894	0.6734673	-3.4199780
C	-3.0967429	0.0750838	-4.1477130
C	-3.4988685	-1.2302057	-3.8094310
C	-2.8708553	-1.9180659	-2.7589449
S	1.3811974	-1.1502813	2.2656154
C	2.6202835	-1.9466649	1.2673402
C	2.9505136	-1.5057682	-0.0401134
C	3.9774719	-2.1323515	-0.7615906
C	4.7086825	-3.2024131	-0.2105752
C	4.3943629	-3.6409189	1.0887593
C	3.3633454	-3.0243151	1.8164973
S	1.9073245	1.5544841	-2.0923851
C	2.5136118	2.9596309	-1.2641206
C	3.1581199	4.0291630	-1.9719493
C	3.6537011	5.1672255	-1.3212050
C	3.5391617	5.3121825	0.0773549
C	2.9100247	4.2750024	0.8004958
C	2.4120142	3.1358180	0.1561480
H	3.2532505	3.9262470	-3.0659595
H	4.1408247	5.9613861	-1.9175170
H	3.9281065	6.2082581	0.5898248
H	2.8044191	4.3575251	1.8970513
H	1.9275662	2.3359450	0.7382897
H	3.1113968	-3.3730699	2.8312807
H	4.9539661	-4.4775530	1.5428127
H	5.5168208	-3.6863125	-0.7844025
H	4.2087914	-1.7541964	-1.7710854
H	2.4245573	-0.6444214	-0.4949880
H	-3.1923655	-2.9373185	-2.4903401
H	-4.3170390	-1.7203139	-4.3653861
H	-3.5905324	0.6169990	-4.9713993
H	-1.6949212	1.6857266	-3.6718756
H	-0.5658941	0.4802549	-1.8568925
H	-4.0194644	2.1467051	2.9571920
H	-3.1631869	-1.4962477	0.7594534
H	-5.5546235	-2.1567385	0.9283422
H	-7.2223987	-0.6798221	2.1145402

H -6.4225489 1.4902497 3.1267091

**2d**

Zn 0.4304058 -0.6241934 0.0782517  
S 0.2007346 1.3939496 -1.0159327  
S 2.4034667 -1.7613280 0.3557234  
S -1.1864080 -1.9649447 1.0429284  
C -1.0235905 2.3424812 -0.1414944  
C -1.7646779 1.8654782 0.9677700  
C -2.7106161 2.6859776 1.6013299  
C -2.9457458 3.9984068 1.1549396  
C -2.2153194 4.4812911 0.0538714  
C -1.2690443 3.6681476 -0.5862124  
C 3.8091479 -0.7176943 0.0650264  
C 3.7442913 0.6769140 -0.1837614  
C 4.9139605 1.4244149 -0.3905992  
C 6.1814387 0.8155672 -0.3530023  
C 6.2587670 -0.5672568 -0.1043564  
C 5.0949575 -1.3222927 0.1003360  
C -2.6950452 -1.8180835 0.1174127  
C -2.8640810 -0.9743395 -1.0098548  
C -4.0895234 -0.9245230 -1.6918509  
C -5.1804123 -1.7106057 -1.2794216  
C -5.0246252 -2.5520188 -0.1623110  
C -3.8040773 -2.6060011 0.5263037  
H -1.6025371 0.8352192 1.3259922  
H -3.2759142 2.2835692 2.4576647  
H -3.6905521 4.6360797 1.6568277  
H -2.3834030 5.5071586 -0.3140317  
H -0.6994774 4.0521779 -1.4472750  
H 2.7608012 1.1726176 -0.2249514  
H 4.8268151 2.5061704 -0.5855495  
H 7.0952391 1.4084993 -0.5163253  
H 7.2406161 -1.0688479 -0.0709703  
H 5.1632482 -2.4050187 0.2921870  
H -2.0222388 -0.3466650 -1.3439297  
H -4.1893514 -0.2533990 -2.5604728  
H -6.1397633 -1.6668478 -1.8188927  
H -5.8664939 -3.1766089 0.1804176  
H -3.6885529 -3.2665078 1.4001654

**3d**

C 0.2243045 -1.2112883 -0.0000000  
C -0.5538680 0.0000000 -0.0000000  
C 0.2243045 1.2112883 -0.0000000  
C 1.6245919 1.2088057 -0.0000000  
C 2.3551380 0.0000000 0.0000000  
C 1.6245918 -1.2088058 -0.0000000  
H -0.3319399 -2.1637459 0.0000000  
H -0.3319398 2.1637459 0.0000000  
H 2.1652325 2.1735930 0.0000000  
H 3.4576215 -0.0000001 0.0000001  
H 2.1652333 -2.1735925 0.0000000  
S -2.2839027 0.0000000 0.0000000

**1e**

Zn 0.0029668 0.0000491 0.0000450  
S -1.2070771 1.5450615 1.3720704  
S 1.2127445 -1.3710839 1.5459095  
S 1.2127527 1.3711415 -1.5458413

S	-1.2071641	-1.5449654	-1.3719175
C	-2.3761026	0.6665137	2.3303150
C	-2.7084461	-0.7063402	2.1296259
C	-3.6556194	-1.3464193	2.9271569
C	-4.3290398	-0.6522777	3.9714649
C	-4.0107904	0.7193749	4.1761986
C	-3.0630908	1.3548931	3.3774754
C	2.3776309	-2.3343565	0.6673785
C	2.7102705	-2.1360467	-0.7057274
C	3.6548945	-2.9371001	-1.3452104
C	4.3251394	-3.9829303	-0.6502472
C	4.0060520	-4.1857813	0.7214599
C	3.0610000	-3.3835033	1.3563671
C	2.3777535	2.3343162	-0.6673572
C	2.7104677	2.1359340	0.7057201
C	3.6551850	2.9369002	1.3451733
C	4.3254538	3.9827129	0.6502068
C	4.0062925	4.1856373	-0.7214724
C	3.0611483	3.3834448	-1.3563510
C	-2.3761117	-0.6664117	-2.3302558
C	-2.7084061	0.7064645	-2.1296429
C	-3.6555398	1.3465386	-2.9272263
C	-4.3289069	0.6523905	-3.9715623
C	-4.0106772	-0.7192751	-4.1762450
C	-3.0630728	-1.3548084	-3.3774210
H	-2.2137945	-1.2601891	1.3160856
H	-3.8911506	-2.4065029	2.7460488
H	-4.5206472	1.2767989	4.9775591
H	-2.8222467	2.4158473	3.5480052
H	2.2182115	-1.3213154	-1.2601360
H	3.8907510	-2.7577552	-2.4055240
H	4.5133282	-4.9884066	1.2794297
H	2.8198803	-3.5522959	2.4175389
H	2.2183914	1.3212102	1.2601260
H	3.8911000	2.7574998	2.4054642
H	4.5135838	4.9882524	-1.2794436
H	2.8199701	3.5522940	-2.4175001
H	-2.2138012	1.2603180	-1.3160773
H	-3.8910138	2.4066481	-2.7461939
H	-4.5205060	-1.2767083	-4.9776167
H	-2.8222676	-2.4157813	-3.5478886
C	-5.2986748	1.3049648	-4.7923469
C	5.2923745	-4.8070693	-1.3023511
C	5.2927853	4.8067612	1.3022822
C	-5.2988766	-1.3048568	4.7921644
N	6.0934880	5.4920523	1.8320733
N	-6.1012704	-1.8352345	5.4750242
N	-6.1010207	1.8353271	-5.4752746
N	6.0929983	-5.4924367	-1.8321632

#### TS1-2e

C	-4.6025724	0.3185958	-1.5328442
C	-4.5122714	-1.1119367	-1.3883193
C	-5.5989393	-1.8566999	-1.9724127
C	-6.6600741	-1.2448598	-2.6292659
C	-6.7266189	0.1759592	-2.7587784
C	-5.6614224	0.9376156	-2.1875752
S	-3.2018063	-1.8956799	-0.5954786
C	-7.8116102	0.8043031	-3.4322765
N	-8.7145246	1.3224348	-3.9932550

Zn	0.7820482	1.0290837	0.5983989
S	1.4398562	2.0913574	-1.3746303
C	3.1806101	2.3080797	-1.2798224
C	4.0122778	1.7547950	-0.2655533
C	5.3868250	1.9923678	-0.2475826
C	6.0028268	2.7959966	-1.2440480
C	5.1828602	3.3429506	-2.2682506
C	3.8105863	3.1020761	-2.2830052
C	7.4086557	3.0561861	-1.2196461
N	8.5654666	3.2794749	-1.2029415
S	1.7375894	-0.8082850	1.6131618
C	2.5016931	-1.8359179	0.4037991
C	3.1887575	-2.9954726	0.8642552
C	3.8196849	-3.8673082	-0.0215733
C	3.7926269	-3.6192595	-1.4200813
C	3.1056913	-2.4678083	-1.8876246
C	2.4744373	-1.5982072	-0.9969009
C	4.4448966	-4.5119924	-2.3281582
N	4.9881898	-5.2510540	-3.0671903
S	-0.6579835	2.3118066	1.8128258
C	-1.5232985	1.1825716	2.8743285
C	-2.1551559	0.0068206	2.3942168
C	-2.8938664	-0.8107158	3.2534816
C	-3.0284822	-0.4840164	4.6287307
C	-2.4040635	0.6957083	5.1132913
C	-1.6683215	1.5096236	4.2495455
C	-3.7814910	-1.3111956	5.5234851
N	-4.3944015	-1.9779915	6.2763198
H	-2.1215093	-0.2772620	1.3250583
H	-3.3859299	-1.7007693	2.8325492
H	-2.5012903	0.9616984	6.1772562
H	-1.1821679	2.4210416	4.6305717
H	1.9530391	-0.7082086	-1.3836246
H	3.0698836	-2.2600927	-2.9675282
H	4.3433741	-4.7573290	0.3594420
H	3.2132417	-3.1986357	1.9459599
H	3.5609218	1.1210780	0.5155675
H	6.0045899	1.5499992	0.5485066
H	5.6415593	3.9643461	-3.0526619
H	3.1856527	3.5349119	-3.0793591
H	-3.7904444	0.9267493	-1.1044250
H	-5.6860921	2.0361414	-2.2733936
H	-7.4688214	-1.8577707	-3.0605807
H	-5.5635862	-2.9540869	-1.8810237

## 2e

Zn	-0.0014427	-0.0167727	-0.9383372
S	2.2526439	0.4289669	-1.1229722
S	-1.5192930	1.7111550	-1.0859159
S	-0.7363452	-2.1980135	-1.0375109
C	3.1998821	-0.8690649	-0.3920253
C	2.6566935	-1.9850665	0.2970069
C	3.4864106	-2.9577295	0.8587079
C	4.8981740	-2.8554806	0.7597357
C	5.4493021	-1.7416511	0.0731794
C	4.6166577	-0.7740766	-0.4883854
C	-0.8465547	3.1806234	-0.3745491
C	0.4212531	3.2712799	0.2577805
C	0.8679082	4.4749655	0.8066018
C	0.0641998	5.6429891	0.7503390

C	-1.2060180	5.5601633	0.1215824
C	-1.6472314	4.3561016	-0.4269225
C	-2.3562364	-2.3327570	-0.3480190
C	-3.0509962	-1.2816646	0.3057556
C	-4.3254510	-1.4832290	0.8389220
C	-4.9612498	-2.7482214	0.7460400
C	-4.2727257	-3.8051972	0.0949227
C	-3.0009046	-3.5982256	-0.4388294
H	1.5633630	-2.0948135	0.3732774
H	3.0413786	-3.8162709	1.3837247
H	6.5420836	-1.6470009	-0.0146648
H	5.0545693	0.0851680	-1.0190914
H	1.0708203	2.3826537	0.2983654
H	1.8565689	4.5209669	1.2872999
H	-1.8426504	6.4561156	0.0690214
H	-2.6337899	4.3035133	-0.9121788
H	-2.5853799	-0.2858658	0.3751442
H	-4.8455957	-0.6508345	1.3363175
H	-4.7517197	-4.7925024	0.0119535
H	-2.4770331	-4.4248097	-0.9429904
C	-6.2671367	-2.9557922	1.2945241
C	5.7511662	-3.8509040	1.3352200
C	0.5226362	6.8783986	1.3099739
N	0.8976874	7.8959123	1.7676140
N	-7.3405188	-3.1289043	1.7453625
N	6.4571399	-4.6664045	1.8063720

### 3e

C	-0.6083667	-1.2156164	0.0000001
C	0.7813493	-1.2200459	-0.0000001
C	1.5254375	0.0000001	-0.0000001
C	0.7813494	1.2200460	-0.0000002
C	-0.6083667	1.2156164	0.0000003
C	-1.3860128	0.0000000	0.0000001
H	-1.1648053	-2.1667609	0.0000002
H	1.3293380	-2.1769389	0.0000001
H	1.3293371	2.1769395	-0.0000005
H	-1.1648053	2.1667609	0.0000002
S	-3.1010525	-0.0000000	-0.0000001
C	2.9482497	0.0000000	-0.0000000
N	4.1307732	-0.0000001	0.0000000

### 1f

C	-3.0496132	-1.3399667	-3.3549141
C	-2.3665758	-0.6503682	-2.3124930
C	-2.6950539	0.7208090	-2.1168549
C	-3.6503527	1.3687845	-2.9201453
C	-4.3303279	0.6738443	-3.9703145
C	-4.0038582	-0.7052623	-4.1662339
S	-1.2112376	-1.5379739	-1.3529318
Zn	0.0027931	0.0000456	0.0000389
S	1.2162890	1.3523935	-1.5386511
C	2.3684136	2.3161209	-0.6514875
C	2.6973266	2.1224415	0.7198659
C	3.6500158	2.9291836	1.3674137
C	4.3268393	3.9809699	0.6718402
C	3.9998543	4.1750201	-0.7074098
C	3.0482181	3.3602661	-1.3416509
C	5.2940269	4.8044481	1.3214167
N	6.0939198	5.4873970	1.8488216

C	-5.3001291	1.3240139	-4.7902769
N	-6.1021419	1.8520669	-5.4702258
S	-1.2111981	1.5380752	1.3530278
C	-2.3665942	0.6504743	2.3125241
C	-2.6951034	-0.7206870	2.1168308
C	-3.6504603	-1.3686600	2.9200565
C	-4.3304641	-0.6737347	3.9702088
C	-4.0039729	0.7053614	4.1662591
C	-3.0496484	1.3400650	3.3549270
C	-5.3003348	-1.3238925	4.7900974
N	-6.1024057	-1.8519453	5.4699811
S	1.2162676	-1.3523466	1.5387084
C	2.3682848	-2.3161705	0.6515110
C	2.6971253	-2.1225586	-0.7198674
C	3.6497245	-2.9293844	-1.3674469
C	4.3265225	-3.9811880	-0.6718795
C	3.9996200	-4.1752012	0.7073998
C	3.0480637	-3.3603270	1.3416723
C	5.2936135	-4.8047571	-1.3214867
N	6.0934256	-5.4877811	-1.8489156
H	-2.2063864	-1.2849382	1.3079076
C	-3.9525956	-2.7530255	2.6748512
C	-4.6510647	1.4618474	5.2032566
H	-2.8181756	2.4004112	3.5293020
H	2.2108080	-1.3125518	-1.2846032
C	3.9522533	-2.6863949	-2.7521549
C	4.6433506	-5.2138529	1.4644741
H	2.8160969	-3.5331827	2.4021638
H	2.2109924	1.3124447	1.2846015
C	3.9526167	2.6861252	2.7520946
C	4.6436092	5.2136953	-1.4644880
H	2.8161903	3.5331722	-2.4021226
H	-2.2063539	1.2850682	-1.3079256
C	-3.9524525	2.7531707	-2.6750099
C	-4.6509319	-1.4617668	-5.2033122
H	-2.8181568	-2.4003317	-3.5292279
N	5.1524978	6.0532846	-2.1090456
N	4.1961925	2.4796866	3.8819165
N	5.1522310	-6.0534517	2.1090320
N	4.1957712	-2.4800135	-3.8820000
N	-5.1624850	-2.1058147	-6.0416709
N	-4.1956367	3.8827407	-2.4668063
N	-4.1958140	-3.8825758	2.4665826
N	-5.1626471	2.1058823	6.0416170

#### TS1-2f

C	-1.6117286	1.4328631	3.7979759
C	-1.7119493	0.9672025	2.4668961
C	-2.3185570	-0.2913940	2.2290287
C	-2.7867450	-1.0734040	3.3063608
C	-2.6744769	-0.6101621	4.6543950
C	-2.0814499	0.6667561	4.8829182
S	-1.1676845	2.0323401	1.1508170
Zn	0.6932541	1.0011193	0.3727195
S	1.6763028	-0.7294277	1.5431089
C	2.5306411	-1.7590975	0.4041031
C	3.2001102	-2.8976166	0.9266302
C	3.8986310	-3.7888085	0.0944179
C	3.9589415	-3.5736824	-1.3172206
C	3.2924751	-2.4248637	-1.8419036

C	2.5947224	-1.5425046	-0.9958262
C	4.6629998	-4.4770650	-2.1709032
N	5.2431715	-5.2230187	-2.8701869
C	-3.1462419	-1.3962821	5.7528457
N	-3.5298456	-2.0300970	6.6652129
S	1.5804169	2.0970421	-1.4820255
C	3.3070136	2.2970273	-1.2503808
C	4.0589501	1.7618359	-0.1708952
C	5.4455473	1.9815661	-0.0630804
C	6.1482842	2.7555686	-1.0368928
C	5.3918167	3.2941912	-2.1242791
C	4.0097270	3.0637402	-2.2208279
C	7.5533371	2.9878328	-0.9309316
N	8.7096984	3.1848271	-0.8486814
S	-3.5176280	-1.7565630	-0.9062334
C	-4.8843036	-0.9824260	-1.5904787
C	-5.0339869	0.4451814	-1.6541692
C	-6.1404712	1.0620477	-2.2566431
C	-7.2026411	0.2913415	-2.8415499
C	-7.0751997	-1.1378047	-2.7696150
C	-5.9619314	-1.7394498	-2.1665694
C	-8.3214902	0.9099545	-3.4644379
N	-9.2488482	1.4203379	-3.9840635
H	-2.4749463	-0.6542904	1.1918703
C	-3.3944932	-2.3551965	3.0680509
C	-1.9514636	1.1873673	6.2152227
H	-1.1510434	2.4122528	3.9895433
H	2.1012592	-0.6635799	-1.4390907
C	3.3336377	-2.1549885	-3.2532128
C	4.5556405	-4.9233871	0.6833479
H	3.1708163	-3.0879874	2.0088865
H	3.5558057	1.1569706	0.6002154
C	6.1609607	1.4181373	1.0494924
C	6.0387215	4.0891510	-3.1321922
H	3.4546088	3.4902954	-3.0683796
H	-4.2393058	1.0695245	-1.2206761
C	-6.2013874	2.4982658	-2.2907510
C	-8.1012806	-1.9804811	-3.3214963
H	-5.8973052	-2.8363502	-2.1277918
N	-8.9214382	-2.6978294	-3.7620679
N	-6.2284350	3.6729255	-2.3071953
N	-3.8855222	-3.4108875	2.9213511
N	-1.8287967	1.6461415	7.2894243
N	5.0838667	-5.8397540	1.1927465
N	3.3629569	-1.9156927	-4.4019282
N	6.7323561	0.9543559	1.9640567
N	6.5390519	4.7472081	-3.9659162

## 2f

C	-2.9983455	-3.5882399	-0.4279401
C	-2.3578109	-2.3251863	-0.3360601
C	-3.0551121	-1.2765352	0.3115164
C	-4.3414008	-1.4759824	0.8481714
C	-4.9866073	-2.7461856	0.7571560
C	-4.2826752	-3.8026903	0.1022611
S	-0.7401446	-2.1964430	-1.0201984
Zn	-0.0027517	-0.0201899	-0.9259790
S	-1.5156376	1.7088122	-1.0798212
C	-0.8411121	3.1723917	-0.3684121
C	0.4254196	3.2629228	0.2586869

C	0.8830804	4.4737678	0.8121743
C	0.0814163	5.6537232	0.7591495
C	-1.1970762	5.5615081	0.1283884
C	-1.6401092	4.3446066	-0.4194111
C	0.5407248	6.8868868	1.3160104
N	0.9164355	7.9033027	1.7708457
C	-6.2911869	-2.9548990	1.3017059
N	-7.3638477	-3.1266354	1.7501611
S	2.2491987	0.4220790	-1.1056672
C	3.1925894	-0.8749545	-0.3795108
C	2.6540725	-1.9930932	0.3022069
C	3.4886516	-2.9765051	0.8671726
C	4.9093695	-2.8779924	0.7703604
C	5.4516583	-1.7505293	0.0808143
C	4.6052151	-0.7762937	-0.4769545
C	5.7629044	-3.8709312	1.3423125
N	6.4682285	-4.6857846	1.8110323
H	1.5633853	-2.1138280	0.3851828
C	2.8883693	-4.0900103	1.5492253
C	6.8743110	-1.5988030	-0.0549775
H	5.0502932	0.0825163	-0.9995408
H	1.0809870	2.3800330	0.3045070
C	2.1767019	4.5113128	1.4374898
C	-2.0476088	6.7166789	0.0432259
H	-2.6298442	4.3030700	-0.8959078
H	-2.6007216	-0.2768004	0.3874274
C	-5.0035526	-0.3771182	1.4961078
C	-4.8805138	-5.1030964	-0.0277110
H	-2.4795502	-4.4208620	-0.9245219
N	8.0310271	-1.4483090	-0.1860784
N	2.3726760	-4.9876745	2.1021366
N	-5.3439483	-6.1741987	-0.1537225
N	-5.5255506	0.5334308	2.0214329
N	-2.7650709	7.6414958	-0.0448543
N	3.2343573	4.5211325	1.9461365

### 3f

C	1.6425276	-1.2295809	0.0000000
C	0.2409867	-1.2152775	0.0000000
C	-0.5292917	0.0012106	0.0000000
C	0.2502150	1.2111109	0.0000000
C	1.6512867	1.2145320	0.0000000
C	2.4042468	-0.0100732	0.0000000
S	-2.2352944	0.0108821	0.0000000
H	-0.3087336	-2.1677159	0.0000000
H	-0.2898084	2.1690473	0.0000000
C	2.3309442	2.4814417	0.0000000
C	3.8249580	-0.0154357	0.0000000
C	2.3196211	-2.4982448	0.0000000
N	2.8452698	3.5382727	0.0000000
N	5.0044232	-0.0202319	0.0000000
N	2.8436789	-3.5503510	0.0000000