Electronic Supplementary Information

On the dual reactivity of a Janus-type mesoionic dipole: experiments and theoretical validation

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CONTENTS:

Full experimental details.

General

Solvents and reagents were purchased from commercial suppliers and used without further purification. The identity of all compounds was confirmed by their elemental analyses, melting points, NMR and crystallographic data. The cycloaddition reactions were conducted in a professional microwave oven (Milestone Ethos Touch Control MW reactor) using a non-sealed flask. All NMR data were recorded in $CDCl_3$ solutions (500 MHz for ^1H and 125 MHz for ^{13}C). FT-IR spectra were registered in the 4000-6000 cm^{-1} range in KBr disks. Elemental microanalyses were performed by SAIUEx at the University of Extremadura.

Synthetic procedures.

5-Isobutyl-3-phenyl-2-thioxoimidazolidin-4-one (2). Compound **2** was synthetized following previous procedures (80% yield)[7a] and showed spectroscopic properties identical to those of an authentical sample.[7b]

5-Isobutyl-6-oxo-2,7-diphenyl-6,7-dihydro-5*H*-imidazo[2,1-*b*]thiazol-4-ium-3-olate (3). To a stirred solution of **2** (10 mmol) and 2-bromo-2-phenylacetic acid (10 mmol) in benzene or toluene (60 mL) was added dropwise triethylamine (10 mmol). The mixture was heated at reflux for 15 h. The solution was cooled at room temperature and the resulting crystals of triethylammonium bromide were filtered off. The solution was washed with water (5 x 30 mL) and brine (1 x 30 mL). The organic layer was dried over $MgSO_4$, filtered and evaporated to dryness to give a light orange foam, which was dried under vacuum. To this residue acetic anhydride (7 mL) was added dropwise under stirring followed by triethylamine (21 mL), and the resulting solution was kept at room temperature for 5-10 minutes. Then cold diethyl ether was added, which gave rise to the spontaneous crystallization of the mesoionic heterocycle (**3**) that was collected by filtration and washed with diethyl ether (40% yield). Mp 196-198 ºC. IR (KBr) ν_{max} 3499, 3055, 3019, 2963, 2952, 2867, 1755, 1624, 1586, 1497, 1425, 1330, 1129, 749, 690 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$) δ 7.70- 6.99 (m, 10H), 5.03 (t, *J* = 8.0 Hz, 1H), 2.33 (t, *J* = 6.8 Hz, 2H), 2.20-2.10 (m, 1H), 1.01 (d, *J* = 8.0 Hz, 6H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.4, 154.2, 153.6, 134.0, 130.9, 130.3, 129.7, 128.6, 123.7, 123.6, 122.3, 99.9, 87.4, 61.7, 37.7, 24.5, 22.7, 22.2 ppm. Anal. Calcd for $C_{21}H_{20}N_2O_2S$: C, 69.20, H, 5.53; N, 7.69; S, 8.80. Found: C, 69.17, H, 5.51; N, 7.68; S, 8.87.

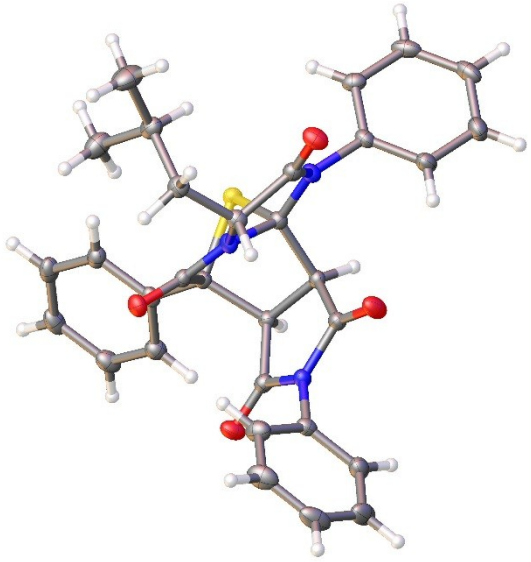
General procedure for the synthesis of compounds 7 and 8. A suspension of the mesoionic heterocycle **3** (1.0 mmol) and the dipolarophile (**5** or **6**) (1.25 mmol) in toluene (5 mL) was heated in a MW oven (300 W) for 8 min until reaching a plateau of 100 ºC and then it was kept at that temperature for 12 min (three cycles). The solvent was removed under reduced pressure and the residue was treated with diethyl ether, which afforded crystals of the resulting product (either **7** or **8**).

3-Isobutyl-1,6,8-triphenyldihydro-6,9b-epithioimidazo[1,2-*a*]pyrrolo[3,4-*c*]pyridine-2,5,7,9(1*H*,3*H*,8*H*,9*aH*)-tetraone (7). Recrystallized from ethanol (45 % yield) had mp 261-263 ºC. IR (KBr) ν_{max} 3473, 3093, 3065, 3036, 2956, 2935, 2913, 2869, 2360, 1749, 1717, 1597, 1499, 1387, 1361, 1200, 1153, 753, 695 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$) δ 7.80-7.16 (m, 15H), 4.36 (d, *J* = 8.5 Hz, 1H), 4.24 (m, 1H), 4.22 (d, *J* = 8.5 Hz, 1H), 2.19-2.10 (m, 3H), 0.99 (t, 6H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.3, 170.2, 170.0, 168.1, 132.8, 130.9, 130.0, 129.4, 129.3, 129. 2, 128.5, 127.1, 126.3, 92.1, 71.3, 57.1, 56.0, 52.1, 37.3, 24.5, 23.5, 21.9 ppm. Anal. Calcd for $C_{31}H_{27}N_3O_4S$: C, 69.25, H, 5.06; N, 7.82; S, 5.96. Found: C, 69.19, H, 5.02; N, 7.80; S, 6.07.

Methyl 4*a*-isobutyl-3,5,7-trioxo-2,6-diphenyl-3,4*a*,5,6,7,7*a*-hexahydro-2*H*-pyrrolo[3',4':4,5]pyrrolo[2,1-*b*]thiazole-8-carboxylate (8). Recrystallized from dichloromethane/ethanol (24 % yield) had mp 212-214 ºC. IR (KBr) ν_{max} 3485, 3430, 3076, 3028, 2958, 2871, 2365, 2198, 2100, 1955, 1883, 1726, 1683, 1591, 1500, 1242, 746, 698 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50-7.26 (m, 10H), 5.39 (s, 1H), 4.56 (s, 1H), 3.86 (s, 3H), 2.56 (dd, J = 11.6 Hz, J = 4.8 Hz, 1H), 2.26 (dd, J = 11.6 Hz, J = 6.4 Hz, 1H), 1.82 (m, 1H), 1.02 (d, J = 5.2 Hz, 3H), 0.97 (d, J = 5.2 Hz, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) 171.9, 171.4, 167.3, 164.2, 156.7, 134.4, 131.2, 129.2, 129.2, 129.0, 128.4, 126.2, 97.4, 71.4, 57.6, 55.6, 51.9, 38.5, 24.9, 23.6, 23.1. Anal. Calcd for $C_{26}H_{24}N_2O_5S$: C, 65.53, H, 5.08; N, 5.88; S, 6.73. Found: C, 65.48, H, 5.07; N, 5.85; S, 6.85.

Crystal Data for Compounds 7 and 8.

Compound 7:

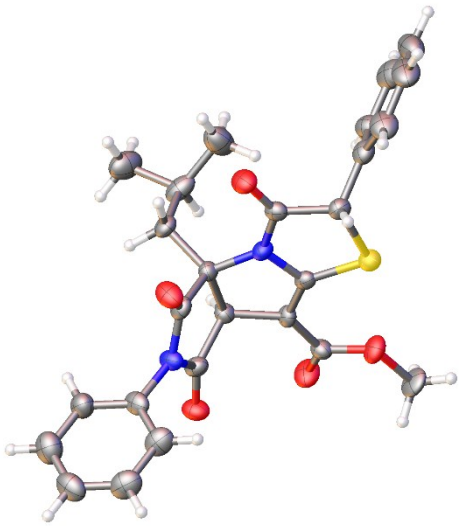


Experimental. Single clear colorless block-shaped crystals of **7** were obtained by recrystallization from ethanol. A suitable crystal (0.15×0.13×0.10) was selected and mounted on a MITIGEN holder in perfluoroether oil on a Rigaku AFC12 FRE-HF diffractometer. The crystal was kept at T = 100(2) K during data collection. Using **Olex2** (Dolomanov et al., 2009), the structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program, using the Direct Methods solution method. The model was refined with version of **ShelXL** (Sheldrick, 2008) using Least Squares minimization.

Crystal Data. $C_{31}H_{27}N_3O_4S$, M_r = 537.61, orthorhombic, $Pna2_1$ (No. 33), a = 11.8735(3) Å, b = 18.6709(4) Å, c = 11.8780(3) Å, $a = b = g = 90^{\circ}$, V = 2633.21(10) Å^3, T = 100(2) K, Z = 4, Z' = 1, m(MoK_a) = 0.166, 27414 reflections measured, 6753 unique (R_{int} = 0.0263) which were used in all calculations. The final wR_2 was 0.0723 (all data) and R_1 was 0.0295 (I > 2(I)).

Compound	**7**
Formula	$C_{31}H_{27}N_3O_4S$
$D_{calc.}$/ g cm^{-3}	1.356
m/mm^{-1}	0.166
Formula Weight	537.61
Colour	clear colorless
Shape	block
Max Size/mm	0.15
Mid Size/mm	0.13
Min Size/mm	0.10
T/K	100(2)
Crystal System	orthorhombic
Flack Parameter	0.02(2)
Hooft Parameter	0.005(15)
Space Group	$Pna2_1$
a/Å	11.8735(3)
b/Å	18.6709(4)
c/Å	11.8780(3)
a/°	90
b/°	90
g/°	90
V/Å^3	2633.21(10)
Z	4
Z'	1
Q_{min}/°	3.263
Q_{max}/°	28.698
Measured Refl.	27414
Independent Refl.	6753
Reflections Used	6471
R_{int}	0.0263
Parameters	354
Restraints	1
Largest Peak	0.240
Deepest Hole	-0.179
GooF	1.038
wR_2 (all data)	0.0723
wR_2	0.0712
R_1 (all data)	0.0315
R_1	0.0295

Compound 8:



Experimental. Single clear colorless prism-shaped crystals of **8** were recrystallized from dichloromethane/ethanol by slow evaporation. A suitable crystal (0.60×0.40×0.08) mm^3 was selected and mounted on a MITIGEN holder with silicon oil on a Rigaku R-AXIS Spider diffractometer. The crystal was kept at T = 120(2) K during data collection. Using **Olex2** (Dolomanov et al., 2009), the structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program, using the Intrinsic Phasing solution method. The model was refined with version 2018/3 of **ShelXL** (Sheldrick, 2015) using Least Squares minimization.

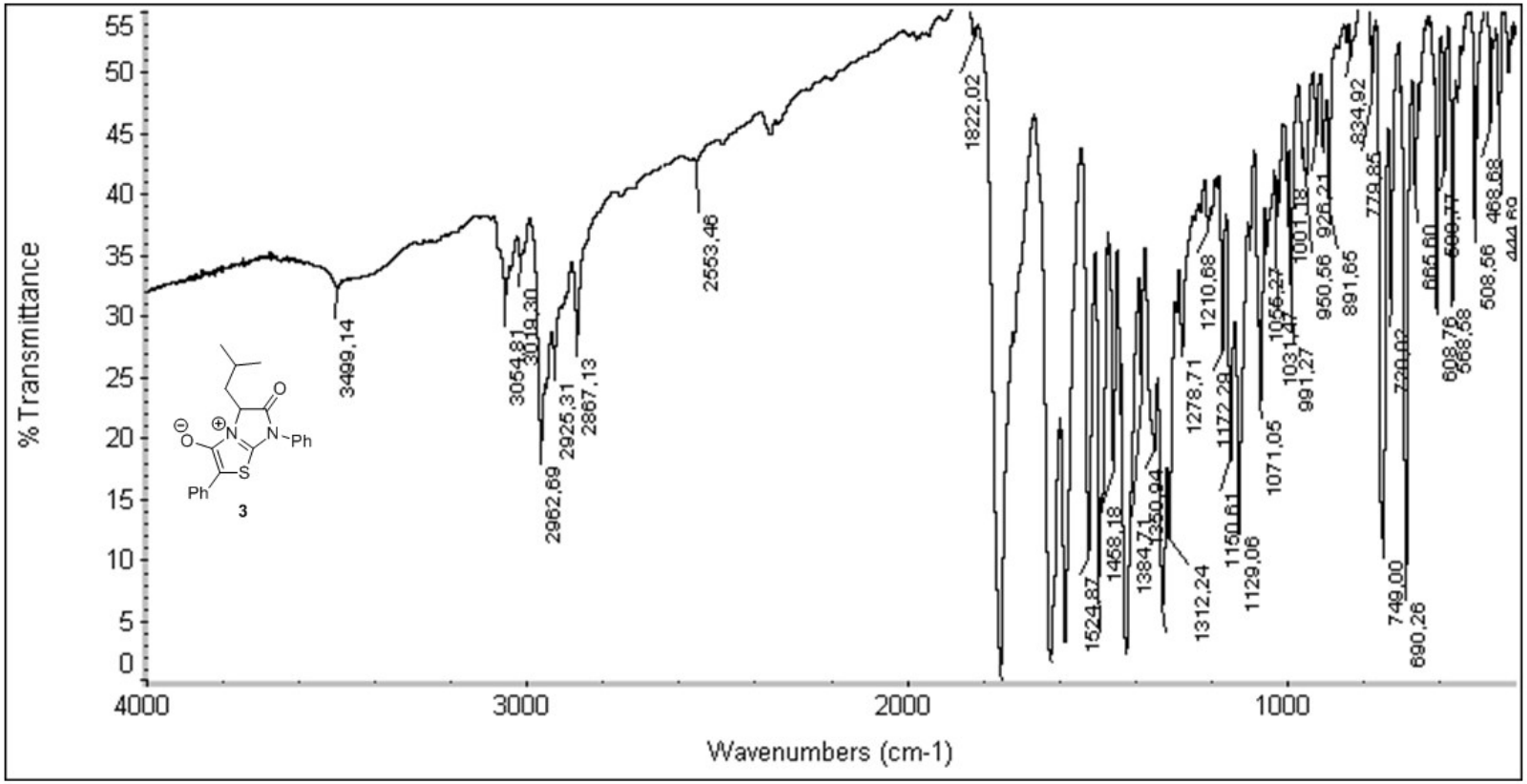
Crystal Data. $C_{26}H_{24}N_2O_5S$, M_r = 476.53, triclinic, P-1 (No. 2), a = 10.5259(11) Å, b = 10.5345(11) Å, c = 10.8340(11) Å, a = 91.068(6)°, b = 104.536(7)°, g = 100.359(7)°, V = 1141.4(2) $Å^3$, T = 120(2) K, Z = 2, Z' = 1, m(CuK_a) = 1.610, 12807 reflections measured, 3963 unique (R_{int} = 0.1150) which were used in all calculations. The final wR_2 was 0.2507 (all data) and R_1 was 0.0839 (I > 2(I)).

Compound	**8**
Formula	$C_{26}H_{24}N_2O_5S$
$D_{calc.}$/ g cm^{-3}	1.387
m/mm^{-1}	1.610
Formula Weight	476.53
Colour	clear colorless
Shape	prism
Size/mm^3	0.60×0.40×0.08
T/K	120(2)
Crystal System	triclinic
Space Group	P-1
a/Å	10.5259(11)
b/Å	10.5345(11)
c/Å	10.8340(11)
a/°	91.068(6)
b/°	104.536(7)
g/°	100.359(7)
V/Å^3	1141.4(2)
Z	2
Z'	1
Wavelength/Å	1.54187
Radiation type	CuK_a
Q_{min}/°	4.225
Q_{max}/°	66.500
Measured Refl.	12807
Independent Refl.	3963
Reflections Used	2625
R_{int}	0.1150
Parameters	311
Restraints	3
Largest Peak	0.660
Deepest Hole	-0.891
GooF	1.133
wR_2 (all data)	0.2507
wR_2	0.2221
R_1 (all data)	0.1098
R_1	0.0839

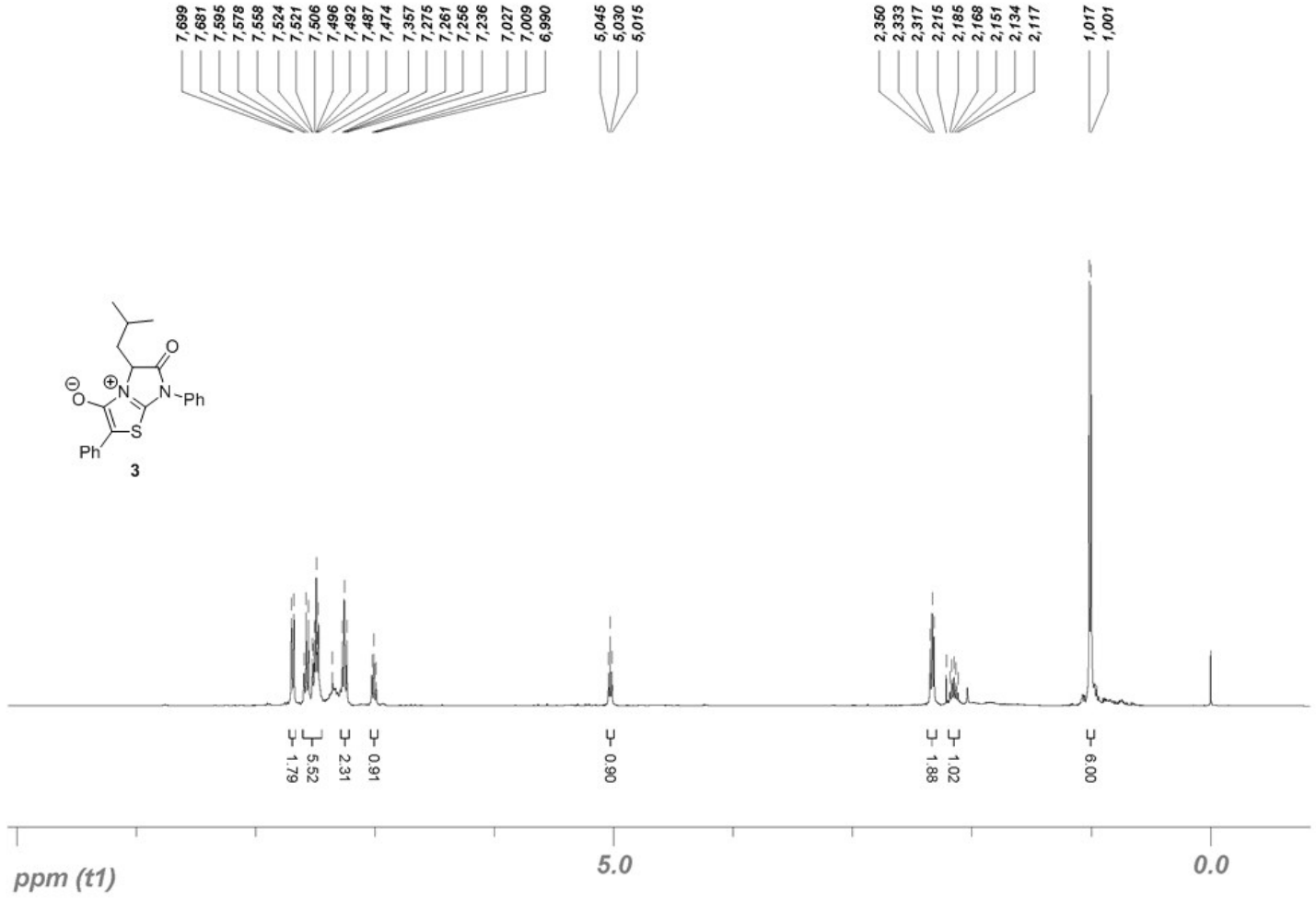
<u>Copies of IR, ^{1}H NMR, ^{13}C NMR and DEPT spectra for synthesized products.</u>

Compound 3:

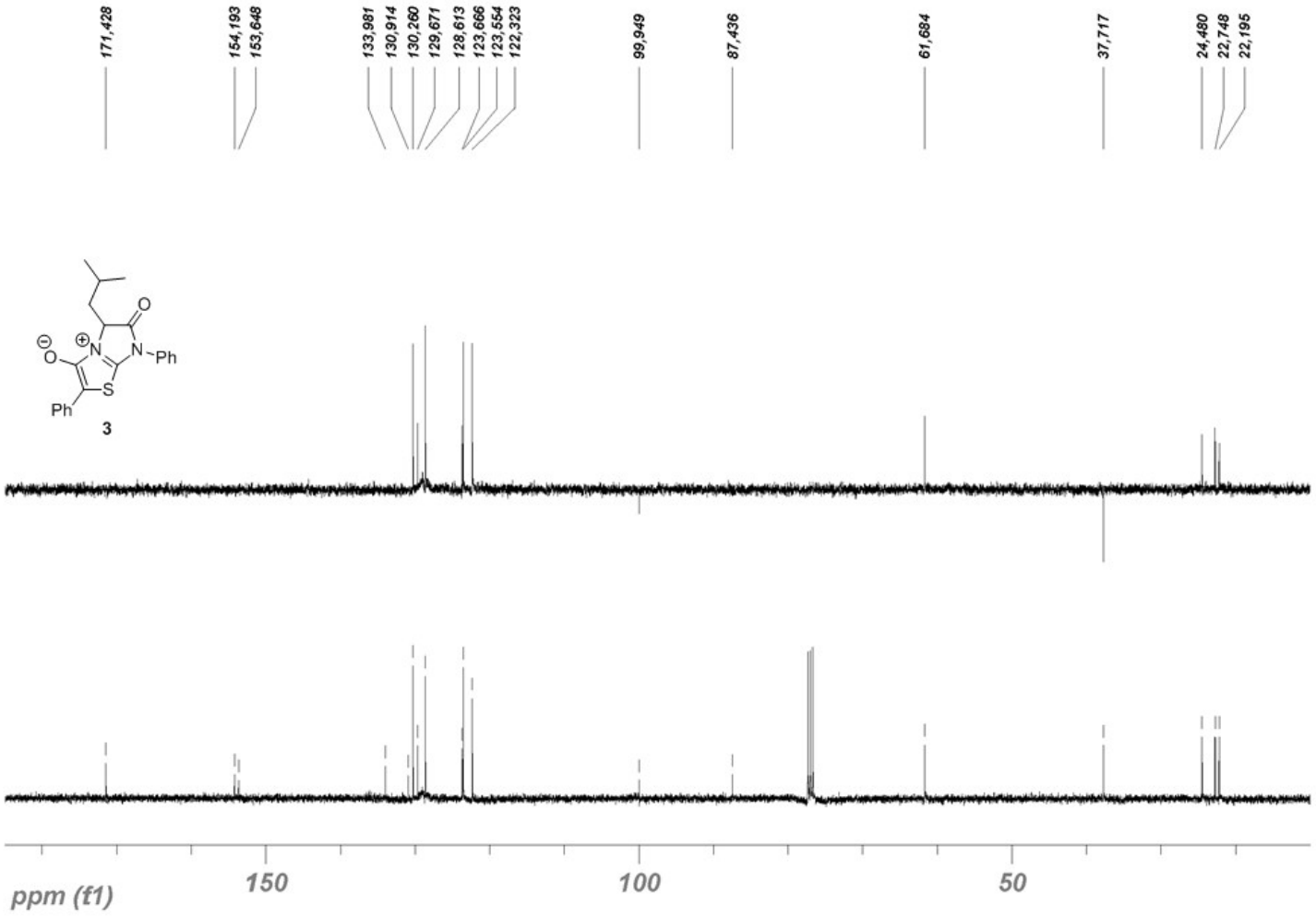
FT-IR spectrum



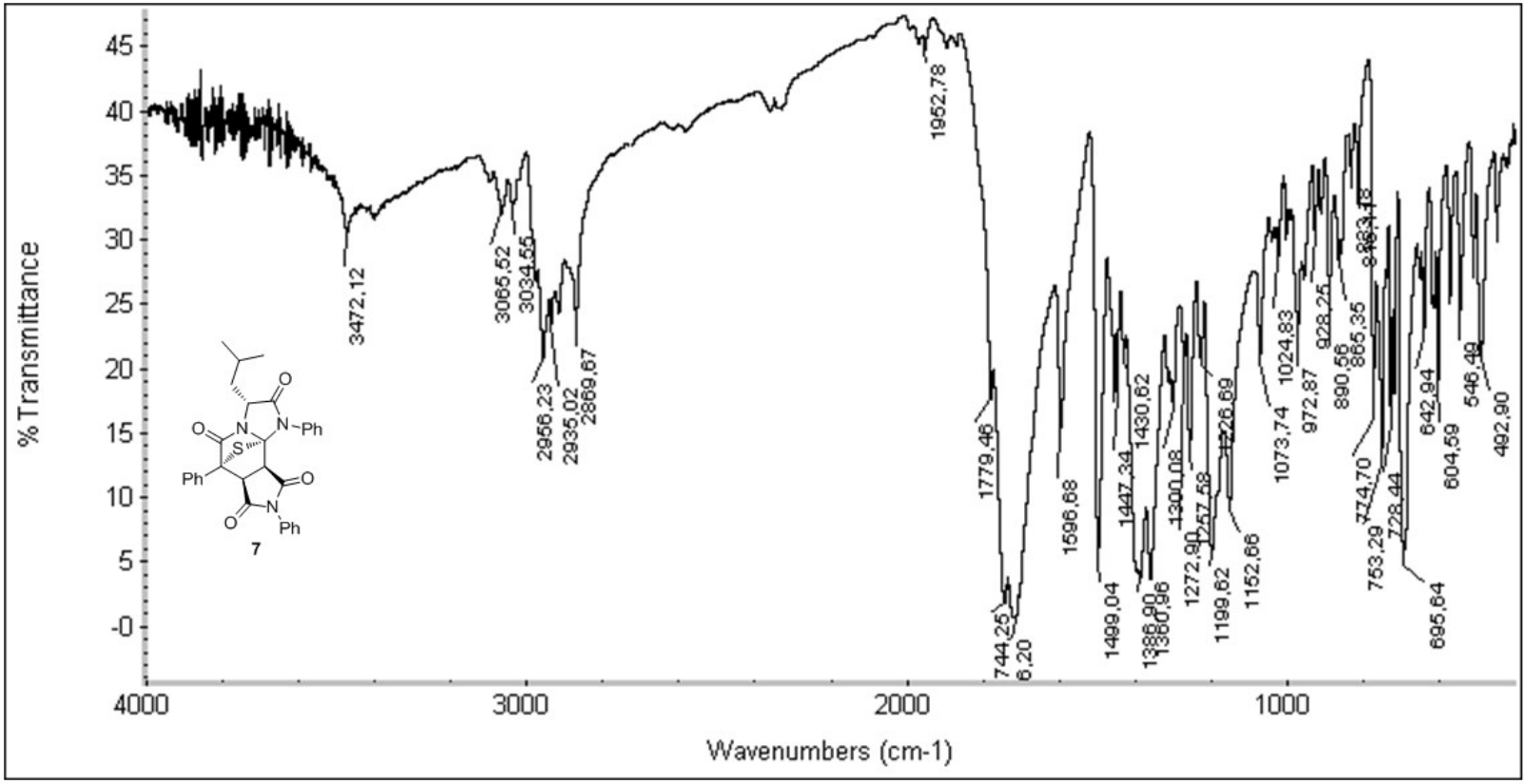
^{1}H NMR spectrum



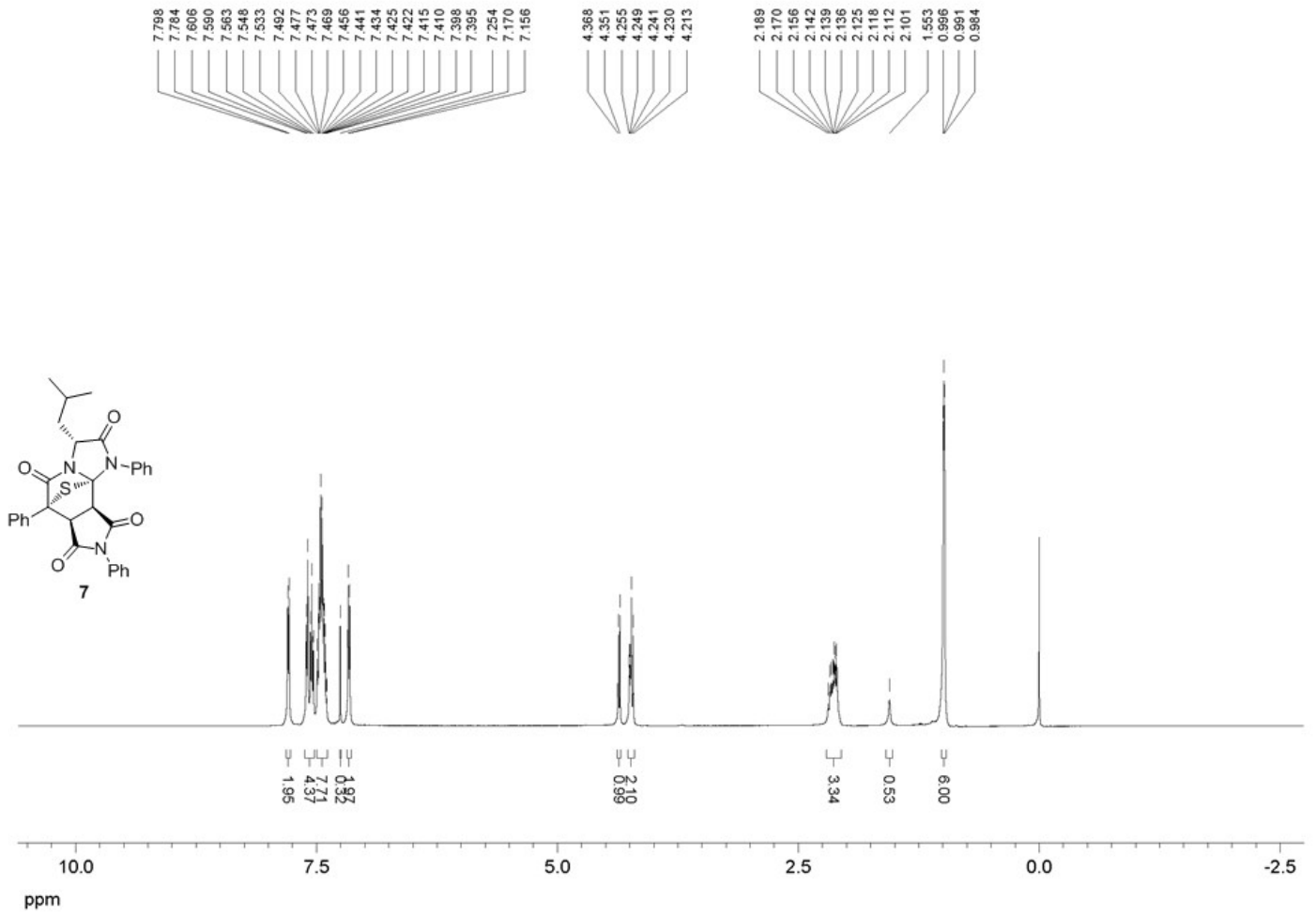
^{13}C NMR and DEPT spectra



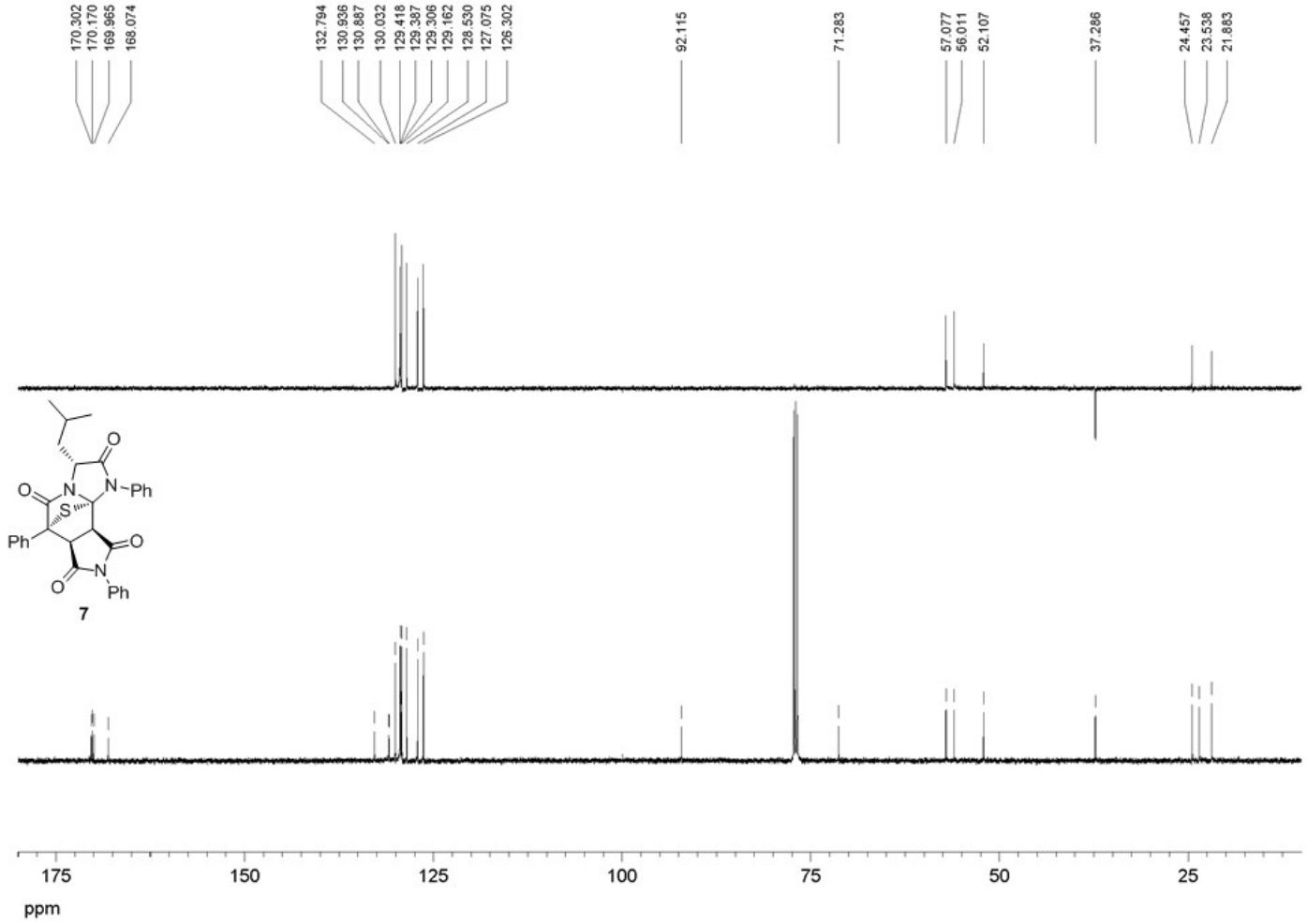
Compound 7:
FT-IR spectrum



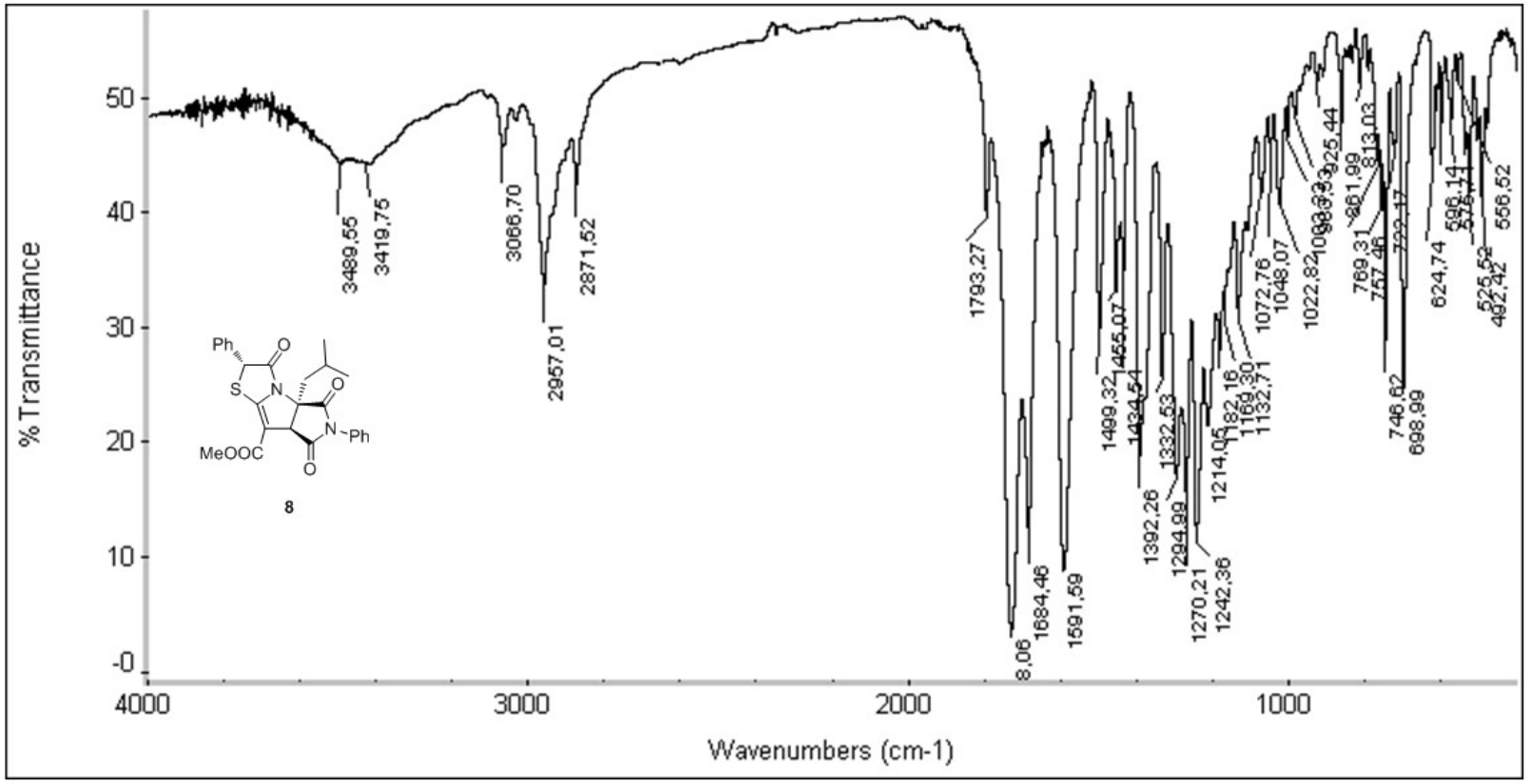
^{1}H NMR spectrum



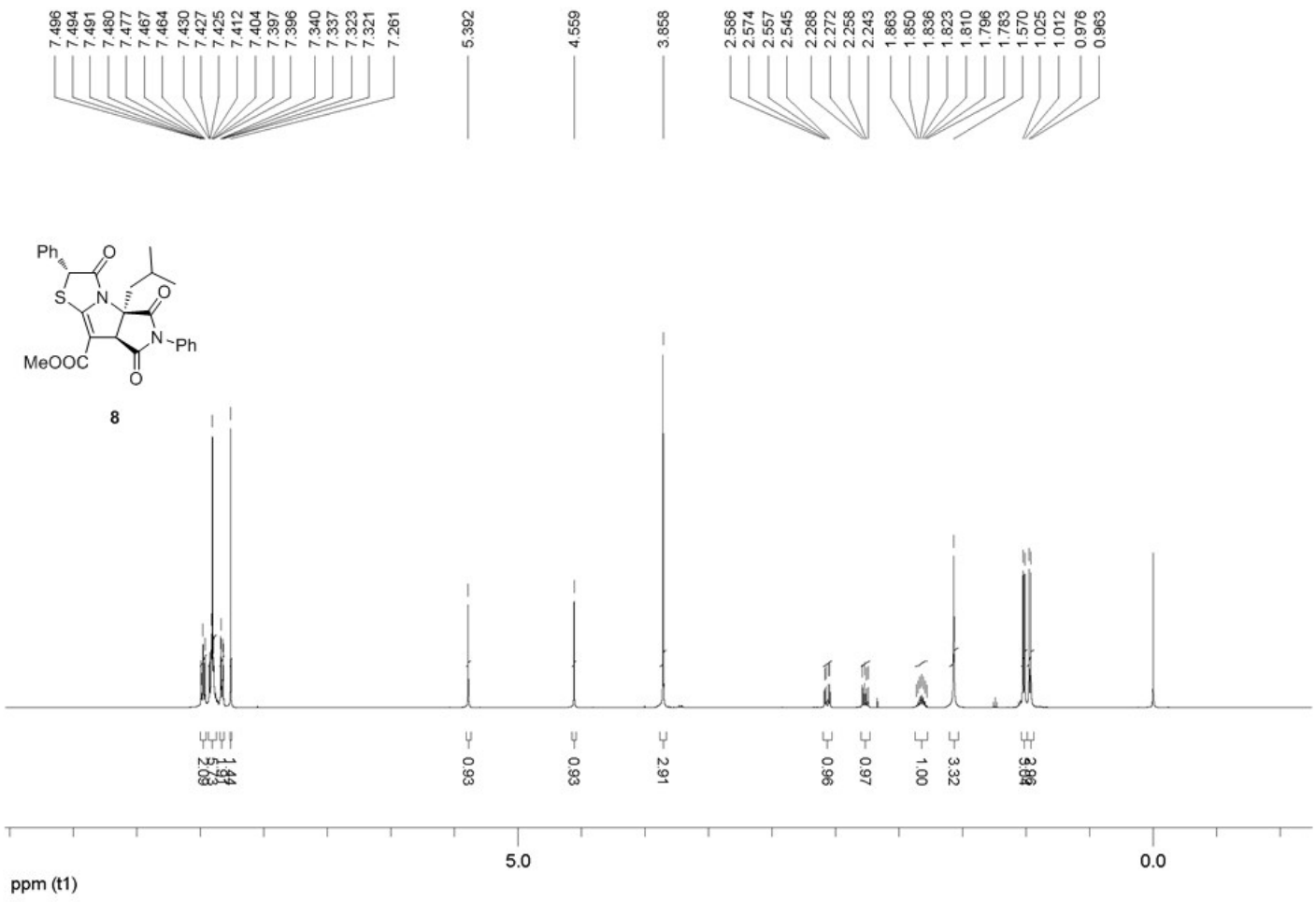
^{13}C NMR and DEPT spectra



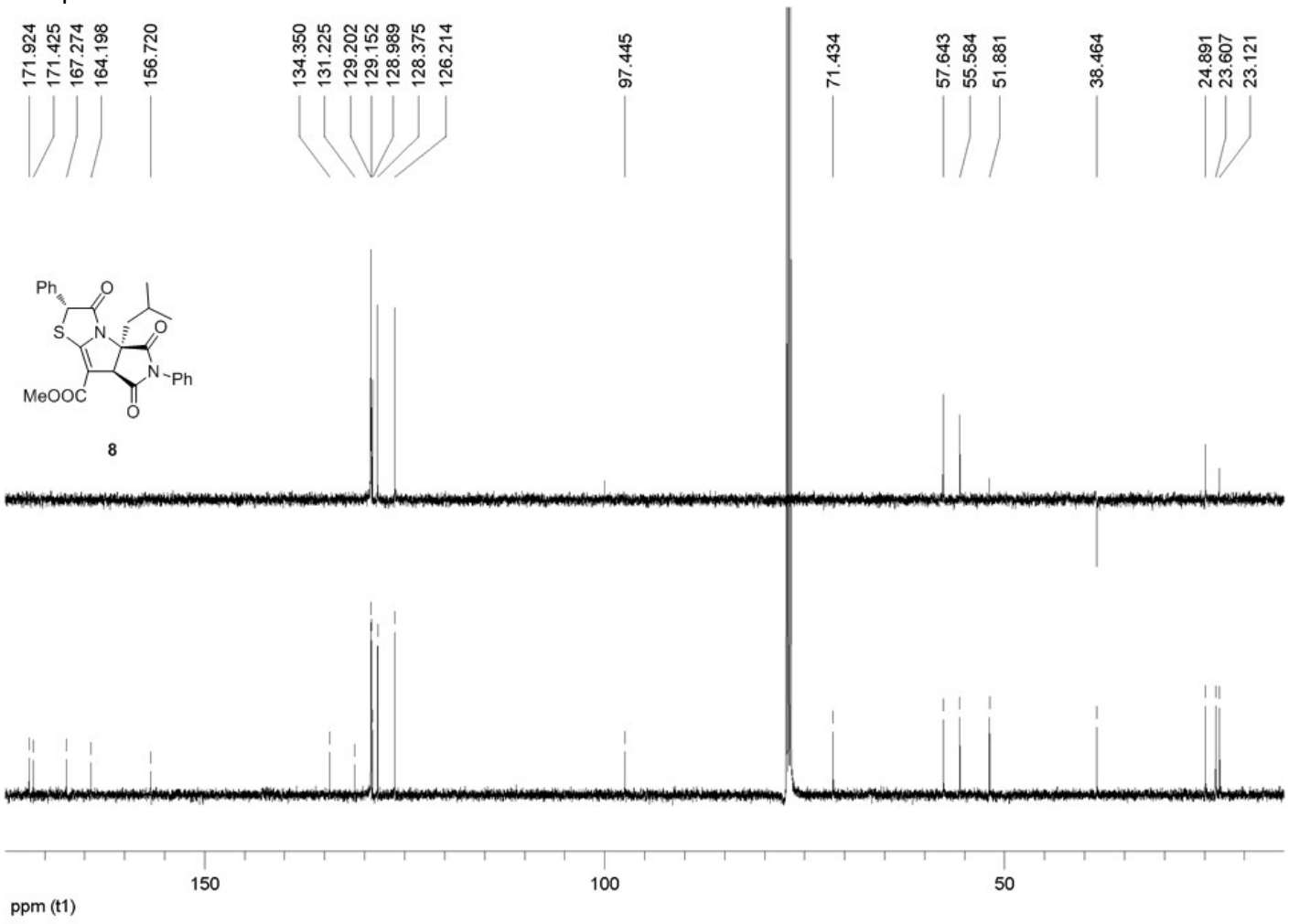
Compound 8:
FT-IR spectrum



^{1}H NMR spectrum



^{13}C NMR and DEPT spectra



Full computational details

All calculations reported in this work were carried out using the Gaussian09 package.[13] For all the geometry optimizations and frequency analysis the two-layer ONIOM[10] method was employed with the M06-2X[11] density functional method in conjunction with the 6-311++G(d,p) and 6-31G basis sets[12] for high- and for low-level, respectively. The geometries were optimized including solvation effects in toluene, which have been determined by the density-based self-consistent reaction field theory of bulk electrostatic, i.e., the well-known solvation model density (SMD)[14] method that takes into account different contributions such as long-range electrostatic polarization (bulk solvent effect). Frequency at 373.1 K on all the stationary points were carried out at the same level of theory as the geometry optimizations to ascertain the nature of the stationary points. Ground and transition states were characterized by none and one imaginary frequency, respectively. All of the relative energies shown are free energies calculated at 373.1 K with respect to the reagents. IRC calculations were carried out for the most asynchronous cycloadditions in order to ensure the saddle points were connected with the corresponding minimums and the saddle points involved in the formation of **8**. Topological analysis of the electron density for dipoles **3** and **4** was carried out with the AIM2000 software at M06-2X/6-311++G(d,p)//ONIOM(M06-2X/6-311++G(d,p):M06-2X/6-31g)-level of theory.

Figures S1 and S2: Topological analysis of ρ(r) for mesoionics 3 and 4.

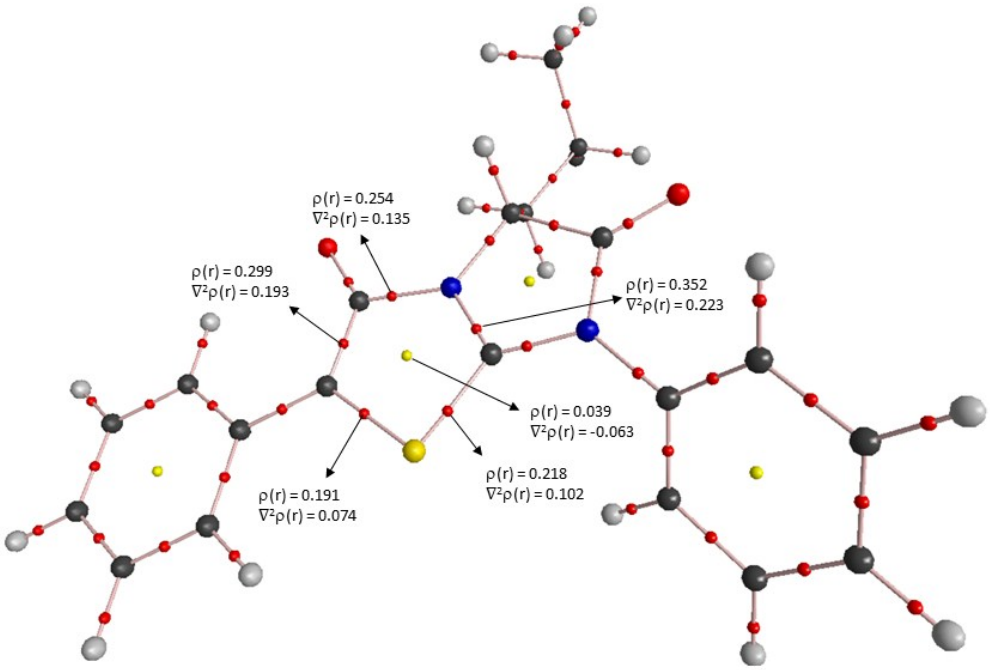


Figure S1. Topological analysis of the electron density of thiazolium-olate **3**.

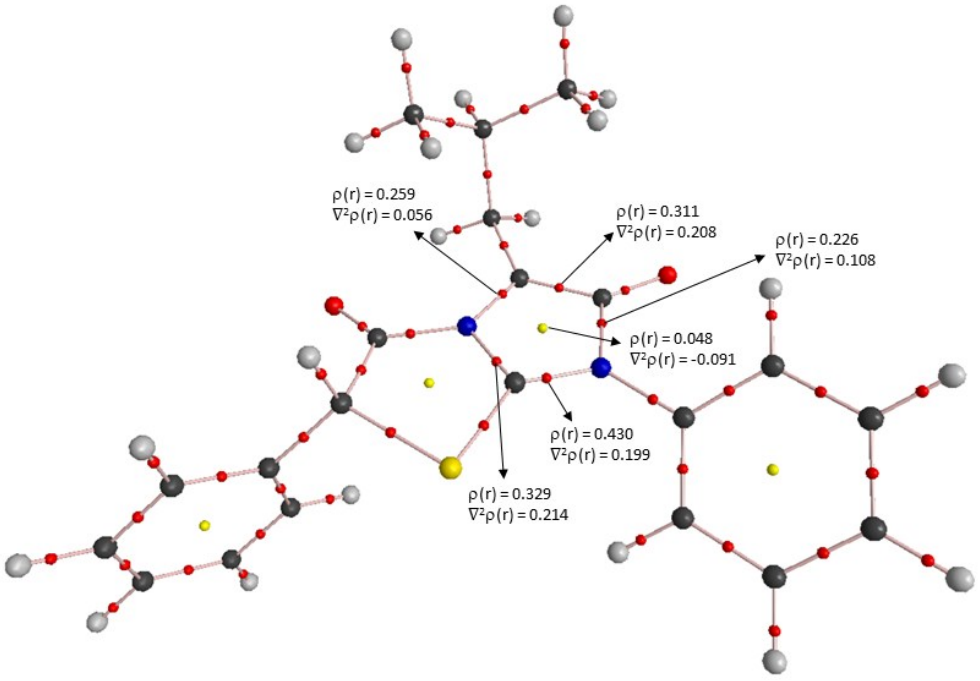


Figure S2. Topological analysis of the electron density of diazolium-olate **4**.

Cartesian coordinates for optimized structures.

Structures 3-23, $I1_8$, $I2_8$, $I3_8$ I_{11} and I_{15}.

Structure **3**:

Energy (Hartrees): -1470.015211

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.616123	0.457845	-0.000061
2	1	0	0.914037	1.502712	-0.000173
3	6	0	1.587389	-0.453420	0.000002
4	1	0	1.492817	-1.528425	0.000112
5	6	0	-0.820496	0.179982	0.000015
6	6	0	-1.703051	1.265551	-0.000032
7	6	0	-1.343030	-1.120609	0.000126
8	6	0	-3.077622	1.060336	0.000036
9	1	0	-1.304546	2.274352	-0.000123
10	6	0	-2.713809	-1.323566	0.000194
11	1	0	-0.677536	-1.975858	0.000157
12	6	0	-3.584582	-0.233981	0.000150
13	1	0	-3.750400	1.909509	-0.000001
14	1	0	-3.108093	-2.332683	0.000282
15	1	0	-4.655698	-0.398360	0.000202
16	7	0	2.980274	-0.033470	-0.000093
17	8	0	3.806454	-0.927525	-0.000074
18	8	0	3.251292	1.151302	-0.000223

Structure **4**:

Energy (Hartrees): -1470.005411

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.434969	-0.338029	-0.084676
2	6	0	1.401522	1.065713	0.004825
3	6	0	1.976160	-0.119961	-0.779874
4	16	0	0.715056	-1.473861	-0.721712
5	7	0	-1.712442	-0.403229	0.224651
6	6	0	-2.570158	-1.531902	0.072734
7	6	0	-2.117312	-2.809250	0.412362
8	6	0	-3.865509	-1.333522	-0.412092
9	6	0	-2.961971	-3.903777	0.232889
10	1	0	-1.129764	-2.947104	0.838990
11	6	0	-4.703360	-2.434805	-0.574112
12	1	0	-4.203646	-0.329811	-0.631390
13	6	0	-4.253905	-3.719299	-0.260981
14	1	0	-2.612986	-4.896055	0.492546
15	1	0	-5.709570	-2.287437	-0.947944
16	1	0	-4.910581	-4.571173	-0.393500
17	6	0	-0.985687	1.690758	0.767916
18	6	0	-2.146074	0.923672	0.784065
19	7	0	0.031230	0.890957	0.207524
20	8	0	2.030831	2.021048	0.354324
21	6	0	-0.851373	3.141788	1.092875
22	1	0	0.149449	3.351149	1.485248
23	6	0	-1.142652	4.103413	-0.087453
24	1	0	-0.996610	5.123005	0.297865
25	8	0	-3.309915	1.111577	1.121116
26	1	0	2.022189	0.210128	-1.821996
27	6	0	3.331702	-0.557973	-0.304520

28	6	0	3.559948	-0.815755	1.053122
29	6	0	4.370693	-0.720220	-1.224010
30	6	0	4.818139	-1.228666	1.482952
31	1	0	2.754477	-0.690500	1.771427
32	6	0	5.631043	-1.137493	-0.792818
33	1	0	4.194659	-0.515688	-2.275361
34	6	0	5.855074	-1.391981	0.559683
35	1	0	4.991680	-1.422272	2.534929
36	1	0	6.432620	-1.259532	-1.511687
37	1	0	6.833418	-1.714475	0.896594
38	1	0	-1.565458	3.358193	1.897093
39	6	0	-2.591064	3.969712	-0.566608
40	1	0	-3.298918	4.147248	0.248843
41	1	0	-2.778873	2.960444	-0.949480
42	1	0	-2.803150	4.683531	-1.370279
43	6	0	-0.162360	3.885706	-1.244523
44	1	0	-0.289979	2.880760	-1.669508
45	1	0	0.876127	3.990922	-0.914838
46	1	0	-0.342139	4.606583	-2.049445

Structure **5**:

Energy (Hartrees): -590.320261

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.989150	-0.646368	0.149650
2	6	0	2.989153	0.646456	-0.149130
3	6	0	1.569526	-1.117534	0.257044
4	6	0	1.569530	1.117349	-0.257747
5	8	0	1.183439	-2.224594	0.511861
6	8	0	1.183447	2.224563	-0.511899
7	6	0	-0.661697	-0.000023	-0.000083
8	6	0	-1.354785	1.038638	0.627636
9	6	0	-1.354961	-1.038639	-0.627682
10	6	0	-2.748585	1.038433	0.616204
11	1	0	-0.808153	1.838523	1.110767
12	6	0	-2.748759	-1.038340	-0.616008
13	1	0	-0.808466	-1.838556	-1.110914
14	6	0	-3.448868	0.000068	0.000160
15	1	0	-3.284971	1.847613	1.097753
16	1	0	-3.285281	-1.847484	-1.097466
17	1	0	-4.532635	0.000102	0.000256
18	7	0	0.763810	-0.000063	-0.000229
19	1	0	3.819760	1.319132	-0.306670
20	1	0	3.819751	-1.318880	0.307919

Structure **6**:

Energy (Hartrees): -534.296220

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.365961	-0.555205	0.000077
2	6	0	0.365961	0.555206	-0.000059
3	1	0	-0.086430	1.539727	-0.000087
4	1	0	0.086431	-1.539726	0.000101
5	6	0	1.853040	0.556223	-0.000193
6	6	0	-1.853040	-0.556223	0.000167
7	8	0	2.506795	1.567755	-0.000100
8	8	0	-2.506794	-1.567755	0.000162
9	8	0	2.380986	-0.669121	-0.000031

10	8	0	-2.380986	0.669121	0.000093
11	6	0	-3.811520	0.728439	-0.000085
12	1	0	-4.211668	0.242859	-0.890834
13	1	0	-4.211818	0.243814	0.891128
14	1	0	-4.062359	1.786326	-0.000631
15	6	0	3.811520	-0.728440	-0.000016
16	1	0	4.062359	-1.786327	-0.000081
17	1	0	4.211758	-0.243264	-0.890948
18	1	0	4.211727	-0.243410	0.891015

Structure **7**:

Energy (Hartrees): -2060.399981

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.587595	-0.859179	-1.657198
2	6	0	0.819746	-1.760768	-0.380656
3	6	0	-1.215739	-0.622941	-0.035999
4	6	0	-0.741491	-0.132250	-1.432153
5	6	0	0.955654	-0.759667	0.810670
6	16	0	-0.887937	-2.444392	-0.119856
7	6	0	1.906932	-2.792763	-0.518640
8	6	0	3.254943	-2.436372	-0.361986
9	6	0	1.589647	-4.115714	-0.854235
10	6	0	4.256268	-3.392453	-0.533081
11	1	0	3.520136	-1.421187	-0.104897
12	6	0	2.594005	-5.067292	-1.025737
13	1	0	0.554298	-4.412694	-0.987398
14	6	0	3.931768	-4.708075	-0.863720
15	1	0	5.293079	-3.103021	-0.407023
16	1	0	2.328267	-6.086397	-1.282229
17	1	0	4.713915	-5.447233	-0.993974
18	8	0	1.966632	-0.500626	1.420164
19	7	0	-0.258551	-0.166270	0.955030
20	6	0	-0.837391	0.744359	1.938109
21	7	0	-2.457992	-0.128929	0.437945
22	6	0	-2.304689	0.756902	1.492481
23	6	0	-3.665680	-0.255718	-0.323024
24	6	0	-4.199579	0.866500	-0.960360
25	6	0	-4.283529	-1.503229	-0.425259
26	6	0	-5.372106	0.732314	-1.702876
27	1	0	-3.691552	1.819831	-0.871385
28	6	0	-5.445287	-1.631088	-1.186290
29	1	0	-3.866954	-2.355546	0.100981
30	6	0	-5.991997	-0.513839	-1.820316
31	1	0	-5.798453	1.599937	-2.192394
32	1	0	-5.928453	-2.597161	-1.272074
33	1	0	-6.901474	-0.613016	-2.401669
34	8	0	-3.184039	1.394520	2.003389
35	1	0	-0.435571	1.756196	1.817049
36	6	0	-0.771178	0.288037	3.401724
37	1	0	-1.467882	0.941097	3.946968
38	1	0	-1.170681	-0.733101	3.459484
39	6	0	0.600671	0.355394	4.097737
40	1	0	1.255511	-0.408368	3.666333
41	6	0	1.271984	1.718262	3.906092
42	1	0	0.604971	2.531036	4.221436
43	1	0	2.184770	1.780232	4.507631
44	1	0	1.557018	1.885392	2.863166
45	6	0	0.407321	0.050982	5.588828
46	1	0	-0.083541	-0.916665	5.738757
47	1	0	1.370082	0.025467	6.108667
48	1	0	-0.212526	0.822358	6.062346
49	1	0	-1.503873	-0.310401	-2.189756
50	1	0	0.610162	-1.500276	-2.536933
51	6	0	-0.388513	1.340647	-1.345530
52	6	0	1.621965	0.249319	-1.792785
53	7	0	0.986654	1.469411	-1.517629
54	6	0	1.691020	2.708968	-1.384703

55	6	0	1.297926	3.818061	-2.133476
56	6	0	2.760584	2.783761	-0.490775
57	6	0	1.985966	5.020934	-1.978832
58	1	0	0.463204	3.738781	-2.819419
59	6	0	3.449518	3.987373	-0.353343
60	1	0	3.043231	1.909483	0.085491
61	6	0	3.062604	5.106017	-1.094407
62	1	0	1.683735	5.888413	-2.553407
63	1	0	4.282886	4.051091	0.336022
64	1	0	3.597041	6.042015	-0.981156
65	8	0	-1.148224	2.243788	-1.111910
66	8	0	2.783289	0.130522	-2.063133

Structure **8**:

Energy (Hartrees): -1888.650053

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.625097	-1.145572	-0.009623
2	6	0	0.494777	-0.495189	0.806498
3	6	0	-0.930830	1.126077	-0.152534
4	6	0	1.008738	0.933887	1.114319
5	6	0	-0.054015	1.856779	0.566157
6	7	0	-0.634911	-0.226996	-0.114652
7	6	0	-1.559991	-1.098071	-0.646150
8	16	0	-2.375438	1.471169	-1.054096
9	6	0	-2.634136	-0.322313	-1.426077
10	1	0	-2.408867	-0.470445	-2.485322
11	8	0	-1.542933	-2.293603	-0.533535
12	6	0	-4.026660	-0.805522	-1.120784
13	6	0	-4.502534	-0.813750	0.196576
14	6	0	-4.853422	-1.254164	-2.153030
15	6	0	-5.785948	-1.274015	0.476033
16	1	0	-3.864848	-0.459886	1.002364
17	6	0	-6.142497	-1.712168	-1.873984
18	1	0	-4.486894	-1.250779	-3.174469
19	6	0	-6.609785	-1.722822	-0.560579
20	1	0	-6.145075	-1.283186	1.498518
21	1	0	-6.776787	-2.059343	-2.681351
22	1	0	-7.609873	-2.079200	-0.342023
23	8	0	1.666966	-2.289478	-0.361842
24	6	0	3.786662	-0.446717	-1.010697
25	6	0	4.541260	-1.578697	-0.694636
26	6	0	4.191158	0.422492	-2.024936
27	6	0	5.708037	-1.844014	-1.408783
28	1	0	4.212629	-2.245325	0.093265
29	6	0	5.367150	0.154083	-2.724794
30	1	0	3.597764	1.298619	-2.254925
31	6	0	6.124134	-0.978969	-2.421991
32	1	0	6.292012	-2.724659	-1.169023
33	1	0	5.688003	0.829262	-3.509212
34	1	0	7.034401	-1.186512	-2.972413
35	7	0	2.587879	-0.177079	-0.275465
36	6	0	0.037408	-1.367043	1.981768
37	1	0	-0.939845	-0.987554	2.308095
38	6	0	0.974606	-1.425533	3.201999
39	1	0	1.025433	-0.425851	3.654853
40	1	0	1.219962	1.110250	2.171284
41	6	0	-0.140128	3.278281	0.866585
42	6	0	2.321985	1.053993	0.342270
43	8	0	3.019233	2.023097	0.257374
44	8	0	0.551071	3.858990	1.665589
45	8	0	-1.124183	3.868813	0.162961
46	6	0	-1.326866	5.259602	0.429228
47	1	0	-0.436024	5.830775	0.165787
48	1	0	-2.166793	5.559338	-0.193135
49	1	0	-1.561049	5.416663	1.482726
50	1	0	-0.119350	-2.379914	1.590978

51	6	0	0.364047	-2.379251	4.237805
52	1	0	-0.657092	-2.084323	4.500659
53	1	0	0.330324	-3.401160	3.842829
54	1	0	0.961249	-2.390419	5.154523
55	6	0	2.401166	-1.871467	2.853294
56	1	0	2.983222	-2.018392	3.768678
57	1	0	2.386887	-2.820272	2.304653
58	1	0	2.939135	-1.129933	2.251048

Structure **9**:

Energy (Hartrees): -2004.357690

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.961897	-0.596203	-0.697221
2	6	0	0.922048	-1.510543	-0.004962
3	6	0	0.069750	0.531298	-0.069233
4	6	0	0.987722	-1.037880	1.513143
5	6	0	0.453070	0.418312	1.457751
6	7	0	-0.292870	-0.812929	-0.397327
7	6	0	-1.542457	-1.124663	-0.814769
8	16	0	-1.319105	1.584836	-0.572253
9	6	0	-2.271095	0.150874	-1.258228
10	8	0	-2.010184	-2.235309	-0.911096
11	8	0	3.095217	-0.876610	-0.989186
12	6	0	2.041501	1.876085	-0.961186
13	6	0	1.649531	3.019988	-0.252350
14	6	0	3.119203	1.941909	-1.853979
15	6	0	2.336817	4.218830	-0.438603
16	1	0	0.820880	2.992292	0.447262
17	6	0	3.802352	3.144327	-2.021005
18	1	0	3.414153	1.059830	-2.404882
19	6	0	3.417109	4.286884	-1.317448
20	1	0	2.024767	5.097766	0.113242
21	1	0	4.635760	3.186969	-2.712699
22	1	0	3.949375	5.220343	-1.456301
23	7	0	1.350497	0.648705	-0.785397
24	6	0	0.993313	-3.012828	-0.217162
25	1	0	1.794117	-3.389038	0.430048
26	6	0	1.222536	-3.555794	-1.656966
27	1	0	0.687700	-4.514445	-1.688478
28	1	0	1.230698	1.141901	1.690784
29	1	0	0.310862	-1.693503	2.061602
30	6	0	-0.715876	0.739039	2.359391
31	6	0	2.382733	-1.232042	2.070077
32	8	0	3.124993	-0.130174	1.994319
33	8	0	2.782406	-2.289055	2.483120
34	8	0	-0.821219	1.784142	2.943280
35	8	0	-1.620503	-0.241238	2.416284
36	6	0	4.512070	-0.283059	2.325884
37	1	0	4.973380	-1.009494	1.656665
38	1	0	4.956445	0.698980	2.186608
39	1	0	4.618876	-0.610597	3.360052
40	6	0	-2.769472	0.032994	3.233343
41	1	0	-3.350669	0.845887	2.796653
42	1	0	-3.348517	-0.887369	3.252809
43	1	0	-2.455925	0.302783	4.241733
44	1	0	0.053249	-3.412346	0.177467
45	6	0	0.631462	-2.684639	-2.774439
46	1	0	-0.452879	-2.591138	-2.677870
47	1	0	1.074472	-1.681843	-2.795898
48	1	0	0.838904	-3.146388	-3.745569
49	6	0	2.703847	-3.858454	-1.931131
50	1	0	3.298823	-2.942409	-1.941440
51	1	0	3.115612	-4.522635	-1.163364
52	1	0	2.813956	-4.357687	-2.900025
53	1	0	-2.153392	0.185505	-2.345366
54	6	0	-3.728869	0.209838	-0.901127

55	6	0	-4.602785	0.939443	-1.714363
56	6	0	-4.224333	-0.422225	0.244615
57	6	0	-5.953126	1.046924	-1.382315
58	1	0	-4.223577	1.422972	-2.609802
59	6	0	-5.575401	-0.319692	0.573321
60	1	0	-3.554515	-1.011432	0.860955
61	6	0	-6.441775	0.418148	-0.236505
62	1	0	-6.620815	1.615905	-2.018911
63	1	0	-5.953815	-0.819777	1.458098
64	1	0	-7.491947	0.495907	0.020767

Structure **10**:

Energy (Hartrees): -2060.325214

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.357922	1.177261	-1.236071
2	6	0	-0.532449	1.630276	-0.025198
3	6	0	-0.759109	-0.718872	-0.212068
4	6	0	0.268081	-0.356055	-1.317513
5	6	0	-1.986028	1.262775	-0.441401
6	16	0	-0.196693	0.325473	1.238915
7	6	0	1.689657	-0.850901	-1.091999
8	6	0	1.830084	1.473299	-0.994132
9	6	0	-0.341340	3.052429	0.413026
10	6	0	-0.753513	4.086696	-0.438617
11	6	0	0.275555	3.371866	1.625433
12	6	0	-0.552861	5.416241	-0.075415
13	1	0	-1.242495	3.853152	-1.377050
14	6	0	0.477077	4.704057	1.986622
15	1	0	0.611456	2.584824	2.293309
16	6	0	0.063763	5.729062	1.137411
17	1	0	-0.877995	6.208077	-0.740274
18	1	0	0.959832	4.936248	2.928827
19	1	0	0.221563	6.764509	1.416572
20	7	0	2.512582	0.257503	-0.895031
21	8	0	2.339309	2.555292	-0.914360
22	8	0	2.064250	-1.990420	-1.121558
23	6	0	3.916073	0.164700	-0.632202
24	6	0	4.461553	0.893297	0.426718
25	6	0	4.720267	-0.652412	-1.428827
26	6	0	5.828644	0.806307	0.682536
27	1	0	3.821508	1.521593	1.034305
28	6	0	6.084489	-0.741811	-1.156007
29	1	0	4.279510	-1.217501	-2.240318
30	6	0	6.641125	-0.012106	-0.104734
31	1	0	6.257257	1.373918	1.500099
32	1	0	6.710748	-1.379368	-1.768726
33	1	0	7.702999	-0.080740	0.101229
34	8	0	-2.900757	2.028457	-0.612329
35	7	0	-2.011555	-0.090656	-0.611721
36	6	0	-3.141524	-1.013027	-0.627494
37	7	0	-1.121742	-2.075727	0.016039
38	6	0	-2.475942	-2.304893	-0.158066
39	6	0	-0.243150	-3.085172	0.538646
40	6	0	0.017092	-4.220431	-0.227541
41	6	0	0.315361	-2.937978	1.808477
42	6	0	0.855432	-5.211247	0.277184
43	1	0	-0.428631	-4.313083	-1.210838
44	6	0	1.170797	-3.924282	2.299141
45	1	0	0.073151	-2.074943	2.417942
46	6	0	1.441663	-5.059682	1.535863
47	1	0	1.061802	-6.094441	-0.315630
48	1	0	1.614422	-3.807999	3.280848
49	1	0	2.104637	-5.825547	1.921247
50	8	0	-3.037454	-3.350358	0.030344
51	1	0	-3.486574	-1.175347	-1.655217
52	6	0	-4.321279	-0.622050	0.277116

53	1	0	-4.733496	-1.544558	0.707811
54	1	0	-3.936214	-0.018135	1.107863
55	6	0	-5.455118	0.124223	-0.451721
56	1	0	-5.005020	0.899629	-1.082025
57	6	0	-6.266281	-0.835689	-1.330289
58	1	0	-6.757612	-1.596109	-0.711437
59	1	0	-7.042282	-0.295821	-1.882521
60	1	0	-5.642233	-1.357774	-2.064391
61	6	0	-6.362316	0.810425	0.574655
62	1	0	-5.806493	1.557474	1.150503
63	1	0	-7.198306	1.316806	0.081572
64	1	0	-6.779376	0.077171	1.276347
65	1	0	-0.093992	-0.736663	-2.274136
66	1	0	0.038811	1.697627	-2.141494

Structure $\mathbf{I_{11}}$:

Energy (Hartrees): -2060.329541

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.059651	0.403692	1.929184
2	6	0	-1.042041	-0.170640	-0.844384
3	6	0	0.045798	1.964587	-0.164143
4	6	0	0.551433	1.608505	1.337507
5	1	0	-1.042435	0.348016	2.370707
6	1	0	0.435873	2.550988	1.880804
7	6	0	-1.483432	1.962285	-0.069479
8	6	0	2.036195	1.237355	1.206409
9	6	0	0.869791	-0.620177	2.026996
10	8	0	0.796422	-1.797808	2.394499
11	8	0	2.911107	1.978958	0.812717
12	7	0	2.156838	-0.084802	1.538823
13	6	0	3.309218	-0.874093	1.283935
14	6	0	3.649994	-1.936025	2.132380
15	6	0	4.098329	-0.605989	0.156034
16	6	0	4.765821	-2.721668	1.840931
17	1	0	3.030207	-2.146492	2.992070
18	6	0	5.218045	-1.388484	-0.114802
19	1	0	3.845570	0.224252	-0.489793
20	6	0	5.555920	-2.452757	0.722326
21	1	0	5.021416	-3.543908	2.500115
22	1	0	5.824249	-1.164815	-0.985571
23	1	0	6.427041	-3.061332	0.507455
24	6	0	0.612740	3.257010	-0.703760
25	6	0	0.290486	4.452266	-0.042935
26	6	0	1.482521	3.301262	-1.798291
27	6	0	0.816767	5.664584	-0.486012
28	1	0	-0.378831	4.439653	0.808178
29	6	0	2.012205	4.514940	-2.233456
30	1	0	1.765190	2.393970	-2.319987
31	6	0	1.679724	5.701175	-1.581263
32	1	0	0.555954	6.579192	0.033658
33	1	0	2.689209	4.528004	-3.079550
34	1	0	2.092537	6.644141	-1.920360
35	7	0	-1.559598	-1.379467	-1.063246
36	7	0	-1.966923	0.696989	-0.417809
37	6	0	-2.965493	-1.344303	-0.778799
38	6	0	-3.280378	0.066382	-0.279456
39	1	0	-3.982421	0.541572	-0.969803
40	6	0	-0.804793	-2.552429	-1.422090
41	6	0	-1.061169	-3.184536	-2.637968
42	6	0	0.161100	-3.019712	-0.529565
43	6	0	-0.316529	-4.314437	-2.973004
44	1	0	-1.824495	-2.800238	-3.304296
45	6	0	0.912321	-4.137924	-0.891773
46	1	0	0.309405	-2.547383	0.440239
47	6	0	0.673986	-4.783465	-2.106512
48	1	0	-0.505524	-4.822053	-3.911030

49	1	0	1.674642	-4.501374	-0.213357
50	1	0	1.256396	-5.656411	-2.376919
51	6	0	-3.813334	0.082206	1.162589
52	1	0	-3.089152	-0.423725	1.810578
53	1	0	-3.868271	1.132234	1.476709
54	6	0	-5.201267	-0.567510	1.323114
55	1	0	-5.112097	-1.641215	1.118345
56	6	0	-6.233528	0.026043	0.356502
57	1	0	-6.251352	1.120727	0.428752
58	1	0	-6.035408	-0.251242	-0.684364
59	1	0	-7.235175	-0.340494	0.600618
60	6	0	-5.657710	-0.387833	2.775984
61	1	0	-6.606905	-0.904028	2.947321
62	1	0	-4.921727	-0.788864	3.480123
63	1	0	-5.804144	0.674603	3.004034
64	8	0	-3.698350	-2.267295	-0.919295
65	8	0	-2.187009	2.844709	0.327503
66	16	0	0.487643	0.477301	-1.190603

Structure **11**:

Energy (Hartrees): -2060.395895

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.015075	-0.251687	-1.131971
2	6	0	0.929157	-0.224388	0.096252
3	6	0	-0.139402	1.895973	0.158059
4	6	0	-0.642813	1.154509	-1.132412
5	1	0	0.572116	-0.481620	-2.022783
6	1	0	-0.406641	1.751399	-2.015761
7	6	0	1.390996	2.068290	-0.037505
8	6	0	-2.144203	0.913843	-1.084469
9	6	0	-1.192617	-1.213697	-1.050419
10	8	0	-1.141730	-2.411881	-1.075204
11	8	0	-3.005975	1.745662	-1.126678
12	7	0	-2.366098	-0.462988	-0.995784
13	6	0	-3.668500	-1.038259	-0.855559
14	6	0	-4.068427	-2.076793	-1.697523
15	6	0	-4.521332	-0.551416	0.137064
16	6	0	-5.335322	-2.636604	-1.535634
17	1	0	-3.393815	-2.446383	-2.459263
18	6	0	-5.790476	-1.108587	0.281308
19	1	0	-4.191038	0.255647	0.780327
20	6	0	-6.197898	-2.153314	-0.550677
21	1	0	-5.647180	-3.448241	-2.182140
22	1	0	-6.457536	-0.729998	1.046634
23	1	0	-7.183075	-2.589028	-0.431225
24	6	0	-0.874434	3.156854	0.503993
25	6	0	-0.726113	4.275455	-0.327163
26	6	0	-1.732273	3.231378	1.604332
27	6	0	-1.426689	5.448360	-0.056192
28	1	0	-0.054008	4.232468	-1.176562
29	6	0	-2.432943	4.407165	1.874243
30	1	0	-1.865210	2.371858	2.253930
31	6	0	-2.283272	5.516829	1.044346
32	1	0	-1.303445	6.308202	-0.704518
33	1	0	-3.096039	4.451042	2.730440
34	1	0	-2.829153	6.429823	1.252789
35	7	0	1.727340	-1.350992	0.435985
36	7	0	1.910262	0.810699	-0.190670
37	6	0	3.081188	-1.051318	0.501314
38	6	0	3.277716	0.403520	0.095815
39	1	0	3.658604	0.955840	0.962009
40	6	0	1.217116	-2.642212	0.801403
41	6	0	0.380109	-2.786099	1.907614
42	6	0	1.588943	-3.749456	0.039240
43	6	0	-0.112929	-4.049802	2.232447
44	1	0	0.122882	-1.928604	2.519249

45	6	0	1.110377	-5.011110	0.382251
46	1	0	2.243312	-3.612831	-0.813772
47	6	0	0.250462	-5.161532	1.471903
48	1	0	-0.773252	-4.163721	3.084012
49	1	0	1.397966	-5.873541	-0.207322
50	1	0	-0.131005	-6.142569	1.730247
51	6	0	4.203707	0.585732	-1.113810
52	1	0	3.766901	0.043984	-1.962977
53	1	0	4.187294	1.654802	-1.365648
54	6	0	5.661699	0.141495	-0.902585
55	1	0	5.678850	-0.947261	-0.776813
56	6	0	6.276659	0.774507	0.351309
57	1	0	6.150221	1.864594	0.341341
58	1	0	5.825255	0.379076	1.266769
59	1	0	7.349447	0.561608	0.399233
60	6	0	6.477126	0.506387	-2.149230
61	1	0	7.505381	0.141656	-2.063279
62	1	0	6.039420	0.072724	-3.055008
63	1	0	6.513950	1.594888	-2.278928
64	8	0	3.948023	-1.826262	0.808613
65	8	0	2.018858	3.094613	-0.058938
66	16	0	-0.148584	0.553498	1.429593

Structure **12**:

```
Energy (Hartrees): -2060.402197

No imaginary frequencies.
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.667120	0.027652	-1.345624
2	6	0	-1.364792	0.112363	0.024877
3	6	0	-0.040196	2.079865	-0.038924
4	6	0	0.305755	1.211516	-1.301371
5	6	0	0.294906	1.242792	1.216588
6	6	0	0.493600	3.485373	-0.060761
7	6	0	1.804845	3.746654	0.361028
8	6	0	-0.290440	4.538904	-0.546696
9	6	0	2.313216	5.043687	0.300248
10	1	0	2.423699	2.941630	0.732326
11	6	0	0.222691	5.834405	-0.606921
12	1	0	-1.305678	4.352500	-0.882340
13	6	0	1.525805	6.090250	-0.181086
14	1	0	3.327619	5.233308	0.631330
15	1	0	-0.397951	6.640141	-0.981673
16	1	0	1.924943	7.097184	-0.224000
17	7	0	-2.335266	-0.850315	0.391684
18	7	0	-0.348880	0.022722	1.071144
19	6	0	-2.153612	-1.314544	1.683614
20	6	0	-0.832473	-0.758132	2.211514
21	1	0	-1.054056	-0.081798	3.046720
22	6	0	-3.543101	-1.044007	-0.357936
23	6	0	-4.730461	-0.474859	0.107578
24	6	0	-3.515205	-1.790323	-1.537443
25	6	0	-5.904616	-0.651663	-0.622619
26	1	0	-4.729470	0.088916	1.034098
27	6	0	-4.692945	-1.949182	-2.268456
28	1	0	-2.583343	-2.249657	-1.852352
29	6	0	-5.884730	-1.382108	-1.812661
30	1	0	-6.831063	-0.219626	-0.263487
31	1	0	-4.681556	-2.527364	-3.184834
32	1	0	-6.799202	-1.515680	-2.379098
33	6	0	0.079530	-1.887339	2.695128
34	1	0	-0.506039	-2.450951	3.432676
35	1	0	0.281424	-2.567807	1.856119
36	6	0	1.404432	-1.412441	3.325730
37	1	0	1.224854	-0.440957	3.804070
38	6	0	2.503700	-1.233421	2.270185
39	1	0	2.837543	-2.211988	1.904295
40	1	0	2.159526	-0.654274	1.408372

41	1	0	3.371994	-0.718641	2.693241
42	6	0	1.867647	-2.407207	4.397500
43	1	0	2.830806	-2.102947	4.819918
44	1	0	1.143578	-2.479525	5.215516
45	1	0	1.991528	-3.407841	3.965300
46	8	0	-2.893479	-2.053678	2.274112
47	8	0	0.957669	1.565311	2.164042
48	16	0	-1.891910	1.922853	0.039319
49	6	0	0.197655	-1.207912	-1.477854
50	6	0	1.686566	0.565600	-1.256683
51	7	0	1.535224	-0.819077	-1.426441
52	1	0	0.249385	1.849764	-2.183929
53	1	0	-1.397298	0.065878	-2.152787
54	6	0	2.634114	-1.733269	-1.517360
55	6	0	2.576126	-2.956290	-0.844889
56	6	0	3.750813	-1.396186	-2.286929
57	6	0	3.645063	-3.845364	-0.946703
58	1	0	1.704013	-3.211302	-0.257355
59	6	0	4.818388	-2.288203	-2.371503
60	1	0	3.788400	-0.445334	-2.802725
61	6	0	4.768493	-3.513523	-1.705219
62	1	0	3.598112	-4.795472	-0.427783
63	1	0	5.687268	-2.024421	-2.962659
64	1	0	5.599090	-4.205855	-1.776847
65	8	0	-0.198826	-2.336520	-1.601016
66	8	0	2.736258	1.125465	-1.103893

Structure **13**:

Energy (Hartrees): -2060.387089

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.321997	0.800239	0.946529
2	6	0	0.300012	1.739487	-0.117670
3	6	0	0.464794	-0.337375	-0.882655
4	6	0	-0.736081	1.711712	-1.302210
5	6	0	-0.612652	0.280765	-1.857389
6	7	0	1.293532	0.813856	-0.656025
7	6	0	2.534103	0.891745	-1.194619
8	16	0	1.560653	-1.652410	-1.483235
9	6	0	3.001441	-0.505825	-1.638464
10	1	0	3.274008	-0.439184	-2.693201
11	8	0	3.221210	1.881574	-1.270956
12	6	0	4.193765	-0.931620	-0.815511
13	6	0	4.068989	-1.120525	0.566791
14	6	0	5.437527	-1.100490	-1.427165
15	6	0	5.181744	-1.471384	1.326827
16	1	0	3.097308	-1.000288	1.039953
17	6	0	6.552284	-1.456067	-0.664684
18	1	0	5.534988	-0.949722	-2.497428
19	6	0	6.425725	-1.641601	0.711128
20	1	0	5.080336	-1.615489	2.396293
21	1	0	7.514392	-1.587377	-1.146249
22	1	0	7.290201	-1.917895	1.303823
23	8	0	-0.921997	1.131726	1.937825
24	6	0	-0.669997	-1.673133	1.023949
25	6	0	-1.003034	-2.765345	0.214448
26	6	0	-0.828419	-1.758215	2.414334
27	6	0	-1.496925	-3.932115	0.795914
28	1	0	-0.912559	-2.710638	-0.863807
29	6	0	-1.334336	-2.927015	2.978714
30	1	0	-0.568533	-0.916843	3.040875
31	6	0	-1.669141	-4.018856	2.176676
32	1	0	-1.755727	-4.769767	0.159225
33	1	0	-1.459983	-2.981934	4.053892
34	1	0	-2.060967	-4.925581	2.621935
35	7	0	-0.148466	-0.479176	0.451724
36	6	0	0.773663	3.099606	0.344467

37	1	0	-0.107022	3.643288	0.709836
38	6	0	1.881919	3.070669	1.428661
39	1	0	2.382239	2.091820	1.385439
40	1	0	1.140092	3.629717	-0.542329
41	6	0	2.931923	4.146956	1.127054
42	1	0	3.715020	4.148960	1.892147
43	1	0	2.466586	5.140619	1.120507
44	1	0	3.397805	3.969833	0.154305
45	6	0	1.314028	3.270416	2.840678
46	1	0	0.546348	2.532618	3.083037
47	1	0	0.862010	4.266223	2.924318
48	1	0	2.113142	3.203410	3.586502
49	1	0	-0.481880	2.496403	-2.014967
50	1	0	-0.255769	0.219599	-2.884163
51	6	0	-2.176547	1.849846	-0.851282
52	6	0	-2.008696	-0.302910	-1.741992
53	8	0	-2.379894	-1.364399	-2.163520
54	8	0	-2.695769	2.824369	-0.386334
55	7	0	-2.806316	0.615069	-1.056365
56	6	0	-4.146684	0.343948	-0.632039
57	6	0	-5.095212	-0.102455	-1.551631
58	6	0	-4.473563	0.529951	0.712152
59	6	0	-6.392084	-0.368532	-1.114343
60	1	0	-4.818104	-0.245181	-2.588733
61	6	0	-5.776776	0.275744	1.134886
62	1	0	-3.711913	0.864551	1.408398
63	6	0	-6.735303	-0.175105	0.224697
64	1	0	-7.133013	-0.723030	-1.821083
65	1	0	-6.039534	0.422817	2.175675
66	1	0	-7.746414	-0.377869	0.558589

Structure **14**:

Energy (Hartrees): -2060.389780

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.128902	0.852292	1.750882
2	6	0	0.184209	0.040594	1.633631
3	6	0	-0.354055	0.719212	-0.411516
4	6	0	1.209291	1.202711	1.342235
5	6	0	0.838619	1.674176	-0.084776
6	7	0	0.047816	-0.478189	0.268687
7	6	0	-0.222355	-1.693366	-0.290412
8	16	0	-0.735441	0.265920	-2.115768
9	6	0	-0.826634	-1.528071	-1.695725
10	8	0	-0.024468	-2.767847	0.217878
11	8	0	-1.665418	1.224737	2.761624
12	6	0	-2.295087	2.307718	0.130272
13	6	0	-2.090509	3.526875	0.785852
14	6	0	-3.289163	2.187098	-0.844344
15	6	0	-2.879414	4.627905	0.455788
16	1	0	-1.339907	3.605152	1.564866
17	6	0	-4.064597	3.297389	-1.178299
18	1	0	-3.448532	1.231309	-1.328305
19	6	0	-3.861732	4.516676	-0.530252
20	1	0	-2.726526	5.570197	0.968522
21	1	0	-4.832146	3.204314	-1.937420
22	1	0	-4.470524	5.375695	-0.787328
23	7	0	-1.480372	1.173216	0.450231
24	6	0	0.512053	-0.936345	2.745988
25	1	0	0.831262	-0.349253	3.615858
26	6	0	-0.637677	-1.897518	3.153195
27	1	0	-1.384284	-1.918694	2.345719
28	1	0	1.386955	-1.512511	2.427300
29	6	0	-0.093406	-3.320756	3.329457
30	1	0	-0.890750	-4.004315	3.639412
31	1	0	0.680924	-3.334679	4.106859
32	1	0	0.335146	-3.689429	2.395420

33	6	0	-1.324712	-1.441880	4.448392
34	1	0	-1.704863	-0.422077	4.368895
35	1	0	-0.610306	-1.480679	5.280149
36	1	0	-2.158283	-2.108118	4.694431
37	1	0	0.546584	2.719780	-0.180815
38	1	0	1.170826	1.963696	2.122445
39	6	0	2.624697	0.669517	1.218622
40	6	0	2.076591	1.403600	-0.923470
41	7	0	3.019650	0.757254	-0.118231
42	8	0	3.301665	0.242047	2.112638
43	8	0	2.236771	1.700581	-2.073584
44	6	0	4.289782	0.295511	-0.589865
45	6	0	5.077129	1.113036	-1.403341
46	6	0	4.724440	-0.980446	-0.223912
47	6	0	6.308773	0.640947	-1.856210
48	1	0	4.726590	2.096775	-1.686935
49	6	0	5.963450	-1.435681	-0.670131
50	1	0	4.101173	-1.603030	0.406450
51	6	0	6.756092	-0.628584	-1.488494
52	1	0	6.919347	1.270363	-2.492761
53	1	0	6.304505	-2.422713	-0.381340
54	1	0	7.716684	-0.988014	-1.838608
55	1	0	-0.176363	-2.055991	-2.395410
56	6	0	-2.219120	-2.109561	-1.735384
57	6	0	-2.527134	-3.134228	-2.632187
58	6	0	-3.208357	-1.637389	-0.861243
59	6	0	-3.811452	-3.682835	-2.659626
60	1	0	-1.762809	-3.506224	-3.306769
61	6	0	-4.487865	-2.186527	-0.886895
62	1	0	-2.972407	-0.836840	-0.163275
63	6	0	-4.792557	-3.210213	-1.788976
64	1	0	-4.041457	-4.478203	-3.359327
65	1	0	-5.245221	-1.818126	-0.204520
66	1	0	-5.789019	-3.636352	-1.810000

Structure $\mathbf{I_{15}}$:

Energy (Hartrees): -2060.335013

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.717656	-1.867180	0.057816
2	6	0	0.592607	-1.858426	-0.698337
3	6	0	0.665213	-0.420380	1.079707
4	6	0	0.402534	-0.762125	-1.976869
5	6	0	0.839455	0.591949	-1.639169
6	7	0	1.437561	-1.198109	0.290542
7	6	0	2.747062	-0.724545	0.141454
8	16	0	1.457894	0.751421	2.037864
9	6	0	3.052855	0.355811	1.196933
10	8	0	3.520870	-1.145247	-0.662325
11	8	0	-1.698115	-2.521864	-0.087815
12	6	0	-1.720658	-0.198469	1.712345
13	6	0	-1.940688	1.175827	1.601221
14	6	0	-2.597110	-1.033802	2.404524
15	6	0	-3.069362	1.719998	2.213106
16	1	0	-1.284667	1.802208	0.999929
17	6	0	-3.725510	-0.473487	3.000634
18	1	0	-2.405118	-2.098149	2.461325
19	6	0	-3.961538	0.899474	2.905212
20	1	0	-3.262770	2.781407	2.116818
21	1	0	-4.419528	-1.111087	3.534822
22	1	0	-4.845908	1.328384	3.361680
23	7	0	-0.603979	-0.789128	1.026937
24	6	0	1.067690	-3.216220	-1.186821
25	1	0	0.202593	-3.691987	-1.670484
26	6	0	1.651752	-4.148247	-0.110397
27	1	0	2.561173	-3.671632	0.283602
28	1	0	1.824808	-3.058922	-1.962274

29	6	0	2.054716	-5.473359	-0.768627
30	1	0	2.538828	-6.136028	-0.044854
31	1	0	1.171530	-5.990167	-1.161853
32	1	0	2.750126	-5.309747	-1.598073
33	6	0	0.691250	-4.401650	1.057302
34	1	0	0.490504	-3.491430	1.635319
35	1	0	-0.265924	-4.795262	0.697145
36	1	0	1.120609	-5.133048	1.749505
37	1	0	0.885557	-1.272153	-2.809860
38	1	0	1.854794	0.954466	-1.647602
39	6	0	-1.096626	-0.589967	-2.235166
40	6	0	-0.255733	1.397166	-1.348807
41	8	0	-0.347904	2.542540	-0.890577
42	8	0	-1.815516	-1.380123	-2.796836
43	7	0	-1.459691	0.610629	-1.660016
44	6	0	-2.797094	1.043697	-1.460991
45	6	0	-3.139650	2.392663	-1.608024
46	6	0	-3.764905	0.115241	-1.051711
47	6	0	-4.442643	2.806700	-1.327814
48	1	0	-2.382953	3.102842	-1.910752
49	6	0	-5.063682	0.540218	-0.785985
50	1	0	-3.495509	-0.928248	-0.935935
51	6	0	-5.408179	1.887869	-0.916227
52	1	0	-4.700878	3.854180	-1.438135
53	1	0	-5.804637	-0.183521	-0.465122
54	1	0	-6.419210	2.215695	-0.701863
55	1	0	3.690492	-0.126673	1.943618
56	6	0	3.750670	1.565598	0.619534
57	6	0	5.149519	1.578470	0.633006
58	6	0	3.046319	2.631881	0.045658
59	6	0	5.845830	2.645668	0.066707
60	1	0	5.691711	0.752257	1.081942
61	6	0	3.749818	3.697796	-0.515440
62	1	0	1.958470	2.640341	0.021173
63	6	0	5.145866	3.707220	-0.507564
64	1	0	6.929454	2.647710	0.078277
65	1	0	3.201066	4.518350	-0.962274
66	1	0	5.684440	4.538948	-0.946971

Structure **15**:

Energy (Hartrees): -2060.386467

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.566069	1.024044	0.891107
2	6	0	-0.240796	1.670563	-0.261250
3	6	0	-0.586021	-0.519891	-0.375819
4	6	0	0.518912	1.239838	-1.567085
5	6	0	0.274695	-0.278008	-1.657884
6	7	0	-1.350890	0.707942	-0.366224
7	6	0	-2.601893	0.669041	0.187563
8	16	0	-1.774576	-1.876362	-0.337010
9	6	0	-3.096028	-0.779307	0.338035
10	8	0	-3.269932	1.624295	0.491803
11	8	0	1.344567	1.572039	1.630619
12	6	0	0.804902	-1.321655	1.688430
13	6	0	1.099845	-2.608129	1.225833
14	6	0	1.006546	-0.998699	3.037201
15	6	0	1.591913	-3.564773	2.113666
16	1	0	0.964796	-2.866181	0.183208
17	6	0	1.514410	-1.959127	3.908738
18	1	0	0.777691	-0.003897	3.394780
19	6	0	1.805756	-3.245844	3.454229
20	1	0	1.816754	-4.559169	1.746276
21	1	0	1.675127	-1.698930	4.948564
22	1	0	2.196604	-3.990622	4.137393
23	7	0	0.280787	-0.323954	0.816657
24	6	0	-0.548117	3.152912	-0.156746

25	1	0	0.374413	3.683012	-0.426660
26	6	0	-1.054214	3.667073	1.218126
27	1	0	-1.364355	2.804930	1.824581
28	1	0	-1.283863	3.374302	-0.939715
29	6	0	-2.276040	4.573601	1.026531
30	1	0	-2.632947	4.951530	1.990234
31	1	0	-2.013149	5.439445	0.405736
32	1	0	-3.091115	4.028015	0.546580
33	6	0	0.049232	4.425869	1.969084
34	1	0	0.933668	3.802866	2.115268
35	1	0	0.343101	5.316965	1.400433
36	1	0	-0.311220	4.759181	2.948139
37	1	0	0.122777	1.808419	-2.408660
38	1	0	-0.274025	-0.595126	-2.543157
39	6	0	2.022131	1.403864	-1.478882
40	6	0	1.659482	-0.898504	-1.634575
41	8	0	1.922764	-2.064663	-1.752979
42	8	0	2.633322	2.433046	-1.424663
43	7	0	2.590974	0.122522	-1.455658
44	6	0	3.993919	-0.102020	-1.274516
45	6	0	4.710503	-0.850133	-2.208122
46	6	0	4.616727	0.439697	-0.149329
47	6	0	6.074877	-1.057853	-2.007514
48	1	0	4.206030	-1.266870	-3.071498
49	6	0	5.983269	0.238082	0.033609
50	1	0	4.031681	1.005187	0.567652
51	6	0	6.712074	-0.510995	-0.892376
52	1	0	6.638537	-1.642448	-2.724890
53	1	0	6.474382	0.660699	0.901860
54	1	0	7.773824	-0.670385	-0.743796
55	1	0	-3.178045	-0.957566	1.413256
56	6	0	-4.432626	-0.994655	-0.323307
57	6	0	-5.537384	-1.383413	0.437690
58	6	0	-4.581218	-0.782115	-1.699593
59	6	0	-6.782134	-1.559243	-0.170925
60	1	0	-5.424809	-1.545705	1.504807
61	6	0	-5.822373	-0.955341	-2.305876
62	1	0	-3.719565	-0.484656	-2.290723
63	6	0	-6.925791	-1.345912	-1.541133
64	1	0	-7.635231	-1.860279	0.425961
65	1	0	-5.931705	-0.786138	-3.370857
66	1	0	-7.891764	-1.481892	-2.013733

Structure **16**:

Energy (Hartrees): -2060.390562

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.595227	-1.140779	0.067232
2	6	0	-1.137816	-1.577085	0.356003
3	6	0	-1.068418	0.514997	-0.385796
4	6	0	-0.540081	-1.709606	-1.092160
5	6	0	-0.561770	-0.267546	-1.642857
6	7	0	-0.539857	-0.279622	0.692132
7	6	0	-0.255049	0.343050	1.877589
8	16	0	-0.573988	2.227818	-0.067390
9	6	0	-0.061251	1.849084	1.666487
10	8	0	-0.094347	-0.197135	2.941382
11	8	0	-3.575107	-1.839128	0.060055
12	6	0	-3.524615	0.898323	-1.001953
13	6	0	-3.190468	1.786237	-2.033360
14	6	0	-4.868564	0.701540	-0.657534
15	6	0	-4.198731	2.469302	-2.713240
16	1	0	-2.157511	1.960502	-2.312928
17	6	0	-5.864852	1.382304	-1.353817
18	1	0	-5.124052	0.021549	0.143156
19	6	0	-5.537758	2.268722	-2.381190
20	1	0	-3.928857	3.157272	-3.505872

21	1	0	-6.902025	1.222709	-1.082798
22	1	0	-6.318006	2.799231	-2.913781
23	7	0	-2.511616	0.196970	-0.292932
24	6	0	-0.929501	-2.748248	1.301824
25	1	0	-1.122360	-3.664398	0.729713
26	6	0	-1.791014	-2.755786	2.594220
27	1	0	-2.201693	-1.749334	2.755175
28	1	0	0.134575	-2.768391	1.558502
29	6	0	-0.915912	-3.110292	3.803173
30	1	0	-1.514174	-3.136475	4.720066
31	1	0	-0.468175	-4.102845	3.667979
32	1	0	-0.116908	-2.377801	3.931932
33	6	0	-2.955062	-3.751613	2.489327
34	1	0	-3.594127	-3.534275	1.632058
35	1	0	-2.564695	-4.771609	2.383723
36	1	0	-3.566932	-3.722958	3.397162
37	1	0	-0.748311	2.358505	2.344704
38	6	0	1.361177	2.259042	1.953408
39	6	0	1.626380	3.427139	2.671561
40	6	0	2.426774	1.477094	1.489820
41	6	0	2.944693	3.813284	2.922895
42	1	0	0.802282	4.032188	3.036204
43	6	0	3.741299	1.857999	1.746218
44	1	0	2.226085	0.563769	0.933214
45	6	0	4.002491	3.029656	2.462704
46	1	0	3.142798	4.721263	3.480748
47	1	0	4.558395	1.239553	1.391251
48	1	0	5.025770	3.325683	2.663512
49	1	0	-1.216539	-0.103632	-2.497005
50	1	0	-1.085199	-2.446584	-1.682953
51	6	0	0.939265	-2.073883	-1.062521
52	6	0	0.866595	0.042092	-2.032380
53	7	0	1.678446	-1.009629	-1.593316
54	8	0	1.405389	-3.106641	-0.667123
55	8	0	1.241591	1.012146	-2.628538
56	6	0	3.101214	-1.023271	-1.762071
57	6	0	3.749886	-2.189375	-2.176458
58	6	0	3.828279	0.145551	-1.515147
59	6	0	5.135805	-2.183016	-2.330694
60	1	0	3.182896	-3.091183	-2.364331
61	6	0	5.212009	0.141198	-1.683395
62	1	0	3.316427	1.050062	-1.210896
63	6	0	5.869839	-1.021873	-2.086431
64	1	0	5.639291	-3.089138	-2.646501
65	1	0	5.771986	1.050388	-1.497187
66	1	0	6.946168	-1.022534	-2.212752

Structure **17**:

Energy (Hartrees): -2004.365485

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.563325	0.551999	-0.229987
2	6	0	0.573286	-0.371264	0.044803
3	6	0	-1.636426	-0.369482	1.052954
4	6	0	-0.275660	-1.094551	1.135088
5	1	0	-0.359118	-2.146204	0.860491
6	16	0	-0.551021	-0.420017	-1.435942
7	7	0	0.646809	1.038751	0.377716
8	6	0	-0.549736	1.665791	0.165471
9	8	0	-0.769512	2.844732	0.291487
10	6	0	-2.906600	1.014404	-0.715206
11	6	0	-3.587904	2.025290	-0.021843
12	6	0	-3.534183	0.386388	-1.797920
13	6	0	-4.865675	2.411127	-0.423668
14	1	0	-3.113504	2.516887	0.817730
15	6	0	-4.814560	0.773472	-2.194784
16	1	0	-3.027478	-0.412895	-2.329588

17	6	0	-5.481819	1.789381	-1.510781
18	1	0	-5.380041	3.198430	0.115148
19	1	0	-5.286013	0.282891	-3.038639
20	1	0	-6.475368	2.092982	-1.820124
21	6	0	2.004809	1.572787	0.306578
22	6	0	2.800016	0.315031	-0.062340
23	1	0	2.328031	1.915995	1.295793
24	6	0	2.206140	2.689867	-0.742588
25	1	0	1.227748	3.091381	-1.021944
26	6	0	3.080664	3.847234	-0.231859
27	1	0	2.606880	4.233837	0.683158
28	7	0	1.928208	-0.756864	-0.133734
29	6	0	2.282885	-2.016000	-0.728333
30	6	0	2.577461	-2.051838	-2.093778
31	6	0	2.309593	-3.177047	0.044743
32	6	0	2.897270	-3.268746	-2.693065
33	1	0	2.560489	-1.132954	-2.670490
34	6	0	2.621348	-4.392194	-0.567205
35	1	0	2.097018	-3.112445	1.106267
36	6	0	2.914081	-4.439416	-1.931073
37	1	0	3.130897	-3.302519	-3.750608
38	1	0	2.642415	-5.299630	0.024891
39	1	0	3.158831	-5.385490	-2.400267
40	8	0	3.979563	0.267463	-0.288899
41	1	0	-1.796100	0.276509	1.916558
42	6	0	-2.852151	-1.272931	0.989614
43	6	0	0.441281	-1.028053	2.471731
44	8	0	-3.852557	-1.078408	1.626210
45	8	0	1.279595	-1.828225	2.799924
46	8	0	0.089917	0.015006	3.217472
47	8	0	-2.702360	-2.279761	0.130614
48	6	0	0.792539	0.162702	4.460524
49	1	0	1.859674	0.289026	4.275637
50	1	0	0.629343	-0.711387	5.091030
51	1	0	0.378529	1.052993	4.926463
52	6	0	-3.854045	-3.110798	-0.059474
53	1	0	-4.700971	-2.508832	-0.390756
54	1	0	-4.110632	-3.621250	0.869637
55	1	0	-3.573061	-3.831029	-0.823942
56	1	0	2.657748	2.265736	-1.649033
57	6	0	3.109009	4.972106	-1.271529
58	1	0	3.706655	5.817244	-0.915360
59	1	0	2.100857	5.337536	-1.492389
60	1	0	3.555727	4.616889	-2.208060
61	6	0	4.504605	3.392525	0.107221
62	1	0	5.003357	2.998847	-0.785391
63	1	0	4.520834	2.597808	0.859141
64	1	0	5.093883	4.233556	0.487617

Structure **18**:

Energy (Hartrees): -2004.365053

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.694201	-0.392699	-0.369704
2	6	0	0.612878	-0.043040	-0.039208
3	6	0	-1.241873	-1.426450	0.717541
4	1	0	-1.340028	-2.419808	0.281888
5	6	0	0.252599	-1.128334	1.014054
6	16	0	-0.298122	-0.548128	-1.588269
7	7	0	-0.097507	1.152718	0.371313
8	6	0	-1.439899	1.052424	0.162889
9	8	0	-2.260033	1.919616	0.332534
10	6	0	-3.054374	-0.601724	-0.971468
11	6	0	-3.831403	-1.727444	-0.672463
12	6	0	-3.549809	0.342956	-1.884639
13	6	0	-5.080661	-1.902344	-1.272235
14	1	0	-3.484129	-2.475616	0.029638

15	6	0	-4.794137	0.164439	-2.482362
16	1	0	-2.958954	1.220522	-2.121654
17	6	0	-5.564892	-0.960225	-2.176794
18	1	0	-5.670469	-2.778023	-1.027263
19	1	0	-5.163628	0.902617	-3.184717
20	1	0	-6.534570	-1.098078	-2.641476
21	6	0	0.757435	2.320323	0.519500
22	6	0	2.132670	1.717359	0.225646
23	1	0	0.748953	2.669554	1.558150
24	6	0	-2.092999	-1.392018	1.974744
25	8	0	-2.737970	-2.320963	2.383047
26	6	0	0.423151	3.486011	-0.440606
27	1	0	-0.572880	3.312811	-0.860089
28	6	0	0.437637	4.858149	0.251860
29	1	0	-0.264394	4.804676	1.097450
30	7	0	1.967943	0.384625	-0.114988
31	6	0	3.060543	-0.466683	-0.486356
32	6	0	3.123622	-1.003649	-1.774618
33	6	0	4.066452	-0.730400	0.444914
34	6	0	4.202395	-1.814442	-2.128126
35	1	0	2.345281	-0.778537	-2.495277
36	6	0	5.152157	-1.526211	0.078240
37	1	0	3.993466	-0.311009	1.441388
38	6	0	5.220849	-2.068875	-1.206435
39	1	0	4.254169	-2.231801	-3.126840
40	1	0	5.938503	-1.722267	0.797223
41	1	0	6.065647	-2.686491	-1.488825
42	8	0	3.182464	2.302314	0.255060
43	1	0	0.374312	-0.662607	1.992265
44	8	0	-2.031816	-0.203800	2.569404
45	6	0	-2.841621	-0.036855	3.741177
46	1	0	-2.684133	0.989331	4.062611
47	1	0	-2.527314	-0.735460	4.517074
48	1	0	-3.890990	-0.203038	3.497489
49	6	0	1.162825	-2.340180	1.020208
50	8	0	1.843073	-2.635042	1.967729
51	8	0	1.142816	-3.013678	-0.124323
52	6	0	2.103311	-4.071793	-0.235547
53	1	0	1.873563	-4.866713	0.475263
54	1	0	3.105502	-3.684115	-0.045651
55	1	0	2.020761	-4.437946	-1.256007
56	1	0	1.134911	3.494541	-1.276372
57	6	0	1.828767	5.214903	0.787362
58	1	0	2.549956	5.277742	-0.035560
59	1	0	2.208940	4.468086	1.491077
60	1	0	1.806635	6.183198	1.298275
61	6	0	-0.056261	5.935740	-0.718745
62	1	0	-0.074400	6.917757	-0.235395
63	1	0	-1.066376	5.715709	-1.079282
64	1	0	0.609310	6.002414	-1.587929

Structure **19**:

Energy (Hartrees): -2004.371213

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.514215	-0.907222	0.770741
2	6	0	1.846446	-0.081872	-0.514613
3	6	0	-0.515176	-0.123062	-0.318014
4	6	0	-0.025276	-0.908118	0.931866
5	7	0	-1.914581	0.025283	-0.549354
6	7	0	-0.054041	1.238812	-0.127714
7	16	0	0.587177	-0.749191	-1.704779
8	6	0	-1.073705	2.235920	-0.399236
9	1	0	-0.832569	2.783942	-1.317413
10	6	0	-2.289714	1.360428	-0.671535
11	6	0	-2.834469	-1.052455	-0.758439
12	6	0	-4.076438	-1.006180	-0.115323

13	6	0	-2.516328	-2.125848	-1.594568
14	6	0	-5.005588	-2.020631	-0.330364
15	1	0	-4.308583	-0.173917	0.536337
16	6	0	-3.449846	-3.147015	-1.791389
17	1	0	-1.558642	-2.176428	-2.097639
18	6	0	-4.696930	-3.094290	-1.170099
19	1	0	-5.969975	-1.972670	0.161707
20	1	0	-3.196712	-3.977244	-2.440079
21	1	0	-5.422324	-3.882225	-1.335406
22	8	0	-3.398548	1.748867	-0.931442
23	6	0	-1.259397	3.208461	0.774530
24	1	0	-0.296593	3.718391	0.912100
25	1	0	-1.441618	2.617618	1.681057
26	6	0	-2.370443	4.258078	0.598377
27	1	0	-3.338751	3.743717	0.595529
28	6	0	-2.236576	5.022673	-0.723727
29	1	0	-1.232697	5.453842	-0.825988
30	1	0	-2.960183	5.843343	-0.765257
31	1	0	-2.428175	4.375579	-1.585447
32	6	0	-2.333699	5.223995	1.789200
33	1	0	-1.387823	5.778731	1.805057
34	1	0	-2.426174	4.688580	2.740290
35	1	0	-3.149877	5.950823	1.728171
36	6	0	1.291508	1.362075	-0.345029
37	8	0	1.898417	2.396470	-0.435752
38	6	0	3.260056	-0.148705	-1.017132
39	6	0	4.216228	-0.985744	-0.430222
40	6	0	3.627604	0.632289	-2.124600
41	6	0	5.516522	-1.035322	-0.937678
42	1	0	3.965725	-1.601543	0.425008
43	6	0	4.923947	0.579507	-2.628192
44	1	0	2.896993	1.287508	-2.585163
45	6	0	5.874371	-0.254939	-2.034890
46	1	0	6.245862	-1.688745	-0.472796
47	1	0	5.192631	1.189711	-3.482586
48	1	0	6.884174	-0.295675	-2.426887
49	1	0	-0.342945	-0.332194	1.802130
50	1	0	1.853001	-1.929452	0.605864
51	6	0	-0.615775	-2.301243	1.036478
52	8	0	-0.168501	-3.289983	0.522742
53	8	0	-1.718994	-2.273110	1.782705
54	6	0	2.184371	-0.314414	1.997832
55	8	0	1.984720	0.801581	2.396043
56	8	0	3.007725	-1.180546	2.588841
57	6	0	-2.470387	-3.491890	1.827171
58	1	0	-3.357899	-3.271031	2.414728
59	1	0	-1.883086	-4.278955	2.302211
60	1	0	-2.746582	-3.795638	0.816331
61	6	0	3.705421	-0.686094	3.741020
62	1	0	4.324507	-1.510590	4.085011
63	1	0	2.995784	-0.392393	4.514790
64	1	0	4.323854	0.168807	3.466191

Structure **20**:

Energy (Hartrees): -2004.372946

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.571633	-0.368357	0.960771
2	6	0	1.755581	0.489049	-0.351562
3	6	0	-0.472964	-0.301041	-0.342447
4	6	0	0.147773	-0.954119	0.916507
5	1	0	1.702530	0.285890	1.824514
6	1	0	0.175548	-2.040489	0.800942
7	7	0	-1.806012	-0.614186	-0.733591
8	7	0	-0.497174	1.132899	-0.098382
9	16	0	0.873911	-0.497246	-1.638616
10	6	0	-1.716775	1.749963	-0.604770
11	1	0	-1.503862	2.295680	-1.531897

12	6	0	-2.560219	0.528322	-0.951094
13	6	0	-2.286573	-1.950562	-0.871382
14	6	0	-3.636985	-2.241454	-0.635274
15	6	0	-1.403385	-2.980367	-1.216159
16	6	0	-4.092064	-3.551395	-0.765698
17	1	0	-4.321092	-1.450816	-0.363819
18	6	0	-1.871110	-4.289419	-1.330533
19	1	0	-0.354825	-2.777692	-1.399048
20	6	0	-3.216238	-4.581390	-1.113107
21	1	0	-5.139136	-3.766328	-0.585917
22	1	0	-1.175828	-5.077111	-1.596199
23	1	0	-3.578260	-5.598183	-1.208956
24	8	0	-3.701761	0.559303	-1.337007
25	6	0	-2.367816	2.674580	0.430360
26	1	0	-1.618517	3.435600	0.687143
27	1	0	-2.558316	2.087259	1.338226
28	6	0	-3.660309	3.375613	-0.024217
29	1	0	-4.435603	2.614860	-0.168574
30	6	0	-3.471011	4.121593	-1.350710
31	1	0	-2.607117	4.796402	-1.299273
32	1	0	-4.355193	4.725548	-1.578629
33	1	0	-3.323224	3.432234	-2.188031
34	6	0	-4.116770	4.341371	1.075914
35	1	0	-3.380019	5.141713	1.215569
36	1	0	-4.240902	3.826688	2.034906
37	1	0	-5.072988	4.805154	0.814169
38	6	0	0.763607	1.675078	-0.236125
39	8	0	1.011294	2.850920	-0.279394
40	6	0	3.180369	0.851781	-0.654743
41	6	0	3.803328	1.875079	0.073045
42	6	0	3.928597	0.116698	-1.581128
43	6	0	5.151356	2.160255	-0.133843
44	1	0	3.233439	2.448162	0.794287
45	6	0	5.279393	0.404312	-1.784887
46	1	0	3.463623	-0.687915	-2.142182
47	6	0	5.893299	1.426269	-1.062075
48	1	0	5.623104	2.956479	0.430404
49	1	0	5.845884	-0.169318	-2.509532
50	1	0	6.941538	1.651961	-1.221611
51	6	0	2.641172	-1.441223	1.006198
52	8	0	2.545474	-2.528527	0.500861
53	8	0	3.719307	-1.010768	1.655132
54	6	0	-0.637608	-0.622305	2.177308
55	8	0	-0.166608	-0.149219	3.176472
56	8	0	-1.922158	-0.947225	2.045810
57	6	0	-2.746618	-0.732426	3.199579
58	1	0	-2.404800	-1.356682	4.025656
59	1	0	-3.751094	-1.019323	2.898408
60	1	0	-2.720185	0.315310	3.499386
61	6	0	4.865381	-1.867576	1.602215
62	1	0	4.647214	-2.826582	2.073317
63	1	0	5.648174	-1.344243	2.145520
64	1	0	5.164992	-2.025192	0.565015

Structure **21**:

Energy (Hartrees): -2004.362182

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.843064	0.566746	1.646612
2	6	0	0.125589	1.490319	0.869767
3	6	0	-0.541740	-0.091607	-0.524818
4	6	0	-0.848104	2.275476	-0.098938
5	6	0	-1.293548	1.176408	-1.099327
6	7	0	0.671973	0.502063	-0.048553
7	6	0	1.843068	0.311761	-0.701165
8	16	0	-0.041048	-1.419118	-1.662859
9	6	0	1.729162	-0.905918	-1.634497

10	1	0	2.009734	-0.577377	-2.636497
11	8	0	2.865550	0.933090	-0.542102
12	6	0	2.658181	-1.998955	-1.160315
13	6	0	2.417995	-2.657695	0.052243
14	6	0	3.790807	-2.324354	-1.910074
15	6	0	3.302266	-3.633190	0.505498
16	1	0	1.532527	-2.410095	0.631959
17	6	0	4.675950	-3.304457	-1.455777
18	1	0	3.980789	-1.809127	-2.846164
19	6	0	4.432603	-3.960201	-0.249502
20	1	0	3.110360	-4.140138	1.444103
21	1	0	5.551323	-3.554054	-2.044313
22	1	0	5.117839	-4.722557	0.103029
23	8	0	-1.265798	0.743963	2.758776
24	6	0	-2.214901	-1.398268	0.933156
25	6	0	-2.863742	-1.953980	-0.177883
26	6	0	-2.585720	-1.802343	2.224178
27	6	0	-3.869832	-2.902585	0.003281
28	1	0	-2.602729	-1.655360	-1.186782
29	6	0	-3.601438	-2.741895	2.388402
30	1	0	-2.093446	-1.375968	3.085598
31	6	0	-4.247159	-3.300364	1.284981
32	1	0	-4.356030	-3.328514	-0.867193
33	1	0	-3.882143	-3.041362	3.391572
34	1	0	-5.030800	-4.035760	1.421791
35	7	0	-1.176952	-0.446522	0.757996
36	6	0	1.112236	2.297016	1.689486
37	1	0	0.536437	2.971628	2.335555
38	6	0	2.099635	1.451572	2.536550
39	1	0	2.156321	0.444671	2.097983
40	1	0	-0.908631	1.358900	-2.101499
41	1	0	-1.682624	2.699314	0.458408
42	6	0	-2.798338	1.019168	-1.160424
43	6	0	-0.074638	3.411760	-0.730043
44	8	0	-0.169753	4.560902	-0.394850
45	8	0	0.781136	2.971877	-1.656405
46	8	0	-3.558577	1.377746	-0.303167
47	8	0	-3.172907	0.415700	-2.289842
48	6	0	1.695383	3.942162	-2.183061
49	1	0	2.332857	3.400159	-2.876700
50	1	0	2.292629	4.370200	-1.377150
51	1	0	1.152427	4.734469	-2.699149
52	6	0	-4.579076	0.156876	-2.413750
53	1	0	-5.133343	1.095786	-2.429220
54	1	0	-4.923189	-0.457033	-1.579806
55	1	0	-4.698072	-0.371269	-3.356600
56	1	0	1.686184	2.923099	0.995725
57	6	0	3.499693	2.074616	2.468447
58	1	0	4.210307	1.501465	3.072603
59	1	0	3.478359	3.100008	2.858262
60	1	0	3.859617	2.096677	1.436752
61	6	0	1.649458	1.327762	3.998649
62	1	0	0.644314	0.910627	4.086200
63	1	0	1.646599	2.316646	4.473434
64	1	0	2.342441	0.690851	4.558414

Structure **22**:

Energy (Hartrees): -2004.361844

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.258922	-0.166412	-1.267808
2	6	0	-0.592874	-1.405338	-0.627289
3	6	0	-0.147248	0.326834	0.670405
4	6	0	-1.494587	-1.671570	0.660020
5	6	0	-1.203421	-0.439680	1.559469
6	7	0	0.536798	-0.738423	0.001817
7	6	0	1.773155	-1.104192	0.429809

8	16	0	1.135042	1.337678	1.473516
9	6	0	2.446843	0.089831	1.130717
10	1	0	2.844692	-0.267395	2.081883
11	8	0	2.333164	-2.150516	0.214477
12	6	0	3.559677	0.607917	0.248299
13	6	0	3.267790	1.261780	-0.955702
14	6	0	4.890689	0.374958	0.602311
15	6	0	4.300153	1.676163	-1.794187
16	1	0	2.232102	1.448870	-1.227015
17	6	0	5.924699	0.793688	-0.237406
18	1	0	5.117003	-0.139301	1.530792
19	6	0	5.631045	1.444747	-1.435168
20	1	0	4.068172	2.182055	-2.724293
21	1	0	6.955190	0.610980	0.044988
22	1	0	6.433374	1.771178	-2.086993
23	8	0	-2.015558	-0.148053	-2.202641
24	6	0	-1.591806	2.138495	-0.382323
25	6	0	-1.743243	2.800247	0.844217
26	6	0	-2.123327	2.703311	-1.550120
27	6	0	-2.421177	4.017678	0.895802
28	1	0	-1.348060	2.380650	1.763310
29	6	0	-2.807564	3.914453	-1.479310
30	1	0	-2.001854	2.195909	-2.496371
31	6	0	-2.960120	4.578691	-0.261138
32	1	0	-2.529620	4.521447	1.849166
33	1	0	-3.216056	4.342939	-2.387264
34	1	0	-3.488999	5.523171	-0.214858
35	7	0	-0.898859	0.902115	-0.450644
36	6	0	-0.325554	-2.632435	-1.480541
37	1	0	-1.290351	-3.129803	-1.635715
38	6	0	0.371726	-2.446120	-2.857285
39	1	0	0.932095	-3.376754	-3.018511
40	1	0	-2.088959	0.172061	1.715629
41	1	0	-1.122155	-2.596106	1.102771
42	6	0	-0.636749	-0.776539	2.917969
43	6	0	-2.937120	-1.891948	0.257153
44	8	0	-3.647069	-0.766353	0.276196
45	8	0	-3.366056	-2.957468	-0.099307
46	8	0	-1.058399	-0.344672	3.955491
47	8	0	0.420849	-1.589851	2.818520
48	6	0	-4.965590	-0.842342	-0.282909
49	1	0	-4.915276	-1.216585	-1.305368
50	1	0	-5.347158	0.175237	-0.266935
51	1	0	-5.592258	-1.497461	0.322941
52	6	0	1.110690	-1.885607	4.039620
53	1	0	1.459304	-0.963328	4.506926
54	1	0	1.949038	-2.518792	3.758340
55	1	0	0.450625	-2.415072	4.727123
56	1	0	0.279454	-3.299762	-0.857866
57	6	0	1.388196	-1.296520	-2.898719
58	1	0	2.174751	-1.421655	-2.149591
59	1	0	0.903384	-0.325172	-2.740907
60	1	0	1.867278	-1.263408	-3.883020
61	6	0	-0.629970	-2.320975	-4.014845
62	1	0	-1.194476	-1.387981	-3.952578
63	1	0	-1.346002	-3.149843	-4.006166
64	1	0	-0.099281	-2.344148	-4.973000

Structure **23**:

Energy (Hartrees): -2004.362802

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.736343	1.530946	-0.145509
2	6	0	-0.276089	1.748218	0.323533
3	6	0	-0.495852	-0.391449	-0.192992
4	6	0	-0.256338	1.048265	1.744315
5	6	0	-0.389502	-0.455857	1.385329

6	7	0	0.365232	0.717410	-0.480614
7	6	0	1.574093	0.533295	-1.061884
8	16	0	0.120750	-1.781329	-1.189090
9	6	0	1.667884	-0.881011	-1.658899
10	8	0	2.454084	1.354531	-1.160440
11	8	0	-2.630599	2.334703	-0.112318
12	6	0	-2.980414	-0.520103	-0.851633
13	6	0	-3.058446	-1.898551	-0.610970
14	6	0	-4.069504	0.145104	-1.431944
15	6	0	-4.215523	-2.600718	-0.946406
16	1	0	-2.230401	-2.435245	-0.160664
17	6	0	-5.222924	-0.568585	-1.750694
18	1	0	-4.015270	1.207579	-1.619932
19	6	0	-5.305004	-1.941225	-1.513482
20	1	0	-4.258214	-3.667796	-0.759334
21	1	0	-6.060193	-0.043568	-2.195812
22	1	0	-6.204051	-2.489232	-1.768647
23	7	0	-1.802367	0.199747	-0.527237
24	6	0	0.275442	3.156384	0.223990
25	1	0	-0.304404	3.791448	0.905292
26	6	0	0.271044	3.757196	-1.206131
27	1	0	0.203323	2.929009	-1.926554
28	1	0	0.509018	-1.018667	1.632604
29	1	0	-1.080036	1.408876	2.359239
30	6	0	-1.581433	-1.109965	2.052271
31	6	0	1.041927	1.417091	2.427629
32	8	0	1.142077	2.253934	3.282345
33	8	0	2.080221	0.754166	1.907160
34	8	0	-2.544629	-0.522104	2.462291
35	8	0	-1.429143	-2.434004	2.115106
36	6	0	3.384733	1.178961	2.324744
37	1	0	4.085976	0.583598	1.743981
38	1	0	3.520495	2.238563	2.106318
39	1	0	3.516859	1.000517	3.392357
40	6	0	-2.539884	-3.157053	2.665040
41	1	0	-2.704096	-2.863597	3.702284
42	1	0	-3.441709	-2.959155	2.083250
43	1	0	-2.265321	-4.207264	2.605768
44	1	0	1.305822	3.135596	0.598237
45	6	0	1.588575	4.500003	-1.461618
46	1	0	1.599827	4.936527	-2.465699
47	1	0	1.709123	5.317731	-0.740125
48	1	0	2.438335	3.819303	-1.367834
49	6	0	-0.916140	4.704510	-1.429490
50	1	0	-1.873022	4.214887	-1.238242
51	1	0	-0.836169	5.566866	-0.756306
52	1	0	-0.914893	5.082370	-2.457336
53	1	0	1.643578	-0.750903	-2.743390
54	6	0	2.932316	-1.594239	-1.260185
55	6	0	3.768905	-2.130544	-2.241107
56	6	0	3.281015	-1.727978	0.090178
57	6	0	4.943752	-2.794628	-1.881022
58	1	0	3.503288	-2.026193	-3.288277
59	6	0	4.453763	-2.387693	0.449809
60	1	0	2.637474	-1.300379	0.854876
61	6	0	5.287176	-2.924675	-0.536325
62	1	0	5.587052	-3.207026	-2.649706
63	1	0	4.718292	-2.485468	1.496911
64	1	0	6.197796	-3.441208	-0.255298

Structure $\mathbf{I1_8}$:

Energy (Hartrees): -2004.310427

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.391726	-0.637365	-0.310940
2	6	0	0.448690	-0.207018	0.879368
3	6	0	-1.152892	1.015549	-0.306431

4	6	0	0.640887	1.317938	1.166183
5	6	0	-0.085003	2.003012	0.009774
6	7	0	-0.927743	-0.142306	0.269777
7	6	0	-1.736668	-1.205674	-0.244803
8	16	0	-2.468074	1.147023	-1.364492
9	6	0	-2.785993	-0.663088	-1.217926
10	1	0	-2.549954	-1.093855	-2.195234
11	8	0	-1.627702	-2.346526	0.054833
12	6	0	-4.191429	-1.003975	-0.797393
13	6	0	-4.656241	-0.630903	0.470058
14	6	0	-5.031684	-1.698690	-1.669484
15	6	0	-5.951807	-0.955506	0.861775
16	1	0	-4.003382	-0.089759	1.150816
17	6	0	-6.331495	-2.022381	-1.275333
18	1	0	-4.670403	-1.993339	-2.649157
19	6	0	-6.791659	-1.651353	-0.012626
20	1	0	-6.305722	-0.668345	1.844783
21	1	0	-6.979349	-2.564882	-1.953600
22	1	0	-7.800232	-1.904646	0.292476
23	8	0	0.847330	-0.712742	-1.435987
24	6	0	3.674787	-1.083170	-0.774494
25	6	0	4.950230	-1.183770	-0.180100
26	6	0	3.575312	-1.303440	-2.164927
27	6	0	6.081129	-1.482602	-0.931708
28	1	0	5.011213	-1.023462	0.891422
29	6	0	4.716603	-1.605427	-2.911304
30	1	0	2.606644	-1.235061	-2.639054
31	6	0	5.972404	-1.695713	-2.309833
32	1	0	7.048267	-1.554856	-0.444535
33	1	0	4.618631	-1.772765	-3.979631
34	1	0	6.850370	-1.932123	-2.900830
35	7	0	2.623254	-0.769654	0.099105
36	6	0	0.596052	-0.988812	2.185678
37	1	0	1.640259	-0.802373	2.467753
38	6	0	0.344857	-2.508931	2.262352
39	1	0	-0.725975	-2.696401	2.132336
40	1	0	0.554294	2.034966	-0.885373
41	1	0	0.130424	1.554009	2.103814
42	6	0	-0.556926	3.416967	0.291774
43	6	0	2.090110	1.728333	1.353852
44	8	0	2.609864	2.247525	0.245823
45	8	0	2.666762	1.623939	2.400632
46	8	0	-0.233497	4.045932	1.256720
47	8	0	-1.351485	3.851361	-0.682159
48	6	0	4.017068	2.518057	0.293485
49	1	0	4.556804	1.612630	0.572369
50	1	0	4.292947	2.827169	-0.711454
51	1	0	4.221621	3.312334	1.012555
52	6	0	-1.845138	5.196244	-0.541378
53	1	0	-1.011779	5.898365	-0.530159
54	1	0	-2.477273	5.367840	-1.408276
55	1	0	-2.420377	5.288025	0.379637
56	1	0	-0.034135	-0.499493	2.941365
57	6	0	1.104126	-3.329091	1.214855
58	1	0	0.805835	-3.076115	0.194067
59	1	0	2.182542	-3.161253	1.298752
60	1	0	0.901810	-4.395489	1.366223
61	6	0	0.738954	-2.972037	3.673913
62	1	0	1.813250	-2.827200	3.837655
63	1	0	0.200737	-2.415571	4.449613
64	1	0	0.517348	-4.035824	3.806134

Structure $\mathbf{I2_8}$:

Energy (Hartrees): -2004.304794

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.516785	-1.645293	-0.480940

2	6	0	-1.557061	-1.138764	0.601620
3	6	0	-1.018728	0.275277	-1.149974
4	1	0	-2.135418	-2.619771	-0.801341
5	6	0	-3.941841	-1.748287	-0.013577
6	6	0	-4.634020	-2.952076	-0.161058
7	6	0	-4.576520	-0.641987	0.566131
8	6	0	-5.956184	-3.054699	0.273734
9	1	0	-4.138758	-3.807370	-0.609047
10	6	0	-5.894709	-0.748102	1.001281
11	1	0	-4.043425	0.299652	0.673587
12	6	0	-6.585694	-1.954317	0.854557
13	1	0	-6.488411	-3.991610	0.160127
14	1	0	-6.382431	0.106855	1.453978
15	1	0	-7.611751	-2.033623	1.194434
16	8	0	-1.521630	-1.503134	1.729441
17	7	0	-0.707739	-0.137438	0.055888
18	6	0	-0.203740	1.465372	-1.549120
19	6	0	0.442918	0.610730	0.663165
20	6	0	0.990597	1.302058	-0.592113
21	6	0	-1.000839	2.726316	-1.234373
22	8	0	-2.010108	2.748525	-0.576482
23	8	0	-0.409298	3.790089	-1.748719
24	6	0	-1.025434	5.055676	-1.457356
25	1	0	-1.043413	5.225058	-0.380580
26	1	0	-0.406026	5.799875	-1.950125
27	1	0	-2.040727	5.077984	-1.852994
28	1	0	1.496649	2.240922	-0.380508
29	6	0	1.562996	-0.378832	1.086077
30	6	0	2.061632	0.330960	-1.199806
31	7	0	2.494190	-0.412840	0.119100
32	8	0	1.552082	-0.937504	2.167335
33	6	0	3.671933	-1.203515	0.192765
34	6	0	3.655864	-2.457151	0.821651
35	6	0	4.859809	-0.725104	-0.380423
36	6	0	4.820776	-3.221499	0.875908
37	1	0	2.743209	-2.815837	1.278503
38	6	0	6.013456	-1.506504	-0.327967
39	1	0	4.840550	0.235720	-0.875715
40	6	0	6.002921	-2.752968	0.300673
41	1	0	4.801024	-4.186179	1.371035
42	1	0	6.928204	-1.131932	-0.774273
43	1	0	6.906479	-3.350646	0.345278
44	16	0	-2.298417	-0.510432	-1.927491
45	8	0	2.990307	0.845865	-1.875273
46	8	0	1.250589	-0.682689	-1.898293
47	6	0	1.999419	-1.531925	-2.746563
48	1	0	2.644689	-0.950145	-3.407629
49	1	0	2.615995	-2.228531	-2.167986
50	1	0	1.282106	-2.103159	-3.339479
51	1	0	0.101614	1.446814	-2.595689
52	6	0	-0.067147	1.444450	1.845659
53	1	0	-1.083885	1.788786	1.621283
54	1	0	-0.120099	0.773968	2.712810
55	6	0	0.799942	2.667218	2.197931
56	1	0	0.795059	3.352918	1.336825
57	6	0	2.252654	2.291252	2.516539
58	1	0	2.286124	1.538889	3.311980
59	1	0	2.806804	3.173094	2.853944
60	1	0	2.782967	1.883047	1.648946
61	6	0	0.161901	3.400334	3.384670
62	1	0	-0.872524	3.687760	3.166989
63	1	0	0.724067	4.306944	3.628882
64	1	0	0.156618	2.758444	4.273078

Structure **$I3_8$**:

Energy (Hartrees): -2004.381260

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.759568	-0.585571	0.877927
2	6	0	0.544025	0.358354	0.890636
3	6	0	-0.550363	-0.098501	-1.189313
4	6	0	0.912530	1.459032	-0.133280
5	6	0	-0.103199	1.380007	-1.285703
6	7	0	-0.577319	-0.326653	0.227149
7	6	0	-1.528346	-1.162158	0.741156
8	16	0	-2.234331	-0.499630	-1.796680
9	6	0	-2.553077	-1.563884	-0.332531
10	1	0	-2.343744	-2.603852	-0.593941
11	8	0	-1.608491	-1.546244	1.881311
12	6	0	-3.968009	-1.423208	0.163772
13	6	0	-4.410494	-0.198664	0.682293
14	6	0	-4.845306	-2.507683	0.112905
15	6	0	-5.716483	-0.065838	1.145138
16	1	0	-3.725165	0.644554	0.721528
17	6	0	-6.156973	-2.373217	0.574062
18	1	0	-4.501457	-3.457890	-0.282956
19	6	0	-6.593535	-1.153718	1.089622
20	1	0	-6.051647	0.881771	1.551035
21	1	0	-6.832369	-3.219928	0.531997
22	1	0	-7.610523	-1.049033	1.450079
23	8	0	1.843265	-1.639370	1.437647
24	6	0	4.005338	-0.648439	-0.188911
25	6	0	5.196532	0.048329	0.012826
26	6	0	4.009023	-1.959138	-0.667893
27	6	0	6.409395	-0.577469	-0.272668
28	1	0	5.166080	1.066398	0.384408
29	6	0	5.227210	-2.580363	-0.939233
30	1	0	3.068999	-2.478230	-0.813670
31	6	0	6.426051	-1.891158	-0.744660
32	1	0	7.338821	-0.041337	-0.121400
33	1	0	5.238956	-3.600806	-1.303539
34	1	0	7.370649	-2.377814	-0.958699
35	7	0	2.758073	-0.005657	0.088972
36	6	0	0.180253	0.822219	2.310051
37	1	0	-0.670048	1.505284	2.195424
38	6	0	1.266619	1.505257	3.175832
39	1	0	0.722915	1.765171	4.094867
40	1	0	0.338859	1.613789	-2.253287
41	1	0	0.917876	2.455091	0.302769
42	6	0	-1.285718	2.293075	-1.041297
43	6	0	2.316772	1.118822	-0.601654
44	8	0	0.440641	-0.949291	-1.712892
45	8	0	2.947234	1.707584	-1.439014
46	8	0	-1.688476	2.607566	0.048628
47	8	0	-1.831445	2.689678	-2.186270
48	6	0	0.736765	-0.809388	-3.097108
49	1	0	-0.180049	-0.717800	-3.687627
50	1	0	1.389026	0.049251	-3.281114
51	1	0	1.259907	-1.717406	-3.392790
52	6	0	-3.049921	3.436890	-2.068546
53	1	0	-2.884082	4.341036	-1.482821
54	1	0	-3.339521	3.688418	-3.085525
55	1	0	-3.816554	2.822350	-1.593990
56	1	0	-0.172683	-0.057949	2.853612
57	6	0	2.420151	0.579499	3.593588
58	1	0	2.057476	-0.399319	3.919783
59	1	0	3.134644	0.420367	2.777923
60	1	0	2.976288	1.033571	4.420501
61	6	0	1.827947	2.817828	2.611275
62	1	0	2.516106	2.638698	1.776076
63	1	0	1.032419	3.491936	2.274723
64	1	0	2.400492	3.339067	3.385669

Structures TS_7, TS_9, TS_{10}, $TS_{12\text{-}14}$, $TS_{16\text{-}23}$, $TS1_{11}$, $TS2_{11}$, $TS1_{15}$, $TS2_{15}$, $TS1_8$, $TS2_8$, $TS3_8$ and $TS3_8$.

Structure **TS_7**:

Energy (Hartrees): -2060.332291

One imaginary frequency (cm^{-1}): 425.9572i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.344016	-1.227063	-1.842661
2	6	0	0.528782	-2.075564	0.214991
3	6	0	-1.328980	-0.553925	0.400577
4	6	0	-0.798449	-0.435177	-1.827157
5	6	0	0.943259	-0.804282	0.815943
6	16	0	-1.218085	-2.285849	0.388498
7	6	0	1.401365	-3.246405	0.088149
8	6	0	2.801319	-3.094754	0.081980
9	6	0	0.859686	-4.533339	-0.087135
10	6	0	3.622881	-4.208529	-0.084729
11	1	0	3.232293	-2.110686	0.201008
12	6	0	1.688748	-5.638010	-0.253305
13	1	0	-0.216377	-4.680556	-0.092595
14	6	0	3.076341	-5.481268	-0.250796
15	1	0	4.698416	-4.074765	-0.088628
16	1	0	1.250436	-6.621019	-0.382242
17	1	0	3.722672	-6.341874	-0.378980
18	8	0	2.060961	-0.407379	1.098995
19	7	0	-0.199612	-0.005597	0.914254
20	6	0	-0.433114	1.352943	1.412485
21	7	0	-2.392244	0.286158	0.601505
22	6	0	-1.922463	1.525180	1.088625
23	6	0	-3.699127	0.078899	0.049175
24	6	0	-4.141958	0.928385	-0.966765
25	6	0	-4.491430	-0.967738	0.520294
26	6	0	-5.408256	0.722277	-1.512036
27	1	0	-3.490419	1.719994	-1.319871
28	6	0	-5.748754	-1.175467	-0.048218
29	1	0	-4.138049	-1.596247	1.330759
30	6	0	-6.208185	-0.329280	-1.058985
31	1	0	-5.765017	1.379118	-2.296232
32	1	0	-6.370947	-1.988232	0.306772
33	1	0	-7.188999	-0.487121	-1.492167
34	8	0	-2.598867	2.487899	1.285630
35	1	0	0.156416	2.083552	0.849649
36	6	0	-0.261281	1.502352	2.934308
37	1	0	-0.706436	2.473594	3.193024
38	1	0	-0.869894	0.727201	3.419120
39	6	0	1.175062	1.454119	3.481760
40	1	0	1.599064	0.465188	3.276486
41	6	0	2.067292	2.503566	2.815447
42	1	0	1.640700	3.508245	2.931119
43	1	0	3.062651	2.505244	3.271525
44	1	0	2.198355	2.301701	1.748987
45	6	0	1.126202	1.664734	5.000467
46	1	0	0.491115	0.917861	5.489077
47	1	0	2.128610	1.591027	5.433204
48	1	0	0.727433	2.658273	5.239334
49	1	0	-1.792417	-0.702721	-2.153191
50	1	0	0.434882	-2.228567	-2.238133
51	6	0	-0.379984	0.971793	-1.769509
52	6	0	1.528647	-0.319986	-1.893954
53	7	0	1.024726	0.987040	-1.751649
54	6	0	1.831046	2.157998	-1.659231
55	6	0	1.497894	3.296879	-2.399214
56	6	0	2.955299	2.151714	-0.827281
57	6	0	2.294942	4.435606	-2.299351
58	1	0	0.622776	3.289251	-3.035915
59	6	0	3.753172	3.293318	-0.748579

60	1	0	3.187706	1.262536	-0.252652
61	6	0	3.425196	4.436675	-1.479230
62	1	0	2.034452	5.319993	-2.869087
63	1	0	4.627005	3.288331	-0.107241
64	1	0	4.045163	5.323189	-1.411256
65	8	0	-1.081201	1.957500	-1.678564
66	8	0	2.686942	-0.612524	-2.020186

Structure **TS_9**:

Energy (Hartrees): -2004.307146

One imaginary frequency (cm^{-1}): 330.6952i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.072738	0.816746	-0.443098
2	6	0	-0.894891	1.582049	-0.074717
3	6	0	-0.208470	-0.456709	-0.688031
4	6	0	-0.766927	0.575433	1.921406
5	6	0	-0.215893	-0.671071	1.651148
6	7	0	0.171545	0.844450	-0.566574
7	6	0	1.529658	1.110356	-0.763864
8	16	0	0.974306	-1.471432	-1.494519
9	6	0	2.195803	-0.094784	-1.451179
10	8	0	2.047950	2.163328	-0.539964
11	8	0	-3.248801	1.112357	-0.397592
12	6	0	-2.353072	-1.649746	-0.951116
13	6	0	-1.848436	-2.884194	-0.526517
14	6	0	-3.624882	-1.559709	-1.527252
15	6	0	-2.619669	-4.033608	-0.690879
16	1	0	-0.875338	-2.953697	-0.052395
17	6	0	-4.387204	-2.717064	-1.673107
18	1	0	-4.005724	-0.599263	-1.844233
19	6	0	-3.890189	-3.955016	-1.260907
20	1	0	-2.226664	-4.987521	-0.359962
21	1	0	-5.372732	-2.647771	-2.118469
22	1	0	-4.488220	-4.850544	-1.381807
23	7	0	-1.565790	-0.474647	-0.795500
24	6	0	-0.888349	3.061687	0.113194
25	1	0	-1.837784	3.313483	0.603973
26	6	0	-0.758018	3.881454	-1.193177
27	1	0	0.248363	3.707236	-1.598164
28	1	0	-0.845443	-1.550946	1.673978
29	1	0	-0.129719	1.382447	2.262362
30	6	0	1.212227	-0.938723	1.850859
31	6	0	-2.189246	0.730435	2.319426
32	8	0	-2.907376	-0.367614	2.063058
33	8	0	-2.648430	1.736990	2.799336
34	8	0	1.692933	-2.038044	2.000202
35	8	0	1.950335	0.192334	1.855711
36	6	0	-4.319454	-0.253497	2.262803
37	1	0	-4.711887	0.573654	1.672210
38	1	0	-4.741160	-1.197265	1.923520
39	1	0	-4.539769	-0.096995	3.319894
40	6	0	3.286181	0.083016	2.358214
41	1	0	3.839501	-0.700774	1.845072
42	1	0	3.749218	1.052788	2.189077
43	1	0	3.253082	-0.133264	3.428754
44	1	0	-0.079285	3.347835	0.793315
45	6	0	-1.791717	3.462660	-2.243474
46	1	0	-1.637132	2.431247	-2.579537
47	1	0	-2.806926	3.533256	-1.837922
48	1	0	-1.726085	4.110491	-3.123872
49	6	0	-0.893937	5.371217	-0.860146
50	1	0	-1.897551	5.585254	-0.473801
51	1	0	-0.165555	5.679025	-0.102545
52	1	0	-0.736527	5.986703	-1.751521
53	1	0	2.297229	0.229150	-2.494123
54	6	0	3.564441	-0.459570	-0.909906
55	6	0	3.891720	-1.757338	-0.505129
56	6	0	4.546579	0.542009	-0.860281

57	6	0	5.179733	-2.048765	-0.049172
58	1	0	3.146692	-2.542690	-0.516404
59	6	0	5.824918	0.249639	-0.388467
60	1	0	4.304221	1.550083	-1.174481
61	6	0	6.146993	-1.047428	0.017481
62	1	0	5.416880	-3.059424	0.262207
63	1	0	6.571050	1.034982	-0.345299
64	1	0	7.144234	-1.274871	0.376346

Structure **TS_{10}**:

Energy (Hartrees): -2060.325214

One imaginary frequency (cm^{-1}): 376.2524i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.238786	1.563596	-1.485257
2	6	0	-0.614197	1.609357	0.266083
3	6	0	-0.983527	-0.812276	0.406166
4	6	0	0.188740	0.298814	-2.105633
5	6	0	-1.944047	1.195862	-0.228993
6	16	0	0.147207	0.216383	1.131332
7	6	0	1.441130	-0.355450	-1.966293
8	6	0	1.692652	1.776655	-1.097475
9	6	0	-0.432348	2.950207	0.872245
10	6	0	-1.086144	4.062135	0.312283
11	6	0	0.443833	3.156613	1.948431
12	6	0	-0.869763	5.338261	0.829749
13	1	0	-1.768792	3.925262	-0.516056
14	6	0	0.659161	4.434728	2.456327
15	1	0	0.967930	2.322055	2.403726
16	6	0	0.003078	5.532655	1.899889
17	1	0	-1.383190	6.183631	0.385949
18	1	0	1.344138	4.570618	3.285211
19	1	0	0.172854	6.527798	2.294154
20	7	0	2.334810	0.569408	-1.306834
21	8	0	2.188758	2.792211	-0.674492
22	8	0	1.803946	-1.474758	-2.301048
23	6	0	3.678849	0.290227	-0.946252
24	6	0	4.198018	0.803568	0.249215
25	6	0	4.486233	-0.497302	-1.776557
26	6	0	5.517306	0.532948	0.606476
27	1	0	3.575968	1.425031	0.880914
28	6	0	5.799340	-0.775351	-1.399247
29	1	0	4.079132	-0.894142	-2.695901
30	6	0	6.322402	-0.261165	-0.212006
31	1	0	5.913733	0.941184	1.529238
32	1	0	6.417668	-1.389596	-2.044113
33	1	0	7.347107	-0.474163	0.070359
34	8	0	-2.787516	1.869304	-0.772508
35	7	0	-2.043615	-0.206244	-0.135383
36	6	0	-2.977192	-1.182036	-0.705184
37	7	0	-1.082370	-2.150881	0.352828
38	6	0	-2.270801	-2.495071	-0.346030
39	6	0	-0.135149	-3.090565	0.897543
40	6	0	1.097965	-3.261350	0.269147
41	6	0	-0.488516	-3.810266	2.039229
42	6	0	2.004431	-4.169214	0.818694
43	1	0	1.338903	-2.713475	-0.638233
44	6	0	0.422499	-4.722959	2.567762
45	1	0	-1.458720	-3.657397	2.498355
46	6	0	1.668666	-4.897920	1.960726
47	1	0	2.968373	-4.307042	0.344327
48	1	0	0.160765	-5.292944	3.450851
49	1	0	2.376071	-5.605777	2.376672
50	8	0	-2.644342	-3.606351	-0.544772
51	1	0	-3.003066	-1.070655	-1.793673
52	6	0	-4.387043	-1.180354	-0.096954
53	1	0	-4.863564	-2.108176	-0.443702
54	1	0	-4.292236	-1.252400	0.994135
55	6	0	-5.289082	0.009443	-0.468880

56	1	0	-4.865466	0.922407	-0.036501
57	6	0	-5.383607	0.201588	-1.985247
58	1	0	-5.690313	-0.729100	-2.479786
59	1	0	-6.128571	0.967532	-2.222532
60	1	0	-4.432959	0.535133	-2.410812
61	6	0	-6.678736	-0.225098	0.137088
62	1	0	-6.625974	-0.372952	1.221052
63	1	0	-7.331340	0.631372	-0.055881
64	1	0	-7.148080	-1.112865	-0.303955
65	1	0	-0.622452	-0.124853	-2.677861
66	1	0	-0.289379	2.440461	-1.851229

Structure **TS1$_{11}$**:

Energy (Hartrees): -2060.324821

One imaginary frequency (cm^{-1}): 377.9509i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.054992	0.388568	-1.935204
2	6	0	1.161850	-0.085837	0.812125
3	6	0	-0.261733	1.890696	0.449839
4	6	0	-0.754432	1.482805	-1.389909
5	1	0	0.928805	0.390338	-2.374394
6	1	0	-0.640009	2.507952	-1.732729
7	6	0	1.174040	2.150901	0.200155
8	6	0	-2.186305	1.002611	-1.201241
9	6	0	-0.868995	-0.773390	-1.896256
10	8	0	-0.625248	-1.938638	-2.179422
11	8	0	-3.144693	1.674273	-0.905582
12	7	0	-2.172651	-0.362455	-1.420944
13	6	0	-3.293897	-1.223214	-1.294499
14	6	0	-3.503681	-2.236273	-2.238599
15	6	0	-4.192256	-1.060954	-0.232980
16	6	0	-4.598146	-3.088303	-2.108153
17	1	0	-2.803244	-2.357222	-3.052844
18	6	0	-5.293751	-1.908856	-0.122804
19	1	0	-4.035315	-0.267382	0.486841
20	6	0	-5.498932	-2.928133	-1.054282
21	1	0	-4.750242	-3.872526	-2.840930
22	1	0	-5.991348	-1.772959	0.695774
23	1	0	-6.354001	-3.587927	-0.962182
24	6	0	-1.122794	2.987700	0.955481
25	6	0	-0.959259	4.286115	0.441109
26	6	0	-2.146649	2.756903	1.886810
27	6	0	-1.791651	5.320265	0.865295
28	1	0	-0.175839	4.486170	-0.277954
29	6	0	-2.977697	3.793791	2.301959
30	1	0	-2.306354	1.764865	2.298198
31	6	0	-2.802939	5.081954	1.795685
32	1	0	-1.649056	6.315413	0.459671
33	1	0	-3.763404	3.592973	3.021089
34	1	0	-3.450605	5.888596	2.118826
35	7	0	1.912888	-1.191200	0.960672
36	7	0	1.874859	0.939012	0.349417
37	6	0	3.257234	-0.887772	0.595957
38	6	0	3.269818	0.565726	0.116888
39	1	0	3.913785	1.157443	0.773549
40	6	0	1.441952	-2.464997	1.431370
41	6	0	1.992465	-2.998592	2.596723
42	6	0	0.449616	-3.130983	0.710841
43	6	0	1.529511	-4.230429	3.055128
44	1	0	2.767148	-2.459920	3.129925
45	6	0	-0.016803	-4.353867	1.194759
46	1	0	0.067608	-2.720696	-0.221367
47	6	0	0.521119	-4.902452	2.360227
48	1	0	1.951290	-4.659639	3.955788
49	1	0	-0.792666	-4.877640	0.649974
50	1	0	0.158705	-5.856274	2.725226
51	6	0	3.697911	0.707097	-1.352304

52	1	0	3.043111	0.083924	-1.970622
53	1	0	3.531889	1.754243	-1.635151
54	6	0	5.166889	0.329094	-1.621939
55	1	0	5.286867	-0.748481	-1.456055
56	6	0	6.136905	1.071194	-0.695549
57	1	0	5.953211	2.152452	-0.721802
58	1	0	6.061967	0.728921	0.342098
59	1	0	7.169496	0.900071	-1.014902
60	6	0	5.482105	0.633183	-3.091638
61	1	0	6.493127	0.302310	-3.346819
62	1	0	4.780377	0.128556	-3.763755
63	1	0	5.420231	1.711187	-3.282183
64	8	0	4.164190	-1.655430	0.662514
65	8	0	1.715137	3.157172	-0.192495
66	16	0	-0.420957	0.291964	1.280164

Structure **TS2$_{11}$**:

Energy (Hartrees): -2060.329349

One imaginary frequency (cm^{-1}): 125.9205i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.066949	0.283870	-1.806099
2	6	0	1.049246	-0.204518	0.779726
3	6	0	-0.032868	1.937798	0.214100
4	6	0	-0.521486	1.530263	-1.280456
5	1	0	1.035674	0.199171	-2.273213
6	1	0	-0.363058	2.441046	-1.865530
7	6	0	1.496318	1.961720	0.119177
8	6	0	-2.019917	1.209308	-1.174413
9	6	0	-0.916967	-0.693143	-1.961905
10	8	0	-0.876767	-1.857820	-2.361816
11	8	0	-2.883231	1.980520	-0.821216
12	7	0	-2.177899	-0.116142	-1.492631
13	6	0	-3.367104	-0.858322	-1.261517
14	6	0	-3.749950	-1.886627	-2.131482
15	6	0	-4.149379	-0.571974	-0.134166
16	6	0	-4.904459	-2.622931	-1.862365
17	1	0	-3.135409	-2.110727	-2.991620
18	6	0	-5.307545	-1.303945	0.114613
19	1	0	-3.858193	0.230655	0.530561
20	6	0	-5.689038	-2.335473	-0.744690
21	1	0	-5.193721	-3.420819	-2.537194
22	1	0	-5.908792	-1.068339	0.985530
23	1	0	-6.589436	-2.905814	-0.546561
24	6	0	-0.627990	3.228576	0.720469
25	6	0	-0.345420	4.413534	0.024324
26	6	0	-1.483502	3.279508	1.825859
27	6	0	-0.898364	5.622892	0.441563
28	1	0	0.313478	4.396290	-0.834791
29	6	0	-2.040834	4.489704	2.235122
30	1	0	-1.731683	2.379463	2.377550
31	6	0	-1.748781	5.666021	1.546445
32	1	0	-0.667878	6.530110	-0.104761
33	1	0	-2.706480	4.508117	3.090086
34	1	0	-2.182768	6.606571	1.865335
35	7	0	1.587160	-1.412704	0.984535
36	7	0	1.979792	0.685863	0.396774
37	6	0	2.988599	-1.358354	0.705242
38	6	0	3.297103	0.069184	0.248242
39	1	0	3.989969	0.528991	0.958526
40	6	0	0.856410	-2.591978	1.368295
41	6	0	1.145432	-3.211609	2.583997
42	6	0	-0.124122	-3.079688	0.504065
43	6	0	0.420958	-4.346872	2.945053
44	1	0	1.918790	-2.814006	3.230756
45	6	0	-0.853712	-4.203702	0.890426
46	1	0	-0.300007	-2.615781	-0.463277
47	6	0	-0.582375	-4.835910	2.104892

48	1	0	0.635555	-4.843775	3.883371
49	1	0	-1.625089	-4.582357	0.230912
50	1	0	-1.148764	-5.713029	2.395137
51	6	0	3.847889	0.137329	-1.184969
52	1	0	3.156966	-0.384847	-1.855750
53	1	0	3.863425	1.195285	-1.476758
54	6	0	5.263927	-0.449469	-1.340724
55	1	0	5.224750	-1.524472	-1.126890
56	6	0	6.268239	0.201385	-0.381692
57	1	0	6.239701	1.294484	-0.471648
58	1	0	6.080371	-0.065189	0.663699
59	1	0	7.284919	-0.126636	-0.618586
60	6	0	5.711373	-0.261232	-2.795542
61	1	0	6.688042	-0.725216	-2.961492
62	1	0	4.999092	-0.710446	-3.495063
63	1	0	5.797730	0.805112	-3.036223
64	8	0	3.731480	-2.278755	0.821816
65	8	0	2.191783	2.871282	-0.235200
66	16	0	-0.446153	0.461447	1.258059

Structure **TS_{12}**:

Energy (Hartrees): -2060.329467

One imaginary frequency (cm^{-1}): 407.5961i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.844638	-0.085879	-1.701387
2	6	0	-1.409023	-0.647858	0.458284
3	6	0	-1.520247	1.758805	0.511837
4	6	0	-0.825409	1.296258	-1.585857
5	6	0	-0.303342	1.270000	1.169244
6	6	0	-1.930641	3.164626	0.495914
7	6	0	-0.969633	4.185147	0.632419
8	6	0	-3.275785	3.524916	0.294887
9	6	0	-1.358561	5.522409	0.576029
10	1	0	0.069113	3.924770	0.778154
11	6	0	-3.653510	4.862977	0.239185
12	1	0	-4.037882	2.758902	0.184898
13	6	0	-2.695772	5.869439	0.382079
14	1	0	-0.606588	6.295929	0.681071
15	1	0	-4.695898	5.119276	0.088049
16	1	0	-2.989806	6.911842	0.341329
17	7	0	-1.405408	-2.011531	0.587897
18	7	0	-0.327027	-0.125486	1.079915
19	6	0	-0.205175	-2.427207	1.201082
20	6	0	0.511387	-1.161507	1.692143
21	1	0	0.358107	-1.101418	2.778741
22	6	0	-2.315469	-2.884935	-0.094479
23	6	0	-3.630522	-2.992797	0.357380
24	6	0	-1.861950	-3.599249	-1.204647
25	6	0	-4.514498	-3.828459	-0.325538
26	1	0	-3.947324	-2.443252	1.237510
27	6	0	-2.750999	-4.444106	-1.868400
28	1	0	-0.834410	-3.476366	-1.531397
29	6	0	-4.073894	-4.555669	-1.432932
30	1	0	-5.539443	-3.918622	0.013468
31	1	0	-2.411866	-5.010353	-2.727435
32	1	0	-4.760919	-5.211134	-1.955391
33	6	0	2.008790	-1.077184	1.368150
34	1	0	2.238877	-1.699921	0.495102
35	1	0	2.221002	-0.038544	1.099796
36	6	0	2.917288	-1.460765	2.548214
37	1	0	2.661522	-0.798286	3.389113
38	6	0	4.375035	-1.199722	2.153172
39	1	0	4.648085	-1.803079	1.279090
40	1	0	4.533566	-0.147550	1.896241
41	1	0	5.054432	-1.460456	2.970970
42	6	0	2.727593	-2.913296	2.996901
43	1	0	3.400869	-3.145324	3.828880

44	1	0	1.703343	-3.118241	3.323977
45	1	0	2.947574	-3.601461	2.173554
46	8	0	0.144906	-3.562719	1.314265
47	8	0	0.637583	1.887877	1.636097
48	16	0	-2.731336	0.477590	0.461434
49	6	0	0.542137	-0.571322	-1.633878
50	6	0	0.598095	1.732877	-1.537812
51	7	0	1.372928	0.555003	-1.480884
52	1	0	-1.572259	1.991638	-1.940570
53	1	0	-1.620968	-0.704650	-2.126018
54	6	0	2.797500	0.543387	-1.439658
55	6	0	3.517928	-0.379638	-2.203984
56	6	0	3.466340	1.468571	-0.629400
57	6	0	4.911831	-0.375731	-2.149527
58	1	0	2.994126	-1.097334	-2.821081
59	6	0	4.859892	1.475023	-0.601177
60	1	0	2.894639	2.165511	-0.028783
61	6	0	5.587160	0.552301	-1.355953
62	1	0	5.468106	-1.096742	-2.737243
63	1	0	5.375484	2.196683	0.021968
64	1	0	6.670507	0.555726	-1.324275
65	8	0	0.924464	-1.722156	-1.647304
66	8	0	1.031108	2.854078	-1.547423

Structure **TS_{13}**:

Energy (Hartrees): -2060.330637

One imaginary frequency (cm^{-1}): 312.6149i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.476332	1.379035	0.748204
2	6	0	0.549121	1.740561	-0.237718
3	6	0	0.681493	-0.481807	0.199171
4	6	0	-0.384228	1.517044	-1.952741
5	6	0	-0.255694	0.198983	-2.433964
6	7	0	1.382249	0.583768	-0.250105
7	6	0	2.450191	0.256276	-1.086722
8	16	0	1.411469	-2.027122	0.005619
9	6	0	2.763346	-1.243223	-0.996804
10	1	0	2.672329	-1.648667	-2.006287
11	8	0	3.055309	1.047485	-1.745868
12	6	0	4.142736	-1.489617	-0.443482
13	6	0	4.509433	-0.967784	0.803823
14	6	0	5.065903	-2.226830	-1.187737
15	6	0	5.792498	-1.182953	1.298619
16	1	0	3.790849	-0.396146	1.386426
17	6	0	6.352020	-2.442848	-0.688920
18	1	0	4.781232	-2.625866	-2.155784
19	6	0	6.715364	-1.922505	0.552450
20	1	0	6.074191	-0.776455	2.262667
21	1	0	7.065503	-3.014468	-1.270504
22	1	0	7.713754	-2.089379	0.939437
23	8	0	-1.289040	2.035134	1.337034
24	6	0	-1.368915	-0.887943	1.527672
25	6	0	-1.964103	-1.965339	0.869752
26	6	0	-1.729709	-0.531971	2.828210
27	6	0	-2.936803	-2.705124	1.542191
28	1	0	-1.717226	-2.195225	-0.162797
29	6	0	-2.710497	-1.275696	3.481184
30	1	0	-1.262107	0.318485	3.308286
31	6	0	-3.312947	-2.360971	2.841198
32	1	0	-3.417030	-3.532334	1.034057
33	1	0	-3.004160	-1.003700	4.487852
34	1	0	-4.081153	-2.930449	3.351050
35	7	0	-0.403471	-0.077882	0.841165
36	6	0	1.180533	3.105764	-0.174507
37	1	0	0.370341	3.813896	0.046413
38	6	0	2.297956	3.244016	0.880801
39	1	0	3.127047	2.589290	0.573331

40	1	0	1.587635	3.371967	-1.155721
41	6	0	2.804899	4.690567	0.888509
42	1	0	3.647481	4.806290	1.577111
43	1	0	2.009153	5.372658	1.210067
44	1	0	3.136338	5.000868	-0.107701
45	6	0	1.837047	2.824168	2.281772
46	1	0	1.593677	1.755534	2.333737
47	1	0	0.946675	3.387913	2.583046
48	1	0	2.626182	3.014763	3.016373
49	1	0	0.083393	2.376504	-2.421589
50	1	0	0.559552	-0.223277	-3.001848
51	6	0	-1.843898	1.679616	-1.583538
52	6	0	-1.449747	-0.530021	-2.162965
53	8	0	-1.725782	-1.706182	-2.345988
54	8	0	-2.417701	2.707167	-1.329183
55	7	0	-2.381755	0.398662	-1.568709
56	6	0	-3.678491	0.064550	-1.092370
57	6	0	-4.465197	-0.869506	-1.774015
58	6	0	-4.143536	0.648994	0.092728
59	6	0	-5.711651	-1.225240	-1.258071
60	1	0	-4.091845	-1.321089	-2.682724
61	6	0	-5.396486	0.295875	0.588708
62	1	0	-3.521525	1.365592	0.617472
63	6	0	-6.182902	-0.645527	-0.079798
64	1	0	-6.316465	-1.953894	-1.786110
65	1	0	-5.752709	0.750119	1.506360
66	1	0	-7.154504	-0.922914	0.313218

Structure **TS_{14}**:

Energy (Hartrees): -2060.332967

One imaginary frequency (cm^{-1}): 324.7386i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.563500	-1.083595	0.808163
2	6	0	1.152726	-1.336484	1.093220
3	6	0	1.294827	0.516354	-0.166472
4	6	0	0.922135	-2.330828	-0.779929
5	6	0	1.000111	-1.354998	-1.772882
6	7	0	0.505419	-0.156835	0.704697
7	6	0	-0.819031	0.296271	0.795978
8	16	0	0.617179	1.991903	-0.790455
9	6	0	-1.044298	1.458150	-0.175704
10	8	0	-1.638055	-0.169162	1.529734
11	8	0	3.543270	-1.749345	1.053803
12	6	0	3.710161	0.608342	-0.691170
13	6	0	4.534102	-0.282869	-1.382280
14	6	0	3.973762	1.979726	-0.688860
15	6	0	5.626767	0.214937	-2.089862
16	1	0	4.330053	-1.345865	-1.348436
17	6	0	5.061116	2.466509	-1.412658
18	1	0	3.350630	2.653790	-0.111654
19	6	0	5.887485	1.586387	-2.112716
20	1	0	6.272079	-0.470647	-2.625781
21	1	0	5.267501	3.529929	-1.418044
22	1	0	6.736181	1.966701	-2.668995
23	7	0	2.573213	0.107900	0.017107
24	6	0	0.715355	-2.167694	2.256743
25	1	0	1.434789	-2.993942	2.333488
26	6	0	0.679915	-1.403871	3.601924
27	1	0	-0.103233	-0.637553	3.527451
28	1	0	-0.266655	-2.612369	2.066956
29	6	0	0.295622	-2.380909	4.718056
30	1	0	0.203246	-1.860527	5.676495
31	1	0	1.061801	-3.157622	4.828671
32	1	0	-0.658920	-2.873089	4.505442
33	6	0	2.014361	-0.718553	3.913584
34	1	0	2.247894	0.070328	3.189372
35	1	0	2.836409	-1.443192	3.898616

36	1	0	1.984090	-0.255982	4.905441
37	1	0	1.861358	-1.054442	-2.350740
38	1	0	1.653986	-3.103692	-0.577746
39	6	0	-0.530863	-2.674496	-0.619532
40	6	0	-0.337745	-0.975463	-2.177126
41	7	0	-1.245676	-1.742910	-1.379830
42	8	0	-1.008205	-3.566530	0.036136
43	8	0	-0.693641	-0.148224	-2.989640
44	6	0	-2.666596	-1.655197	-1.444205
45	6	0	-3.303864	-1.352453	-2.655313
46	6	0	-3.426401	-1.863554	-0.285515
47	6	0	-4.693643	-1.245249	-2.694429
48	1	0	-2.717627	-1.192729	-3.549123
49	6	0	-4.815651	-1.766257	-0.343513
50	1	0	-2.934395	-2.100254	0.647458
51	6	0	-5.454915	-1.453111	-1.543428
52	1	0	-5.180427	-1.008902	-3.633705
53	1	0	-5.395119	-1.933409	0.557018
54	1	0	-6.535403	-1.375487	-1.582113
55	1	0	-1.556662	1.020745	-1.039959
56	6	0	-1.881386	2.564253	0.405093
57	6	0	-3.199690	2.705067	-0.037004
58	6	0	-1.386453	3.413964	1.401543
59	6	0	-4.019323	3.692584	0.509935
60	1	0	-3.582617	2.037012	-0.802218
61	6	0	-2.205978	4.401287	1.943972
62	1	0	-0.362134	3.306355	1.745732
63	6	0	-3.522942	4.542633	1.498130
64	1	0	-5.040662	3.796012	0.163159
65	1	0	-1.819388	5.059740	2.713016
66	1	0	-4.158291	5.312348	1.920966

Structure $\mathbf{TS1_{15}}$:

Energy (Hartrees): -2060.333031

One imaginary frequency (cm^{-1}): 312.4695i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.688312	1.914437	0.044632
2	6	0	-0.629586	1.923573	-0.607799
3	6	0	-0.627479	0.392820	1.072660
4	6	0	-0.418879	0.657450	-2.087285
5	6	0	-0.844296	-0.632326	-1.709221
6	7	0	-1.425274	1.167102	0.306005
7	6	0	-2.730802	0.681030	0.172966
8	16	0	-1.391016	-0.818238	2.019507
9	6	0	-3.004732	-0.411811	1.223263
10	8	0	-3.525272	1.102019	-0.611910
11	8	0	1.677568	2.564288	-0.136790
12	6	0	1.766048	0.243314	1.667826
13	6	0	1.980417	-1.135850	1.627495
14	6	0	2.667558	1.108420	2.288496
15	6	0	3.124328	-1.654072	2.232345
16	1	0	1.305148	-1.790359	1.082299
17	6	0	3.812040	0.574353	2.878141
18	1	0	2.483183	2.175102	2.291708
19	6	0	4.041017	-0.802671	2.851461
20	1	0	3.310126	-2.720294	2.188054
21	1	0	4.524777	1.237064	3.354049
22	1	0	4.937964	-1.210852	3.302358
23	7	0	0.626878	0.800233	0.996300
24	6	0	-1.169920	3.221615	-1.151450
25	1	0	-0.330695	3.723103	-1.652937
26	6	0	-1.781392	4.161515	-0.092787
27	1	0	-2.668243	3.660412	0.322538
28	1	0	-1.927263	3.014029	-1.915030
29	6	0	-2.236163	5.456545	-0.774724
30	1	0	-2.741774	6.116441	-0.063052
31	1	0	-1.373272	5.996626	-1.181951

32	1	0	-2.927497	5.250702	-1.598376
33	6	0	-0.810880	4.465689	1.053759
34	1	0	-0.571728	3.569450	1.638533
35	1	0	0.128113	4.879352	0.668494
36	1	0	-1.248120	5.196187	1.742092
37	1	0	-0.938328	1.268247	-2.818239
38	1	0	-1.852550	-1.015545	-1.697069
39	6	0	1.079655	0.549511	-2.273379
40	6	0	0.281607	-1.416480	-1.344254
41	8	0	0.348017	-2.531583	-0.836577
42	8	0	1.800157	1.338814	-2.827377
43	7	0	1.460000	-0.639644	-1.660094
44	6	0	2.803303	-1.046756	-1.439279
45	6	0	3.167558	-2.390843	-1.569528
46	6	0	3.751733	-0.095629	-1.038878
47	6	0	4.476245	-2.780523	-1.281230
48	1	0	2.426865	-3.118963	-1.870540
49	6	0	5.057138	-0.496540	-0.766228
50	1	0	3.461402	0.943556	-0.932812
51	6	0	5.424458	-1.839696	-0.879740
52	1	0	4.752351	-3.824692	-1.377922
53	1	0	5.784689	0.243087	-0.451147
54	1	0	6.440358	-2.147501	-0.659019
55	1	0	-3.622027	0.064413	1.990976
56	6	0	-3.723447	-1.610197	0.648129
57	6	0	-5.122226	-1.606845	0.677468
58	6	0	-3.039996	-2.681232	0.058642
59	6	0	-5.838203	-2.661788	0.113125
60	1	0	-5.649168	-0.777357	1.138115
61	6	0	-3.762691	-3.735087	-0.501449
62	1	0	-1.952975	-2.703375	0.027900
63	6	0	-5.158431	-3.728098	-0.476697
64	1	0	-6.921551	-2.651004	0.138468
65	1	0	-3.229833	-4.560385	-0.958729
66	1	0	-5.712471	-4.550757	-0.914001

Structure **TS2$_{15}$**:

Energy (Hartrees): -2060.334654

One imaginary frequency (cm^{-1}): 138.1629i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.705401	1.853454	0.083796
2	6	0	-0.598291	1.841298	-0.684408
3	6	0	-0.673301	0.350581	1.026739
4	6	0	-0.381277	0.701507	-1.914653
5	6	0	-0.770087	-0.644628	-1.498569
6	7	0	-1.453067	1.190182	0.298598
7	6	0	-2.763239	0.725963	0.145891
8	16	0	-1.478383	-0.799321	2.010640
9	6	0	-3.071607	-0.369106	1.187932
10	8	0	-3.539001	1.154383	-0.652948
11	8	0	1.681925	2.520508	-0.051171
12	6	0	1.698604	0.189945	1.738790
13	6	0	1.932984	-1.184734	1.672739
14	6	0	2.545173	1.047724	2.442336
15	6	0	3.040353	-1.705522	2.341289
16	1	0	1.301522	-1.832233	1.069174
17	6	0	3.653761	0.510657	3.094182
18	1	0	2.345052	2.111684	2.466485
19	6	0	3.900759	-0.862747	3.046068
20	1	0	3.241493	-2.768162	2.281917
21	1	0	4.322803	1.166831	3.637771
22	1	0	4.768634	-1.274264	3.547942
23	7	0	0.593646	0.755981	1.016695
24	6	0	-1.064486	3.183161	-1.214700
25	1	0	-0.191070	3.648344	-1.693457
26	6	0	-1.667164	4.139935	-0.169900
27	1	0	-2.588317	3.676505	0.212146

28	1	0	-1.808048	3.007549	-1.999301
29	6	0	-2.045265	5.454145	-0.863781
30	1	0	-2.543397	6.134250	-0.166140
31	1	0	-1.149131	5.957561	-1.244891
32	1	0	-2.720478	5.277687	-1.707304
33	6	0	-0.732276	4.407881	1.014975
34	1	0	-0.548397	3.503677	1.607730
35	1	0	0.233935	4.793583	0.670951
36	1	0	-1.175488	5.149632	1.687261
37	1	0	-0.900092	1.152096	-2.760772
38	1	0	-1.771578	-1.044956	-1.519366
39	6	0	1.116631	0.564494	-2.201392
40	6	0	0.357151	-1.442537	-1.288739
41	8	0	0.479233	-2.592447	-0.863271
42	8	0	1.807713	1.370834	-2.772796
43	7	0	1.521182	-0.631035	-1.638654
44	6	0	2.874333	-1.030968	-1.471355
45	6	0	3.255888	-2.357630	-1.695847
46	6	0	3.815423	-0.093205	-1.026459
47	6	0	4.576591	-2.742399	-1.461919
48	1	0	2.517570	-3.074761	-2.026858
49	6	0	5.133108	-0.487402	-0.808556
50	1	0	3.512396	0.933030	-0.850494
51	6	0	5.518677	-1.813300	-1.019911
52	1	0	4.867154	-3.773045	-1.632692
53	1	0	5.856329	0.242224	-0.462048
54	1	0	6.544249	-2.117364	-0.842909
55	1	0	-3.694387	0.112846	1.947565
56	6	0	-3.801222	-1.554020	0.595719
57	6	0	-5.198813	-1.498217	0.551414
58	6	0	-3.131108	-2.663042	0.064521
59	6	0	-5.924539	-2.538101	-0.028064
60	1	0	-5.716767	-0.639227	0.965732
61	6	0	-3.863391	-3.702084	-0.510428
62	1	0	-2.045849	-2.722817	0.084916
63	6	0	-5.257132	-3.642461	-0.558984
64	1	0	-7.006511	-2.485886	-0.060366
65	1	0	-3.339480	-4.556301	-0.922662
66	1	0	-5.819134	-4.453344	-1.007904

Structure **TS_{16}**:

Energy (Hartrees): -2060.335014

One imaginary frequency (cm^{-1}): 320.3653i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.831486	0.955346	-0.518762
2	6	0	1.523320	1.599151	-0.446839
3	6	0	1.427568	-0.368164	0.664775
4	6	0	0.844463	0.730989	-2.175689
5	6	0	0.866814	-0.659742	-2.070239
6	7	0	0.818893	0.817808	0.499503
7	6	0	-0.418633	0.959902	1.143831
8	16	0	0.626115	-1.500655	1.693190
9	6	0	-0.646991	-0.223523	2.092397
10	8	0	-1.130964	1.909276	1.030329
11	8	0	3.834222	1.267884	-1.112088
12	6	0	3.576687	-1.406041	0.087098
13	6	0	3.086658	-2.683839	-0.200712
14	6	0	4.939604	-1.178938	0.286324
15	6	0	3.981100	-3.751611	-0.267471
16	1	0	2.030127	-2.840069	-0.399271
17	6	0	5.821538	-2.254178	0.200665
18	1	0	5.294697	-0.178660	0.498012
19	6	0	5.345900	-3.539285	-0.069338
20	1	0	3.608334	-4.744402	-0.488527
21	1	0	6.881265	-2.086521	0.350518
22	1	0	6.037925	-4.370774	-0.130395
23	7	0	2.668358	-0.307465	0.166191

24	6	0	1.378870	3.090824	-0.499717
25	1	0	2.111614	3.443826	-1.238325
26	6	0	1.636026	3.811941	0.842400
27	1	0	0.833876	3.525756	1.537079
28	1	0	0.385211	3.359828	-0.872789
29	6	0	1.554388	5.325631	0.616649
30	1	0	1.659200	5.868040	1.561481
31	1	0	2.357358	5.654932	-0.053527
32	1	0	0.597863	5.608342	0.165634
33	6	0	2.985194	3.428001	1.459715
34	1	0	3.023845	2.367951	1.737599
35	1	0	3.802615	3.621086	0.755083
36	1	0	3.174000	4.011270	2.366864
37	1	0	-0.372289	0.164686	3.079340
38	6	0	-2.073626	-0.708934	2.110182
39	6	0	-2.949428	-0.125047	3.033114
40	6	0	-2.548460	-1.663450	1.204623
41	6	0	-4.296196	-0.484431	3.044971
42	1	0	-2.578493	0.614728	3.735321
43	6	0	-3.895814	-2.025601	1.227551
44	1	0	-1.883881	-2.113868	0.472538
45	6	0	-4.770540	-1.437016	2.141353
46	1	0	-4.970285	-0.025440	3.758868
47	1	0	-4.261003	-2.754995	0.514275
48	1	0	-5.817768	-1.717617	2.147970
49	1	0	1.697026	-1.323174	-2.258804
50	1	0	1.493184	1.324649	-2.811262
51	6	0	-0.612949	1.134730	-2.092682
52	6	0	-0.435127	-1.143886	-1.731800
53	7	0	-1.315621	-0.001246	-1.703317
54	8	0	-1.083256	2.221406	-2.321022
55	8	0	-0.812868	-2.276686	-1.485296
56	6	0	-2.737349	-0.076616	-1.632632
57	6	0	-3.449783	0.915960	-0.951551
58	6	0	-3.414579	-1.138206	-2.243116
59	6	0	-4.839627	0.839069	-0.879008
60	1	0	-2.916443	1.732601	-0.483098
61	6	0	-4.804443	-1.209013	-2.155021
62	1	0	-2.856063	-1.903987	-2.764635
63	6	0	-5.521643	-0.223956	-1.473883
64	1	0	-5.386911	1.609257	-0.347730
65	1	0	-5.325423	-2.034113	-2.627750
66	1	0	-6.602472	-0.281988	-1.410655

Structure **TS_{17}**:

Energy (Hartrees): -2004.304820

One imaginary frequency (cm^{-1}): 428.0383i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.570343	0.217604	-0.507526
2	6	0	0.772764	-0.316867	-0.510129
3	6	0	-1.349527	-0.341050	1.515303
4	6	0	-0.063983	-0.884627	1.666204
5	1	0	0.102570	-1.948774	1.563528
6	16	0	-0.588152	-1.070478	-1.237521
7	7	0	0.591903	1.018270	-0.355160
8	6	0	-0.742495	1.424011	-0.317060
9	8	0	-1.088704	2.558975	-0.050238
10	6	0	-3.004502	0.272576	-0.837354
11	6	0	-3.778402	1.397316	-0.498039
12	6	0	-3.644577	-0.833958	-1.424065
13	6	0	-5.148229	1.409067	-0.756397
14	1	0	-3.302819	2.252980	-0.038573
15	6	0	-5.013809	-0.813795	-1.676580
16	1	0	-3.076191	-1.724072	-1.679411
17	6	0	-5.772998	0.309729	-1.344955
18	1	0	-5.729244	2.284396	-0.489355
19	1	0	-5.485715	-1.675637	-2.135301

20	1	0	-6.838845	0.325336	-1.540897
21	6	0	1.865012	1.702820	-0.127121
22	6	0	2.853570	0.533450	-0.256088
23	1	0	1.905506	2.100121	0.888656
24	6	0	2.219792	2.787888	-1.152379
25	1	0	2.101635	2.368703	-2.159435
26	6	0	1.444016	4.112596	-1.033802
27	1	0	0.400466	3.936353	-1.315356
28	7	0	2.102238	-0.615833	-0.560344
29	6	0	2.638970	-1.930976	-0.760309
30	6	0	2.518606	-2.529186	-2.015506
31	6	0	3.266787	-2.580315	0.302626
32	6	0	3.030120	-3.812365	-2.206173
33	1	0	2.044244	-1.991769	-2.830147
34	6	0	3.789000	-3.856587	0.093362
35	1	0	3.318426	-2.086246	1.266366
36	6	0	3.668379	-4.472713	-1.154101
37	1	0	2.938964	-4.288589	-3.175012
38	1	0	4.283615	-4.371275	0.908392
39	1	0	4.072746	-5.466705	-1.306605
40	8	0	4.044425	0.586129	-0.185929
41	1	0	-1.551127	0.631338	1.952487
42	6	0	-2.554292	-1.215031	1.572810
43	6	0	1.000430	-0.161682	2.341145
44	8	0	-3.594332	-0.881892	2.078056
45	8	0	2.125571	-0.589243	2.519674
46	8	0	0.647504	1.081702	2.734544
47	8	0	-2.358589	-2.412255	1.005782
48	6	0	1.630658	1.806748	3.474928
49	1	0	2.574485	1.869948	2.929444
50	1	0	1.813777	1.320438	4.434704
51	1	0	1.211519	2.798307	3.632469
52	6	0	-3.484859	-3.294466	1.031681
53	1	0	-4.343552	-2.829412	0.545553
54	1	0	-3.742982	-3.547018	2.061152
55	1	0	-3.174286	-4.185924	0.491030
56	1	0	3.290197	2.994013	-1.008685
57	6	0	2.057562	5.125996	-2.008420
58	1	0	1.481746	6.056441	-2.014130
59	1	0	2.077820	4.736085	-3.031970
60	1	0	3.087439	5.367696	-1.718277
61	6	0	1.457763	4.651390	0.400506
62	1	0	2.481659	4.691740	0.796071
63	1	0	0.841999	4.033340	1.061065
64	1	0	1.047911	5.666013	0.430644

Structure $\mathbf{TS_{18}}$:

Energy (Hartrees): -2004.301343

One imaginary frequency (cm^{-1}): 434.2607i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.364730	-0.950590	-0.724360
2	6	0	0.783771	0.097214	-0.444780
3	6	0	-0.917624	-1.028518	1.503256
4	1	0	-1.106263	-2.094612	1.482672
5	6	0	0.383145	-0.545096	1.640559
6	16	0	0.269637	-1.377152	-1.199829
7	7	0	-0.218452	1.019788	-0.499733
8	6	0	-1.500552	0.507222	-0.666019
9	8	0	-2.507744	1.196385	-0.659006
10	6	0	-2.459186	-1.898853	-0.942410
11	6	0	-2.186322	-3.277070	-1.041469
12	6	0	-3.796586	-1.467256	-1.004953
13	6	0	-3.215956	-4.194728	-1.215651
14	1	0	-1.164423	-3.635723	-0.960102
15	6	0	-4.822436	-2.396852	-1.176135
16	1	0	-4.021435	-0.413187	-0.917131
17	6	0	-4.541132	-3.757983	-1.286551

18	1	0	-2.985400	-5.251492	-1.288724
19	1	0	-5.848451	-2.049804	-1.220496
20	1	0	-5.343931	-4.474096	-1.419025
21	6	0	0.277516	2.353545	-0.190571
22	6	0	1.790939	2.129309	-0.322837
23	1	0	0.068992	2.571191	0.866592
24	6	0	-2.084694	-0.226819	1.943248
25	8	0	-3.194413	-0.672003	2.091141
26	6	0	-0.247725	3.475536	-1.093733
27	1	0	-0.516391	3.039007	-2.062458
28	6	0	-1.442999	4.244552	-0.501928
29	1	0	-2.177594	3.506777	-0.157168
30	7	0	1.999933	0.756491	-0.498768
31	6	0	3.278559	0.129320	-0.652444
32	6	0	3.496360	-0.732731	-1.729082
33	6	0	4.288828	0.390724	0.273932
34	6	0	4.733413	-1.365160	-1.859671
35	1	0	2.719823	-0.891771	-2.469204
36	6	0	5.526637	-0.229479	0.122476
37	1	0	4.092210	1.047591	1.110730
38	6	0	5.748404	-1.113951	-0.935886
39	1	0	4.904368	-2.040682	-2.689317
40	1	0	6.312107	-0.034303	0.842367
41	1	0	6.710391	-1.601650	-1.041898
42	8	0	2.646485	2.966091	-0.281764
43	1	0	0.532192	0.452609	2.037136
44	8	0	-1.771433	1.064742	2.145597
45	6	0	-2.873745	1.926001	2.446613
46	1	0	-2.451623	2.923454	2.554912
47	1	0	-3.350302	1.618381	3.378513
48	1	0	-3.598651	1.901801	1.632761
49	6	0	1.538144	-1.428070	1.873729
50	8	0	2.591938	-1.042706	2.326026
51	8	0	1.317049	-2.704411	1.525347
52	6	0	2.448301	-3.573208	1.626272
53	1	0	2.808869	-3.617055	2.654260
54	1	0	3.251811	-3.224811	0.974203
55	1	0	2.098740	-4.551984	1.305488
56	1	0	0.576129	4.181974	-1.266338
57	6	0	-1.004740	5.121164	0.677389
58	1	0	-0.299646	5.890559	0.339854
59	1	0	-0.510634	4.545514	1.468671
60	1	0	-1.865620	5.626799	1.127033
61	6	0	-2.088824	5.102098	-1.595003
62	1	0	-2.925197	5.683376	-1.194313
63	1	0	-2.469915	4.478751	-2.410240
64	1	0	-1.360390	5.807178	-2.014678

Structure **TS_{19}**:

Energy (Hartrees): -2004.305449

One imaginary frequency (cm^{-1}): 404.5845i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.302882	-0.407511	1.452635
2	6	0	1.794502	-0.515287	-0.779486
3	6	0	-0.598720	-0.241268	-0.636120
4	6	0	-0.083227	-0.436816	1.537682
5	7	0	-1.961437	-0.049850	-0.818573
6	7	0	0.036489	0.946006	-0.847786
7	16	0	0.431646	-1.546468	-1.148159
8	6	0	-0.889787	2.055648	-1.014976
9	1	0	-0.719715	2.513012	-1.994542
10	6	0	-2.224228	1.312352	-1.044913
11	6	0	-2.973587	-1.057110	-0.724818
12	6	0	-4.129257	-0.791893	0.015883
13	6	0	-2.814908	-2.280011	-1.379928
14	6	0	-5.135364	-1.752139	0.082979
15	1	0	-4.233268	0.154456	0.530050

16	6	0	-3.819425	-3.245681	-1.284554
17	1	0	-1.938231	-2.476396	-1.985788
18	6	0	-4.983188	-2.981828	-0.562922
19	1	0	-6.034997	-1.540881	0.649011
20	1	0	-3.693568	-4.195434	-1.790526
21	1	0	-5.766357	-3.728492	-0.502674
22	8	0	-3.312315	1.787927	-1.211969
23	6	0	-0.791930	3.113351	0.096896
24	1	0	0.228569	3.513986	0.060031
25	1	0	-0.890521	2.618815	1.069054
26	6	0	-1.811444	4.260356	-0.022327
27	1	0	-2.816154	3.856404	0.152097
28	6	0	-1.795645	4.906367	-1.412778
29	1	0	-0.777560	5.205397	-1.692315
30	1	0	-2.422451	5.803839	-1.424780
31	1	0	-2.184797	4.228668	-2.179631
32	6	0	-1.511486	5.300944	1.063215
33	1	0	-0.531103	5.761831	0.894030
34	1	0	-1.501199	4.846952	2.059646
35	1	0	-2.265222	6.094720	1.058395
36	6	0	1.420262	0.889268	-0.962591
37	8	0	2.121055	1.880204	-1.090084
38	6	0	3.155092	-1.052822	-0.867099
39	6	0	3.389345	-2.413021	-0.593345
40	6	0	4.247393	-0.224558	-1.180462
41	6	0	4.678358	-2.934297	-0.642001
42	1	0	2.560874	-3.058535	-0.315624
43	6	0	5.535745	-0.755644	-1.223649
44	1	0	4.077321	0.825118	-1.380674
45	6	0	5.758391	-2.107585	-0.959750
46	1	0	4.840656	-3.983635	-0.424112
47	1	0	6.369769	-0.107491	-1.468798
48	1	0	6.763007	-2.513051	-0.995539
49	1	0	-0.617343	0.468321	1.799962
50	1	0	1.872657	-1.322000	1.568182
51	6	0	-0.757223	-1.712248	1.829658
52	8	0	-0.273327	-2.811456	1.692246
53	8	0	-2.011823	-1.512131	2.265007
54	6	0	2.008892	0.864834	1.737843
55	8	0	1.463402	1.920431	1.953850
56	8	0	3.333240	0.710099	1.699792
57	6	0	-2.784872	-2.695807	2.469752
58	1	0	-3.754973	-2.360626	2.829072
59	1	0	-2.308250	-3.339561	3.210509
60	1	0	-2.896281	-3.239509	1.529086
61	6	0	4.103030	1.911400	1.807837
62	1	0	5.137620	1.611036	1.657429
63	1	0	3.976621	2.356698	2.795938
64	1	0	3.793746	2.622197	1.040868

Structure **TS_{20}**:

Energy (Hartrees): -2004.305209

One imaginary frequency (cm^{-1}): 388.6611i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.441256	0.072646	1.559029
2	6	0	1.764130	0.180969	-0.709735
3	6	0	-0.557479	-0.392746	-0.386254
4	6	0	0.267868	-0.667368	1.690168
5	1	0	1.440584	1.132613	1.790623
6	1	0	0.359617	-1.744862	1.744472
7	7	0	-1.903661	-0.682651	-0.539494
8	7	0	-0.392207	0.958278	-0.498128
9	16	0	0.800996	-1.233606	-1.083331
10	6	0	-1.643404	1.658093	-0.780420
11	1	0	-1.610111	1.961367	-1.835763
12	6	0	-2.639699	0.505077	-0.702083
13	6	0	-2.440775	-2.001977	-0.687579

14	6	0	-3.367277	-2.247551	-1.705828
15	6	0	-2.011057	-3.032769	0.150304
16	6	0	-3.869715	-3.535709	-1.875189
17	1	0	-3.695809	-1.441559	-2.349156
18	6	0	-2.507493	-4.321989	-0.042666
19	1	0	-1.326899	-2.822256	0.961206
20	6	0	-3.438343	-4.576147	-1.050238
21	1	0	-4.593045	-3.725040	-2.659309
22	1	0	-2.171879	-5.122924	0.605269
23	1	0	-3.827703	-5.577564	-1.190633
24	8	0	-3.833478	0.567197	-0.800469
25	6	0	-1.936907	2.881477	0.092607
26	1	0	-1.106060	3.580483	-0.066603
27	1	0	-1.917505	2.580039	1.142222
28	6	0	-3.264044	3.592623	-0.236716
29	1	0	-4.094480	2.942707	0.063484
30	6	0	-3.412008	3.896081	-1.732483
31	1	0	-2.534035	4.436501	-2.108909
32	1	0	-4.291432	4.523523	-1.910125
33	1	0	-3.541724	2.983297	-2.323706
34	6	0	-3.336073	4.887538	0.582587
35	1	0	-2.547772	5.582528	0.268999
36	1	0	-3.205129	4.689958	1.651651
37	1	0	-4.301056	5.385102	0.443626
38	6	0	0.911771	1.380912	-0.737189
39	8	0	1.214657	2.550183	-0.877587
40	6	0	3.192641	0.197105	-1.039069
41	6	0	3.940809	1.382878	-0.902457
42	6	0	3.854330	-0.973282	-1.453410
43	6	0	5.302747	1.391013	-1.195011
44	1	0	3.448127	2.287571	-0.573186
45	6	0	5.215542	-0.955126	-1.749088
46	1	0	3.309371	-1.907458	-1.544294
47	6	0	5.945876	0.228130	-1.624199
48	1	0	5.861867	2.313610	-1.087742
49	1	0	5.703192	-1.866298	-2.076210
50	1	0	7.004393	0.242913	-1.857692
51	6	0	2.735496	-0.628040	1.683829
52	8	0	2.900298	-1.814449	1.525560
53	8	0	3.719212	0.226881	1.977003
54	6	0	-0.933706	-0.087120	2.294396
55	8	0	-1.134005	1.088106	2.496344
56	8	0	-1.842607	-1.039149	2.563308
57	6	0	-3.107054	-0.583927	3.051979
58	1	0	-2.986496	-0.079209	4.011277
59	1	0	-3.715635	-1.477767	3.166886
60	1	0	-3.572462	0.096656	2.337002
61	6	0	5.038119	-0.325845	1.992130
62	1	0	5.130810	-1.063818	2.790666
63	1	0	5.707758	0.511870	2.172468
64	1	0	5.262722	-0.793505	1.032368

Structure **TS_{21}**:

Energy (Hartrees): -2004.304984

One imaginary frequency (cm^{-1}): 318.7748i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.425132	-1.369684	0.972713
2	6	0	0.121196	-1.743382	0.439052
3	6	0	0.407155	0.450283	0.078650
4	6	0	0.929466	-1.820004	-1.639522
5	6	0	1.058030	-0.488268	-2.017083
6	7	0	-0.523468	-0.538732	0.193463
7	6	0	-1.838932	-0.194464	-0.126468
8	16	0	-0.292861	2.051626	-0.104586
9	6	0	-1.889748	1.259851	-0.601035
10	1	0	-1.889367	1.212929	-1.695269
11	8	0	-2.780234	-0.922809	-0.014760

12	6	0	-3.092795	2.010854	-0.104509
13	6	0	-3.390939	2.046130	1.263851
14	6	0	-3.918469	2.681977	-1.009490
15	6	0	-4.507215	2.742926	1.717722
16	1	0	-2.749160	1.528907	1.971612
17	6	0	-5.036086	3.382816	-0.553184
18	1	0	-3.689070	2.654589	-2.070009
19	6	0	-5.331044	3.413659	0.809240
20	1	0	-4.735925	2.763334	2.776775
21	1	0	-5.673195	3.900239	-1.260888
22	1	0	-6.199748	3.956368	1.163948
23	8	0	2.293936	-2.056496	1.460016
24	6	0	2.609457	0.877191	1.133516
25	6	0	2.913994	2.023962	0.393752
26	6	0	3.340603	0.557372	2.282048
27	6	0	3.947097	2.859935	0.816317
28	1	0	2.375195	2.253559	-0.520030
29	6	0	4.379105	1.395169	2.682797
30	1	0	3.107141	-0.339000	2.839400
31	6	0	4.683870	2.549123	1.959125
32	1	0	4.178843	3.749443	0.241720
33	1	0	4.948525	1.143431	3.569613
34	1	0	5.491007	3.196786	2.280016
35	7	0	1.519343	0.043140	0.747760
36	6	0	-0.587023	-2.988322	0.864129
37	1	0	0.172655	-3.778591	0.921380
38	6	0	-1.307624	-2.875638	2.230895
39	1	0	-2.135772	-2.164657	2.110545
40	1	0	0.276947	0.009251	-2.576162
41	1	0	1.819070	-2.405745	-1.434054
42	6	0	2.409899	0.069811	-2.109723
43	6	0	-0.233693	-2.614353	-2.091994
44	8	0	-0.253053	-3.814136	-2.197676
45	8	0	-1.298561	-1.835880	-2.359681
46	8	0	3.410908	-0.442427	-1.668293
47	8	0	2.421574	1.252183	-2.762222
48	6	0	-2.497799	-2.521191	-2.732300
49	1	0	-3.246862	-1.748749	-2.890370
50	1	0	-2.818429	-3.195186	-1.937165
51	1	0	-2.337826	-3.088459	-3.650032
52	6	0	3.716775	1.814818	-2.984287
53	1	0	4.302069	1.169958	-3.642197
54	1	0	4.253634	1.941417	-2.042956
55	1	0	3.544955	2.778345	-3.459858
56	1	0	-1.320142	-3.296988	0.111402
57	6	0	-1.891277	-4.244696	2.595926
58	1	0	-2.467512	-4.187634	3.524636
59	1	0	-1.088148	-4.976754	2.741358
60	1	0	-2.553325	-4.619163	1.808205
61	6	0	-0.380651	-2.366858	3.340236
62	1	0	-0.062956	-1.332456	3.163921
63	1	0	0.519857	-2.986820	3.411552
64	1	0	-0.895275	-2.392812	4.306409

Structure **TS_{22}**:

Energy (Hartrees): -2004.306615

One imaginary frequency (cm^{-1}): 348.1528i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.411818	0.953097	-0.919706
2	6	0	0.422348	1.571725	-0.045756
3	6	0	0.077473	-0.640195	-0.005408
4	6	0	1.542929	1.014061	1.783619
5	6	0	1.421160	-0.370363	1.878924
6	7	0	-0.512045	0.571500	0.192018
7	6	0	-1.762460	0.541800	0.826541
8	16	0	-1.042450	-1.994809	0.101816
9	6	0	-2.368613	-0.861347	0.699674

10	1	0	-2.665016	-1.177742	1.699878
11	8	0	-2.311201	1.484845	1.308123
12	6	0	-3.576840	-0.809795	-0.209940
13	6	0	-3.435217	-0.596477	-1.586497
14	6	0	-4.853521	-0.918507	0.346132
15	6	0	-4.563782	-0.490351	-2.396225
16	1	0	-2.443826	-0.523834	-2.024620
17	6	0	-5.983361	-0.815890	-0.467300
18	1	0	-4.963339	-1.081247	1.413355
19	6	0	-5.840102	-0.600922	-1.837597
20	1	0	-4.448102	-0.324187	-3.460845
21	1	0	-6.970757	-0.905487	-0.029766
22	1	0	-6.717101	-0.522566	-2.469598
23	8	0	2.351460	1.444383	-1.510031
24	6	0	1.979046	-1.476600	-1.339680
25	6	0	2.106460	-2.670858	-0.620830
26	6	0	2.675990	-1.285850	-2.537438
27	6	0	2.928416	-3.682552	-1.117077
28	1	0	1.594123	-2.810480	0.325970
29	6	0	3.501974	-2.301943	-3.012060
30	1	0	2.574962	-0.353630	-3.075286
31	6	0	3.628416	-3.502047	-2.309827
32	1	0	3.025449	-4.607197	-0.560660
33	1	0	4.042691	-2.154447	-3.939558
34	1	0	4.270143	-4.288976	-2.688115
35	7	0	1.124978	-0.444543	-0.859440
36	6	0	0.142457	3.040496	0.001124
37	1	0	1.118924	3.531689	0.091698
38	6	0	-0.603749	3.635961	-1.222555
39	1	0	-0.636528	4.717931	-1.034132
40	1	0	2.256875	-0.986096	1.570969
41	1	0	0.894407	1.656080	2.370060
42	6	0	0.504416	-1.041972	2.796260
43	6	0	2.833505	1.650973	1.415489
44	8	0	3.717416	0.773373	0.935041
45	8	0	3.051835	2.833839	1.519056
46	8	0	0.628718	-2.178567	3.187028
47	8	0	-0.548262	-0.266197	3.145068
48	6	0	4.910947	1.333732	0.379362
49	1	0	4.654531	2.042591	-0.407370
50	1	0	5.463455	0.492960	-0.033856
51	1	0	5.493982	1.829330	1.156643
52	6	0	-1.453548	-0.828900	4.096280
53	1	0	-1.814090	-1.803804	3.763546
54	1	0	-2.274071	-0.118914	4.182550
55	1	0	-0.960602	-0.947136	5.062653
56	1	0	-0.425027	3.268039	0.909021
57	6	0	-2.046284	3.133253	-1.335196
58	1	0	-2.616628	3.323825	-0.422510
59	1	0	-2.070328	2.053242	-1.531379
60	1	0	-2.555540	3.625567	-2.170657
61	6	0	0.143533	3.407363	-2.540912
62	1	0	0.114337	2.350035	-2.829144
63	1	0	1.194271	3.700808	-2.471208
64	1	0	-0.328725	3.981125	-3.345416

Structure **TS_{23}**:

Energy (Hartrees): -2004.304768

One imaginary frequency (cm^{-1}): 333.0177i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.723581	1.542331	0.021637
2	6	0	-0.299961	1.844957	0.132735
3	6	0	-0.501197	-0.274510	-0.573563
4	6	0	-0.166871	0.846616	2.091044
5	6	0	-0.188851	-0.516261	1.812654
6	7	0	0.335425	0.798497	-0.530266
7	6	0	1.631961	0.604654	-1.008715

8	16	0	0.128870	-1.638973	-1.476751
9	6	0	1.743044	-0.755837	-1.701520
10	8	0	2.505563	1.420070	-0.963791
11	8	0	-2.687758	2.216205	0.303155
12	6	0	-2.955371	-0.557578	-0.726212
13	6	0	-2.956877	-1.945344	-0.556257
14	6	0	-4.094211	0.103409	-1.195821
15	6	0	-4.102035	-2.674724	-0.873633
16	1	0	-2.089681	-2.454687	-0.146642
17	6	0	-5.235449	-0.638176	-1.495200
18	1	0	-4.086533	1.178633	-1.308488
19	6	0	-5.244201	-2.025503	-1.342290
20	1	0	-4.099373	-3.750552	-0.741076
21	1	0	-6.119905	-0.125093	-1.854018
22	1	0	-6.134970	-2.594444	-1.580613
23	7	0	-1.773219	0.192531	-0.458387
24	6	0	0.208911	3.251089	0.122352
25	1	0	-0.487568	3.839181	0.734136
26	6	0	0.312786	3.887803	-1.285423
27	1	0	1.109655	3.362660	-1.829017
28	1	0	0.724642	-1.086533	1.715668
29	1	0	-1.037354	1.305517	2.547865
30	6	0	-1.407522	-1.255988	2.143950
31	6	0	1.108561	1.528759	2.412186
32	8	0	1.203438	2.546303	3.049091
33	8	0	2.169442	0.889538	1.887471
34	8	0	-2.477325	-0.760574	2.411432
35	8	0	-1.208306	-2.591894	2.123840
36	6	0	3.436004	1.538319	2.039297
37	1	0	4.150641	0.926298	1.492315
38	1	0	3.403535	2.541907	1.614456
39	1	0	3.706768	1.593242	3.094437
40	6	0	-2.323849	-3.380521	2.544142
41	1	0	-2.561463	-3.171478	3.588735
42	1	0	-3.202107	-3.172181	1.930935
43	1	0	-2.013399	-4.417083	2.430110
44	1	0	1.191349	3.314855	0.601451
45	6	0	0.722534	5.356456	-1.131539
46	1	0	0.877864	5.823556	-2.108990
47	1	0	-0.060328	5.918098	-0.608454
48	1	0	1.650181	5.451485	-0.557545
49	6	0	-0.989592	3.766599	-2.083345
50	1	0	-1.238940	2.721489	-2.301142
51	1	0	-1.827708	4.204157	-1.529994
52	1	0	-0.899325	4.290229	-3.040836
53	1	0	1.806554	-0.528806	-2.769879
54	6	0	2.938651	-1.559562	-1.271745
55	6	0	3.664857	-2.279659	-2.224370
56	6	0	3.311781	-1.617669	0.076704
57	6	0	4.756753	-3.056018	-1.833904
58	1	0	3.377260	-2.232844	-3.270321
59	6	0	4.405822	-2.389733	0.463376
60	1	0	2.754179	-1.049047	0.816990
61	6	0	5.128151	-3.111672	-0.490458
62	1	0	5.315818	-3.611356	-2.577993
63	1	0	4.693090	-2.428992	1.507915
64	1	0	5.977851	-3.712462	-0.187500

Structure **TS1$_8$**:

Energy (Hartrees): -2004.309722

One imaginary frequency (cm^{-1}): 175.8583i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.389330	0.371541	-1.190206
2	6	0	0.774927	-1.051909	-0.933843
3	6	0	-0.350052	-0.280826	0.894329
4	6	0	1.522385	-1.589842	0.337122
5	6	0	0.943138	-0.747027	1.487248

6	7	0	-0.563410	-0.806080	-0.316065
7	6	0	-1.775442	-0.367260	-0.908463
8	16	0	-1.651592	0.506661	1.645623
9	6	0	-2.514129	0.595641	0.020344
10	1	0	-2.285121	1.591702	-0.377620
11	8	0	-2.175714	-0.697859	-1.980257
12	6	0	-3.995343	0.367020	0.101224
13	6	0	-4.501070	-0.910384	0.373580
14	6	0	-4.875968	1.436127	-0.081429
15	6	0	-5.875693	-1.113560	0.458511
16	1	0	-3.818345	-1.743581	0.516006
17	6	0	-6.253765	1.231778	0.006573
18	1	0	-4.484182	2.425178	-0.296727
19	6	0	-6.753901	-0.041569	0.276853
20	1	0	-6.262564	-2.104441	0.665358
21	1	0	-6.932199	2.064174	-0.138373
22	1	0	-7.823749	-0.201583	0.343782
23	8	0	2.411404	0.398731	-1.881054
24	6	0	1.302293	2.575893	-0.262165
25	6	0	0.463229	3.520779	0.359695
26	6	0	2.632379	2.950604	-0.547705
27	6	0	0.925159	4.790377	0.690080
28	1	0	-0.559735	3.231191	0.576965
29	6	0	3.085412	4.227008	-0.214973
30	1	0	3.282995	2.245693	-1.045760
31	6	0	2.244184	5.153107	0.404550
32	1	0	0.256924	5.498799	1.167998
33	1	0	4.109280	4.500826	-0.448305
34	1	0	2.607377	6.142916	0.656880
35	7	0	0.748894	1.309689	-0.502889
36	6	0	0.900826	-2.038020	-2.089167
37	1	0	1.977891	-2.049731	-2.299891
38	6	0	0.162650	-1.811282	-3.425624
39	1	0	-0.897330	-2.030767	-3.277001
40	1	0	1.566652	0.127420	1.699784
41	1	0	1.250289	-2.640062	0.461577
42	6	0	0.771363	-1.459918	2.818450
43	6	0	3.030409	-1.534224	0.180138
44	8	0	3.551025	-0.432712	0.712119
45	8	0	3.664298	-2.390646	-0.374325
46	8	0	-0.079026	-1.188586	3.621918
47	8	0	1.718851	-2.370389	2.990622
48	6	0	4.927387	-0.182285	0.403111
49	1	0	5.055648	-0.140531	-0.678962
50	1	0	5.159686	0.779039	0.854595
51	1	0	5.558924	-0.965344	0.823947
52	6	0	1.708686	-3.051508	4.256980
53	1	0	0.762176	-3.574955	4.391266
54	1	0	2.533569	-3.757555	4.215329
55	1	0	1.854026	-2.335606	5.065837
56	1	0	0.641728	-3.035768	-1.712522
57	6	0	0.278526	-0.384202	-3.970580
58	1	0	-0.149410	0.354487	-3.284950
59	1	0	1.324887	-0.112428	-4.138425
60	1	0	-0.263316	-0.305091	-4.919354
61	6	0	0.722222	-2.813781	-4.445920
62	1	0	1.777067	-2.600553	-4.655433
63	1	0	0.651570	-3.843725	-4.078174
64	1	0	0.170799	-2.753514	-5.389583

Structure **TS2$_8$**:

Energy (Hartrees): -2004.290049

One imaginary frequency (cm^{-1}): 179.2887i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.148910	-1.122776	-0.120167
2	6	0	0.293844	-0.387766	0.945533
3	6	0	-1.074398	0.931316	-0.417741

4	6	0	0.833552	1.052456	0.971223
5	6	0	0.177509	1.724200	-0.243951
6	7	0	-1.036040	-0.175226	0.281861
7	6	0	-2.199528	-0.997849	0.177818
8	16	0	-2.446350	1.204974	-1.377208
9	6	0	-3.072686	-0.492470	-0.969967
10	1	0	-2.801218	-1.109131	-1.834476
11	8	0	-2.444586	-1.905555	0.899369
12	6	0	-4.545756	-0.559180	-0.697487
13	6	0	-5.078948	0.024330	0.458609
14	6	0	-5.390351	-1.207142	-1.602221
15	6	0	-6.446617	-0.046298	0.707680
16	1	0	-4.423915	0.528864	1.163937
17	6	0	-6.761289	-1.276060	-1.351368
18	1	0	-4.977197	-1.661079	-2.497023
19	6	0	-7.289391	-0.696717	-0.198162
20	1	0	-6.855463	0.401329	1.605625
21	1	0	-7.412015	-1.782915	-2.053953
22	1	0	-8.353765	-0.751958	-0.001940
23	8	0	0.648415	-2.043423	-0.776639
24	6	0	3.428338	-1.030827	-0.897836
25	6	0	4.715843	-0.778612	-0.394647
26	6	0	3.289752	-1.716301	-2.116573
27	6	0	5.841901	-1.173278	-1.112027
28	1	0	4.801042	-0.294919	0.572691
29	6	0	4.425810	-2.112476	-2.823270
30	1	0	2.298671	-1.943846	-2.485334
31	6	0	5.703745	-1.838638	-2.333544
32	1	0	6.830040	-0.973502	-0.711203
33	1	0	4.308459	-2.640220	-3.763945
34	1	0	6.581054	-2.148138	-2.890394
35	7	0	2.340962	-0.567190	-0.142819
36	6	0	0.236983	-1.030580	2.350092
37	1	0	0.880698	-0.395240	2.969362
38	6	0	0.722933	-2.482125	2.584627
39	1	0	0.665762	-2.581954	3.679034
40	1	0	0.790790	1.546987	-1.142192
41	1	0	0.536645	1.566284	1.888864
42	6	0	-0.098437	3.216061	-0.215120
43	6	0	2.378221	0.998362	0.945633
44	8	0	2.855156	1.908718	0.013833
45	8	0	2.991121	0.790837	1.992713
46	8	0	-0.882433	3.732546	-0.969519
47	8	0	0.608510	3.844243	0.701343
48	6	0	4.075957	2.557093	0.342664
49	1	0	4.926314	1.876492	0.280328
50	1	0	4.197812	3.349063	-0.396033
51	1	0	4.030510	2.985068	1.345925
52	6	0	0.446436	5.272215	0.751195
53	1	0	-0.593012	5.523903	0.961666
54	1	0	1.093636	5.609308	1.556140
55	1	0	0.751104	5.714366	-0.197339
56	1	0	-0.785276	-0.927858	2.734441
57	6	0	-0.168438	-3.575849	1.986947
58	1	0	-1.191556	-3.514607	2.366595
59	1	0	-0.198288	-3.501017	0.896237
60	1	0	0.236739	-4.559923	2.250270
61	6	0	2.197458	-2.702365	2.199431
62	1	0	2.303290	-2.952147	1.138973
63	1	0	2.804752	-1.813320	2.401571
64	1	0	2.603936	-3.543847	2.771187

Structure $\mathbf{TS3_8}$:

Energy (Hartrees): -2004.299715

One imaginary frequency (cm^{-1}): 220.8068i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.639320	-0.250260	1.235709

2	6	0	0.413018	0.621769	0.833189
3	6	0	-0.781633	0.077010	-1.126737
4	6	0	0.920712	1.412604	-0.387277
5	6	0	-0.223919	1.438595	-1.406674
6	7	0	-0.596139	-0.248941	0.146394
7	6	0	-1.319432	-1.355835	0.619946
8	16	0	-1.924414	-0.856949	-1.977821
9	6	0	-2.225769	-1.908750	-0.489035
10	1	0	-1.882178	-2.919601	-0.718100
11	8	0	-1.266178	-1.776391	1.731870
12	6	0	-3.670672	-1.908792	-0.055697
13	6	0	-4.315323	-0.700159	0.239935
14	6	0	-4.348878	-3.119316	0.097027
15	6	0	-5.634109	-0.711047	0.685851
16	1	0	-3.788056	0.244012	0.116879
17	6	0	-5.670941	-3.125503	0.545419
18	1	0	-3.843950	-4.053533	-0.125780
19	6	0	-6.313559	-1.923366	0.838831
20	1	0	-6.132143	0.223750	0.914743
21	1	0	-6.193605	-4.067192	0.665038
22	1	0	-7.340219	-1.927991	1.186145
23	8	0	1.712592	-0.826530	2.300353
24	6	0	3.723735	-1.001830	0.201549
25	6	0	4.899507	-0.475469	-0.348329
26	6	0	3.701052	-2.316463	0.682913
27	6	0	6.043250	-1.270746	-0.415548
28	1	0	4.887275	0.535252	-0.731632
29	6	0	4.854804	-3.096362	0.622166
30	1	0	2.791941	-2.713499	1.115687
31	6	0	6.028494	-2.578930	0.071165
32	1	0	6.951317	-0.861115	-0.843707
33	1	0	4.833365	-4.110949	1.003869
34	1	0	6.923890	-3.188684	0.025577
35	7	0	2.552465	-0.197670	0.242778
36	6	0	-0.251240	1.274963	2.051022
37	1	0	-1.290772	1.509313	1.792916
38	6	0	0.413291	2.544607	2.628117
39	1	0	0.000556	2.640834	3.641484
40	1	0	0.145398	1.561756	-2.425210
41	1	0	1.341116	2.385341	-0.153905
42	6	0	-1.262333	2.505773	-1.089018
43	6	0	2.054546	0.522127	-0.995564
44	8	0	1.213461	-0.626000	-1.675432
45	8	0	2.885397	1.049106	-1.763247
46	8	0	-2.289473	2.315547	-0.489720
47	8	0	-0.860556	3.681068	-1.545455
48	6	0	1.586110	-0.916759	-3.003862
49	1	0	1.740522	-0.008272	-3.592124
50	1	0	2.511842	-1.499383	-3.027607
51	1	0	0.783008	-1.517182	-3.442216
52	6	0	-1.726881	4.796621	-1.281224
53	1	0	-1.870548	4.917957	-0.207744
54	1	0	-1.220019	5.662311	-1.698894
55	1	0	-2.690102	4.644122	-1.768663
56	1	0	-0.267804	0.496554	2.822915
57	6	0	1.936590	2.426891	2.773672
58	1	0	2.210055	1.541128	3.354383
59	1	0	2.441745	2.358116	1.802424
60	1	0	2.335152	3.309004	3.285179
61	6	0	0.006088	3.819302	1.872362
62	1	0	0.416119	3.858413	0.857422
63	1	0	-1.085829	3.891542	1.805734
64	1	0	0.371344	4.707022	2.399727

Structure **TS4$_8$**:

Energy (Hartrees): -2004.288007

One imaginary frequency (cm^{-1}): 1654.7889i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.520257	-1.059637	-0.446800
2	6	0	0.415145	-0.703603	0.558155
3	6	0	-0.891391	1.019658	-0.419918
4	6	0	0.891558	0.633245	1.170602
5	6	0	0.152885	1.707039	0.372615
6	7	0	-0.809905	-0.347201	-0.167371
7	6	0	-1.902153	-1.119814	-0.503826
8	16	0	-2.588016	1.495586	-0.631132
9	6	0	-2.995732	-0.235500	-1.120080
10	1	0	-2.875642	-0.319101	-2.205155
11	8	0	-2.004593	-2.305799	-0.341942
12	6	0	-4.384231	-0.647658	-0.717968
13	6	0	-4.753762	-0.668610	0.633197
14	6	0	-5.313773	-1.022722	-1.690721
15	6	0	-6.036280	-1.064768	1.003359
16	1	0	-4.034294	-0.373347	1.391758
17	6	0	-6.600139	-1.418654	-1.319883
18	1	0	-5.029913	-1.010368	-2.738213
19	6	0	-6.962553	-1.439869	0.026338
20	1	0	-6.314039	-1.081478	2.050937
21	1	0	-7.314308	-1.710360	-2.081304
22	1	0	-7.961004	-1.747007	0.315672
23	8	0	1.451738	-1.890438	-1.307543
24	6	0	3.893548	-0.428794	-0.798450
25	6	0	5.044149	-0.634281	-0.035165
26	6	0	3.954715	-0.383017	-2.192304
27	6	0	6.271026	-0.788437	-0.679651
28	1	0	4.974854	-0.665108	1.045704
29	6	0	5.184204	-0.551776	-2.826962
30	1	0	3.047157	-0.223021	-2.762361
31	6	0	6.342437	-0.751352	-2.073255
32	1	0	7.168726	-0.943708	-0.092773
33	1	0	5.236649	-0.523778	-3.908996
34	1	0	7.297257	-0.878612	-2.570139
35	7	0	2.630272	-0.276797	-0.146620
36	6	0	0.204334	-1.833719	1.576905
37	1	0	-0.634165	-1.522519	2.213383
38	6	0	1.430553	-2.151691	2.462803
39	1	0	1.949686	-1.216861	2.723711
40	1	0	0.583756	1.819437	-1.014682
41	1	0	0.725232	0.703413	2.247897
42	6	0	-0.180898	3.013980	0.914720
43	6	0	2.382563	0.657242	0.874851
44	8	0	-0.024256	1.283335	-1.888819
45	8	0	3.221637	1.348104	1.378613
46	8	0	-1.027414	3.750537	0.446575
47	8	0	0.573535	3.343670	1.971005
48	6	0	-0.575626	2.068270	-2.944296
49	1	0	-1.418542	1.536865	-3.389178
50	1	0	-0.903771	3.044762	-2.579955
51	1	0	0.203009	2.194741	-3.698086
52	6	0	0.374809	4.659634	2.492169
53	1	0	0.556862	5.408298	1.720334
54	1	0	-0.640546	4.772418	2.874079
55	1	0	1.096018	4.768222	3.298872
56	1	0	-0.109408	-2.739073	1.048369
57	6	0	0.939292	-2.789200	3.770223
58	1	0	0.288722	-2.106913	4.326741
59	1	0	0.371025	-3.702550	3.557502
60	1	0	1.782211	-3.058160	4.414061
61	6	0	2.432597	-3.095306	1.779829
62	1	0	1.937041	-4.033261	1.504490
63	1	0	2.881950	-2.679257	0.874089
64	1	0	3.250795	-3.334285	2.467251