Surpporting Information

for

Theoretical Study on Hydroformylation Catalyzed by Cationic Cobalt(II) Complex

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1. Details of DFT calculations

All the calculations were performed in Gaussian 09 program.[1] The intermediates and transition states were optimized at the ωB97X-D[2]/BS-I level. BS-I denotes that the Co center adopted the LANL2DZ basis set based on the effective nuclear potential energy approximation (ECP)[3] and the 6-31G* basis set for all other atoms. The solvation effect of tetrahydrofuran (ε=7.58) was simulated by the polarizable continuum model of the implicit solvent model based on density (SMD).[4-7] The improved elastic image pair (i-EIP) method was used to assist in searching transition states.[8, 9] All transition states were further confirmed and characterized with one and only one imaginary frequency. The intermediates along the reaction pathway were confirmed by intrinsic reaction coordinates (IRC) calculations.[10] Additionally, single point energies were calculated at the ωB97X-D/BS-II level. BS-II denotes that the SDD basis set was used for the Co center and the 6-311++G** basis set for all the other atoms.[11-15] All energies discussed in the following sections are Gibbs free energies calculated at 298.15 K with a correction coefficient of 1.89 kcal/mol for standard state changes from 1 atm to 1 M.[16, 17] All energies discussed are compared with **A1** in the following parts unless otherwise stated. To verify the reliability of the computational methods, we also compared other functionals, such as M06-L. The intermediates and transition states were optimized at the M06-L/BS-III level. BS-III denotes that the SDD basis set was used for the Co center and the 6-31G** basis set for all the other atoms. Additionally, single point energies were calculated at the M06-L[18]/BS-IV level. BS-IV denotes that the SDD basis set was used for the Co center and the 6-311++G** basis set for all the other atoms. In the calculation of single point energy, the solvation effect was simulated by the polarizable continuum model of the implicit solvent model based on density (SMD). As shown in Figure S1-2 in Supporting Information, the trend of calculated results is consistent using two functionals.

2. The Gibbs free energy profiles of hydorformylation calculated at the M06-L/BS-III//M06-L/BS-IV level

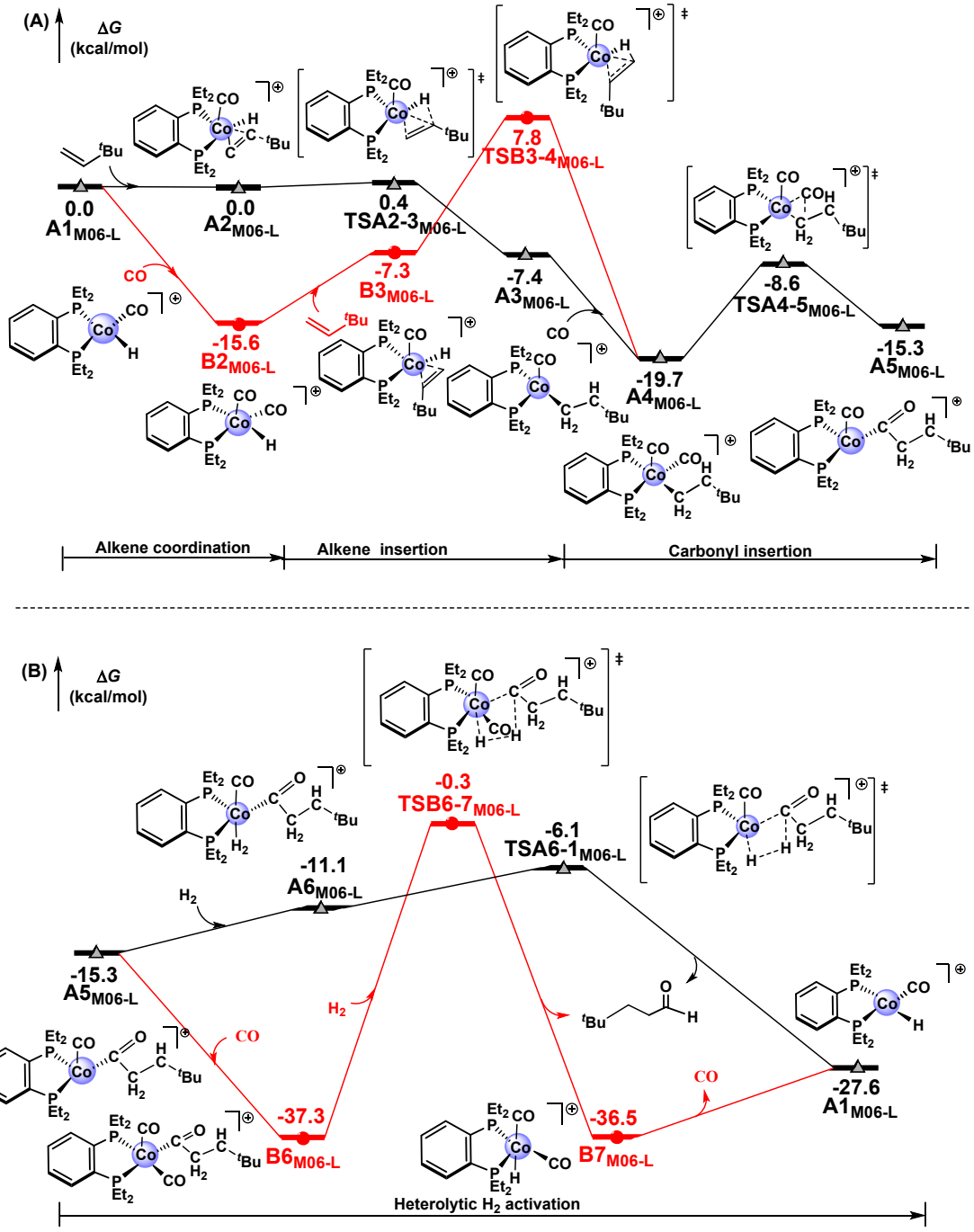


Fig. S1. The Gibbs free energy profiles of the dissociative mechanism (black line) and associative mechanism (pink line) at the M06-L/BS-III//M06-L/BS-IV level.

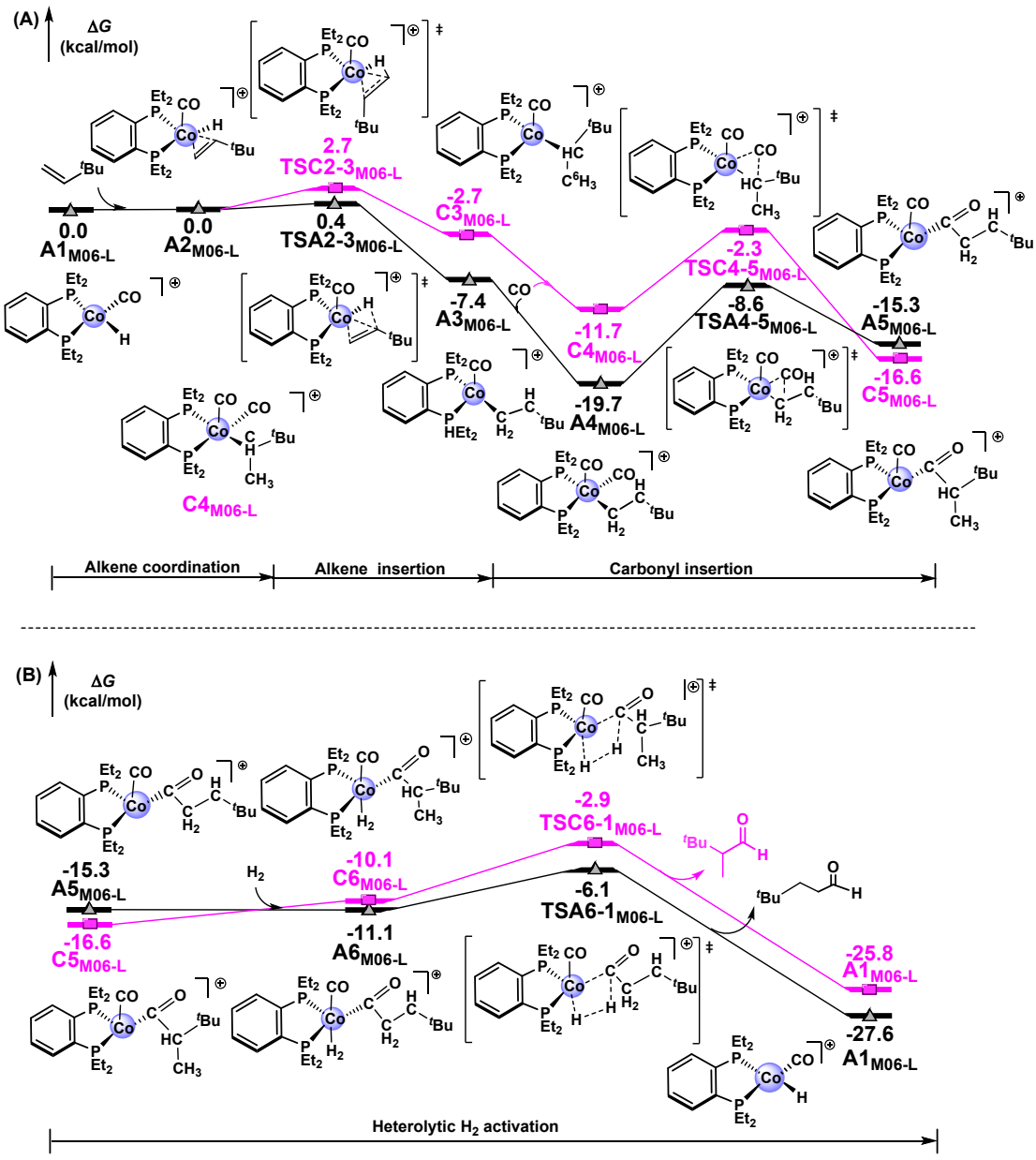


Fig. S2. The Gibbs free energy profile of forming linear aldehyde and branched aldehyde by the dissociative mechanism at the M06-L/BS-III//M06-L/BS-IV level.

3. The Gibbs free energy profiles of spin multiplicity of cobalt(II) complex

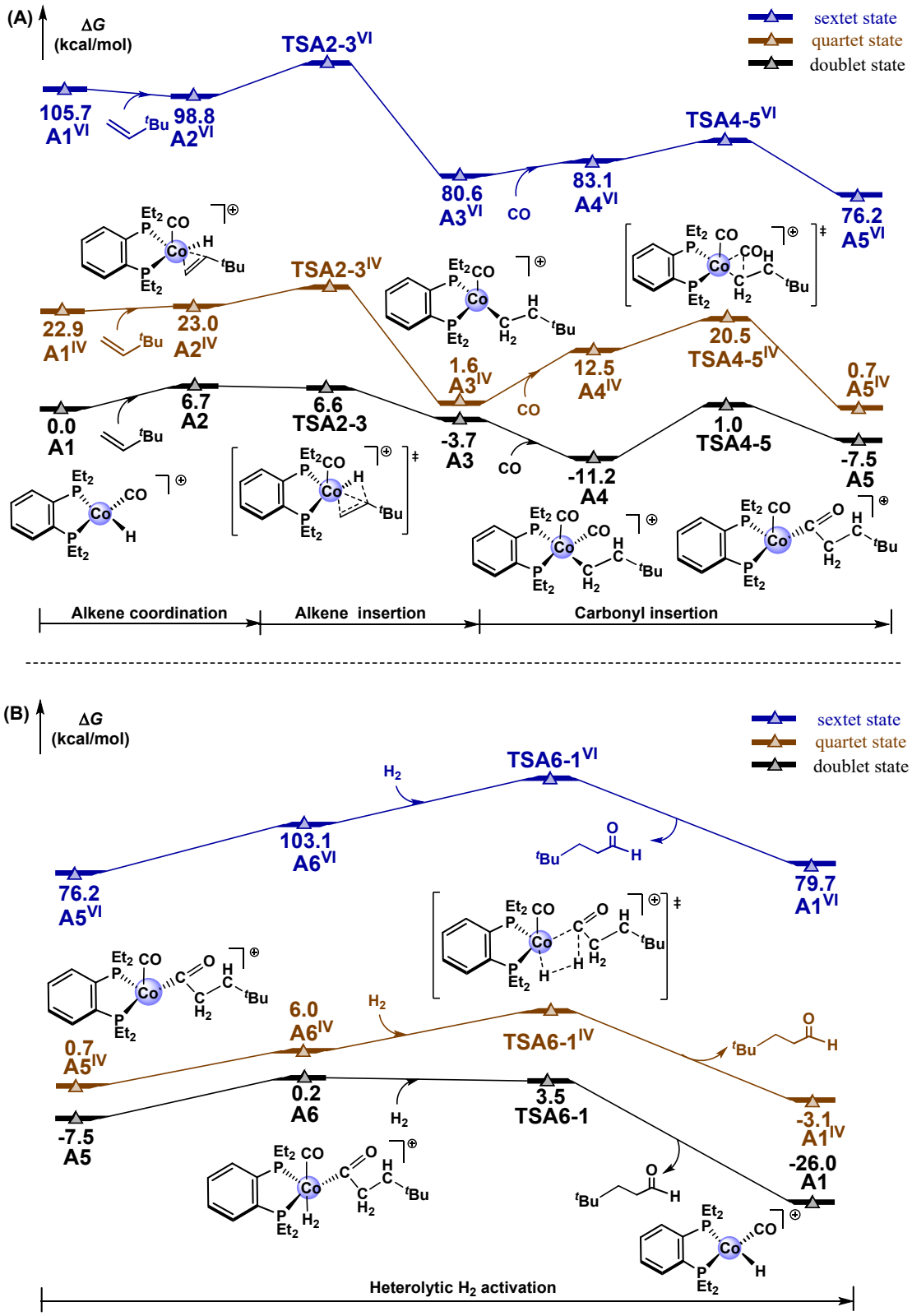


Fig. S3. The Gibbs free energy profile of forming linear aldehyde under dissociative

path.

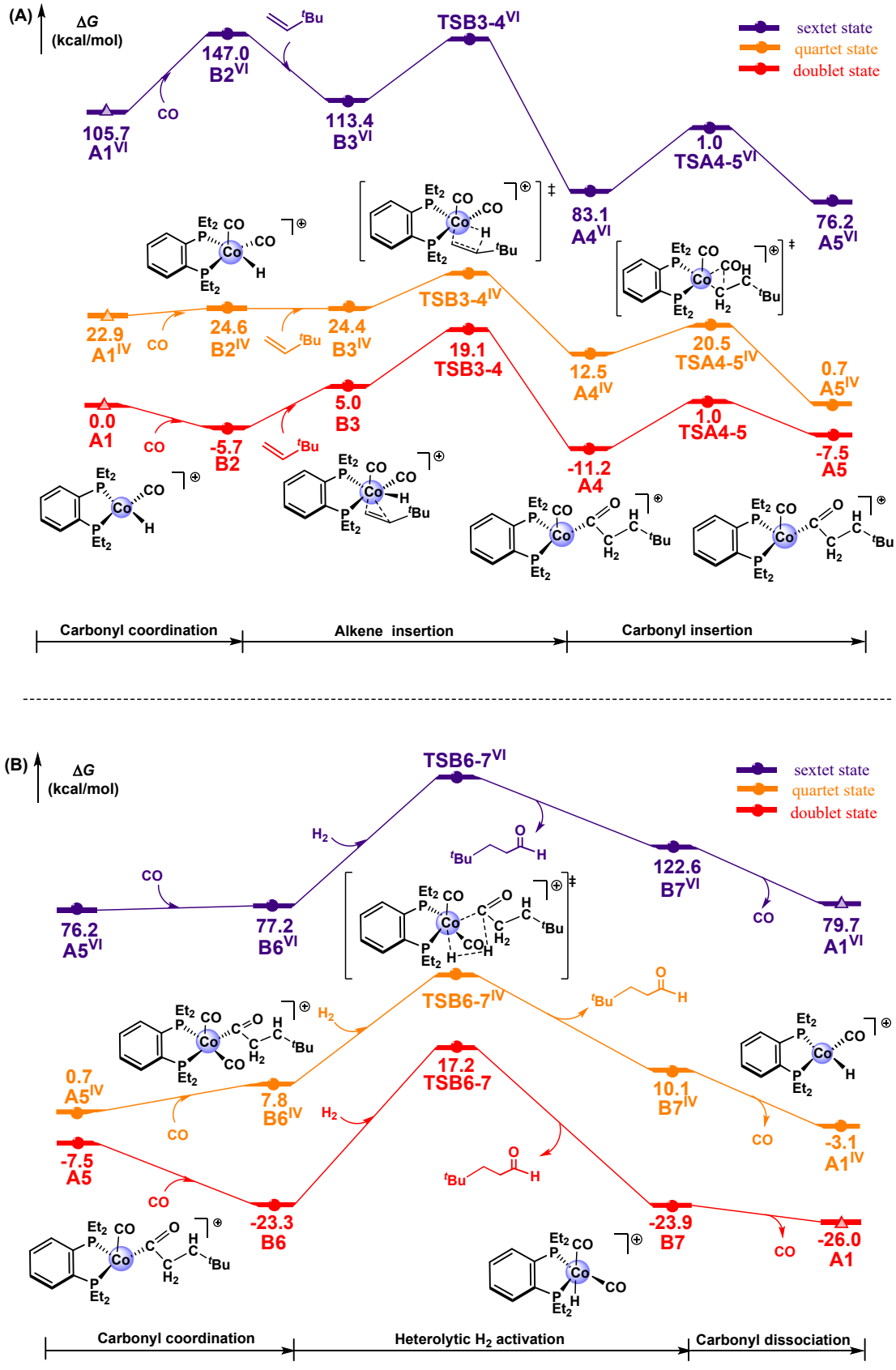


Fig. S4. The Gibbs free energy profile of forming linear aldehyde under associative

path.

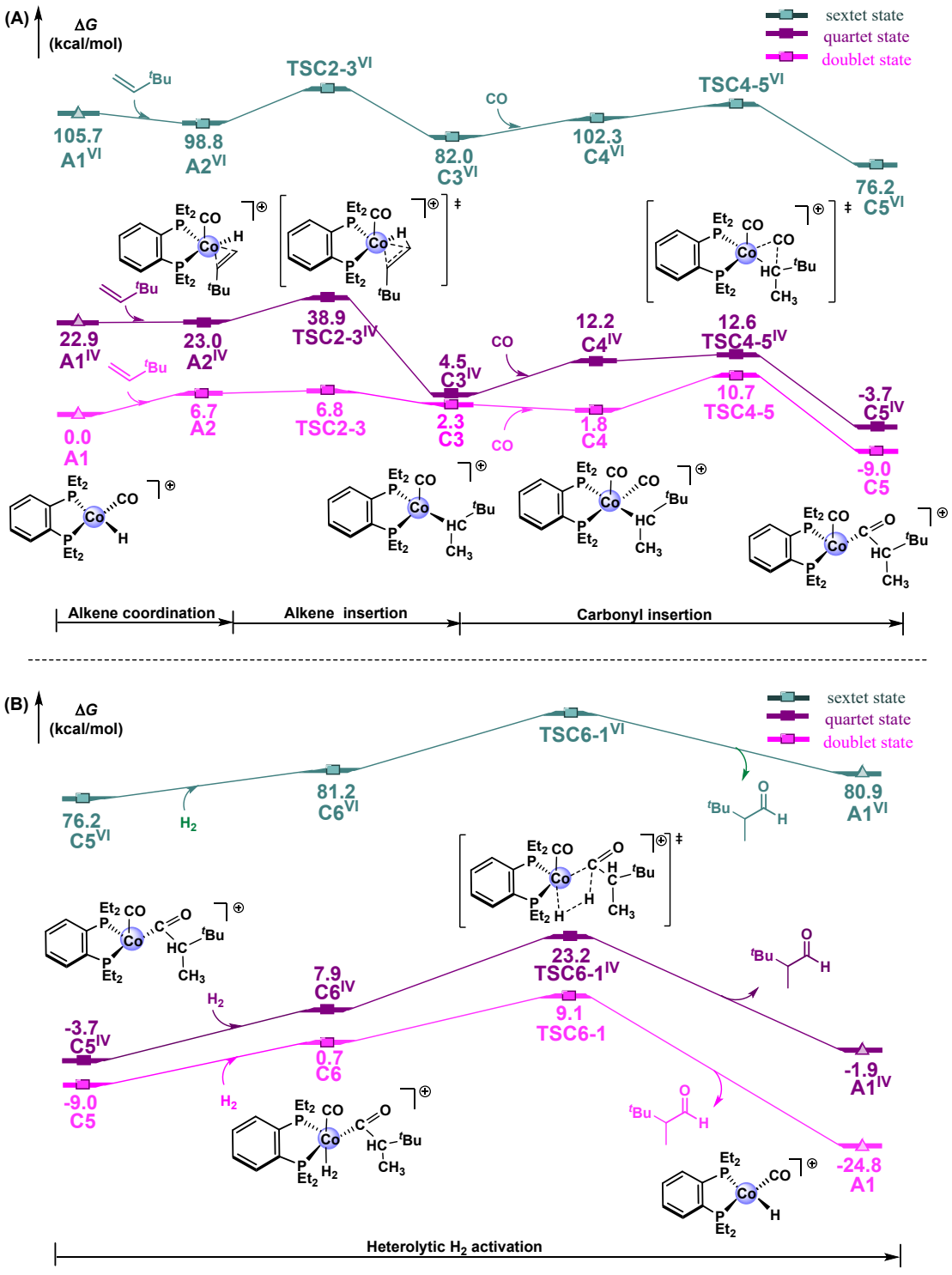


Fig. S5. The Gibbs free energy profile of forming branched aldehyde under dissociative path.

As shown in Fig. S6, the catalytic species of $[HCo(CO)_2(DEPBz)]^+$ at doublet state is still more stable than that at quartet state (the MN15-L functional was used in that it be a good one for the calculation of the spin splitting energy and the optimized geometry of intermediate at different spin states[19]. It is a very interesting phenomenon, we are trying to figure it out and report its nature in the near future. I guess that a new intemediate with a dinuclear structure was formed showing doublet spin state.

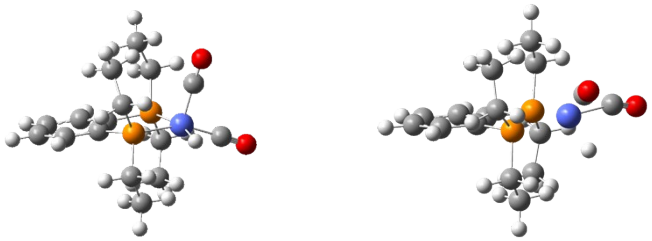


Fig. S6. Comparison of doublet and quartet spin states for $[HCo(CO)_2(DEPBz)]^+$.

4. The Gibbs free energy profiles for formation of catalytic active specie A1

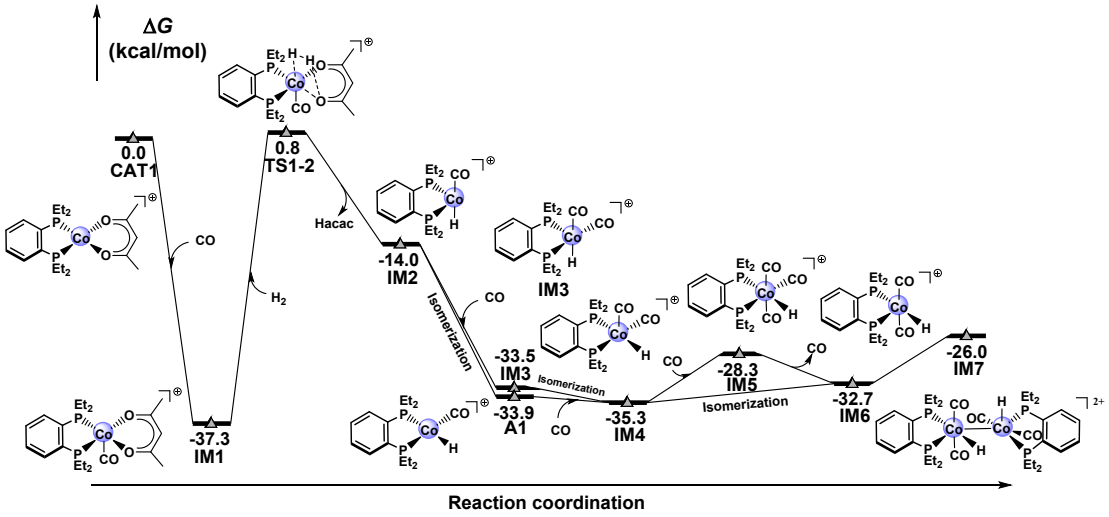


Fig. S7. The formation of catalytic active species **A1**.

5. The way of alkene coordination

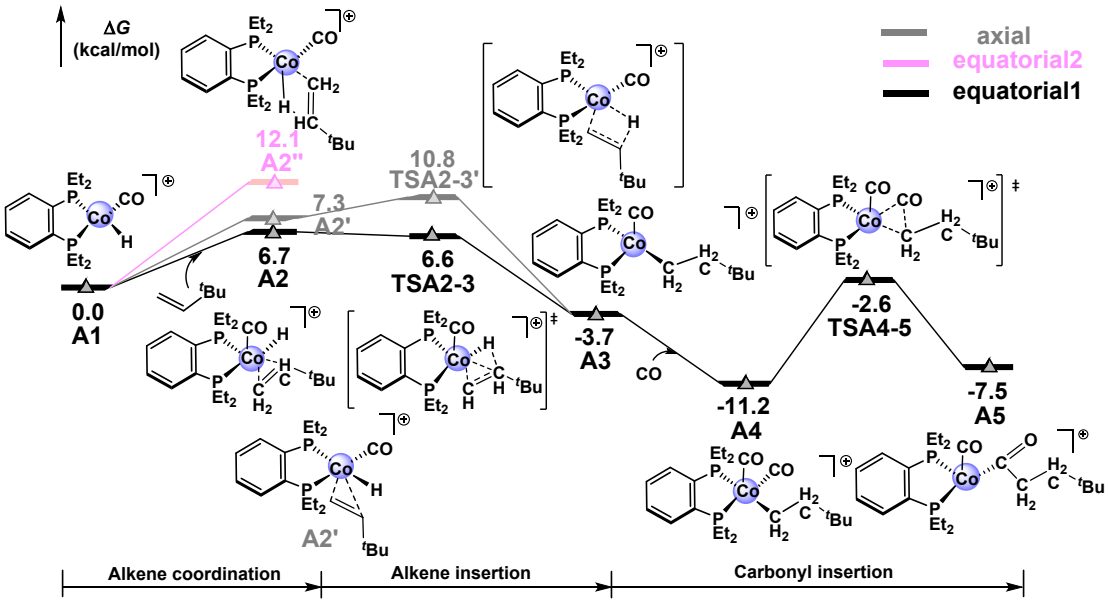


Fig. S8. The way of olefin coordination by dissociative mechanism.

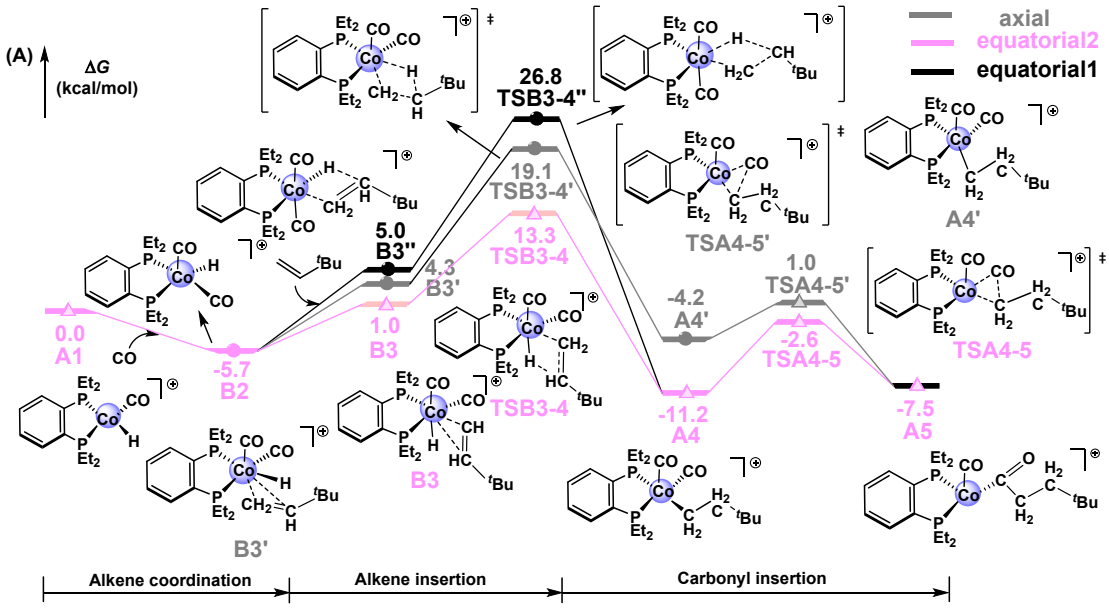


Fig. S9. The way of olefin coordination by associative mechanism.

6. The Mulliken charge analysis

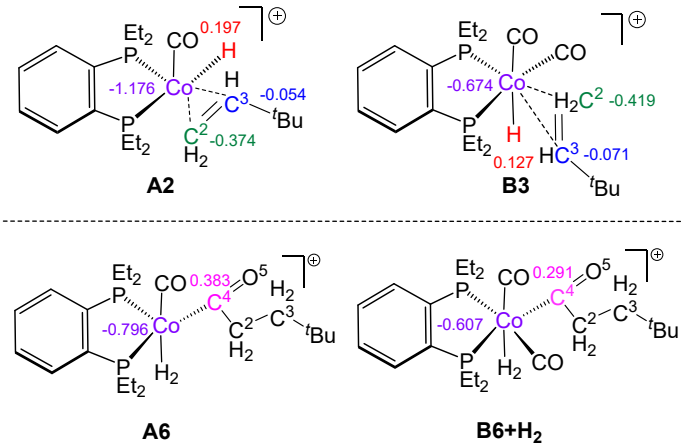


Fig. S10. The Mulliken charge of **A2**, **B3**, **A6** and **B6+H_2**.

7. Regioselectivity

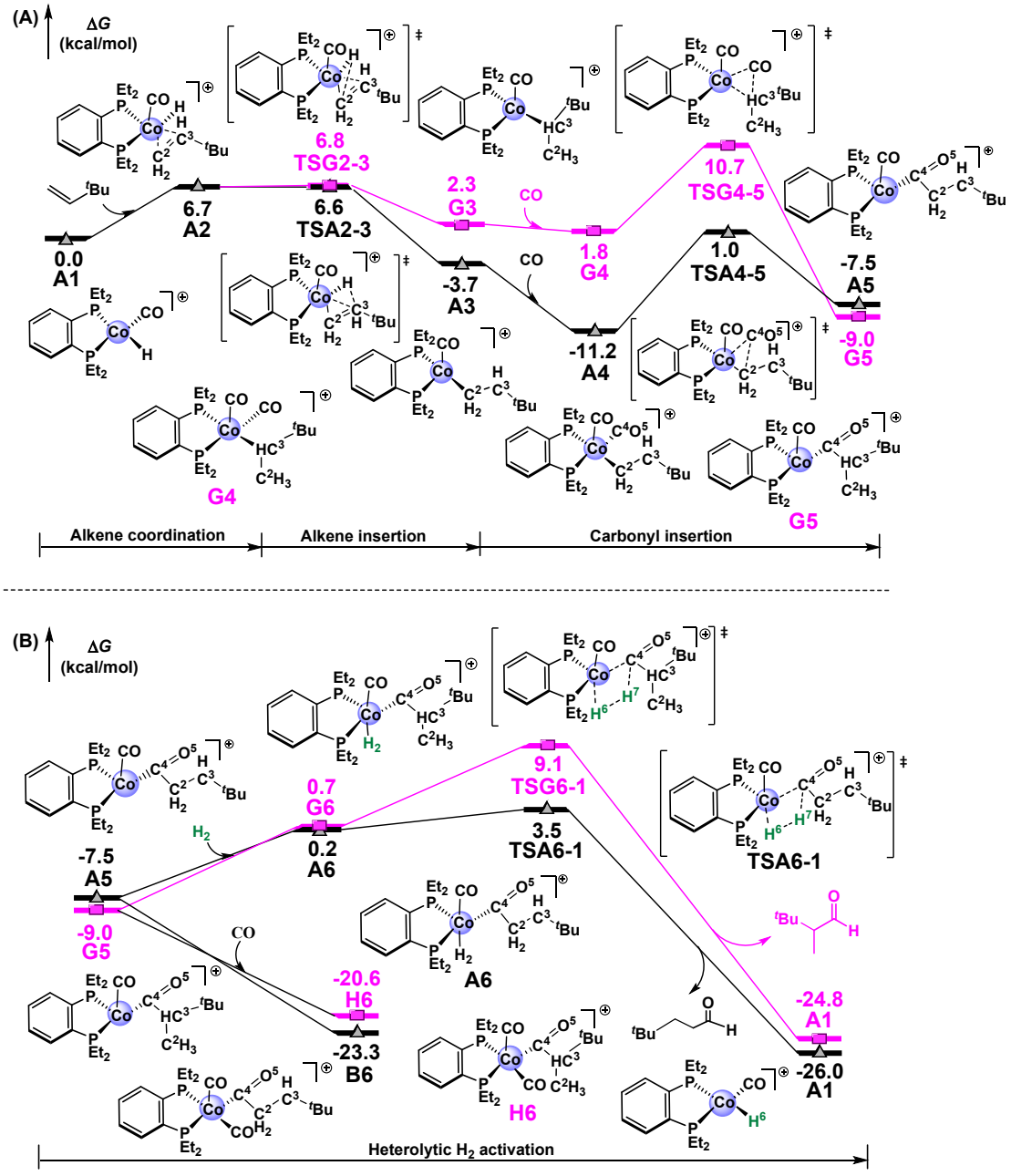


Fig. S11. The Gibbs free energy profile of the dissociative mechanism of forming linear (black line) and branched (pink line) aldehyde.

8. The Gibbs free energy profiles of substituent effect

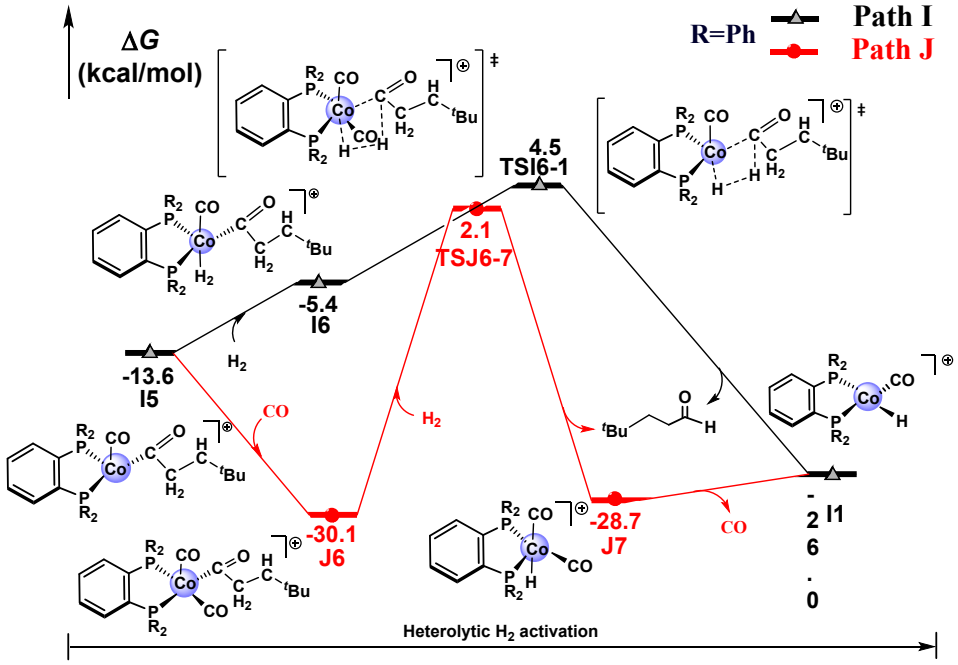


Fig. S12. With -Ph as substituent on phosphine, the Gibbs free energy barrier profile of hydrogen activation step in dissociative (black line) and associative mechanism (red line).

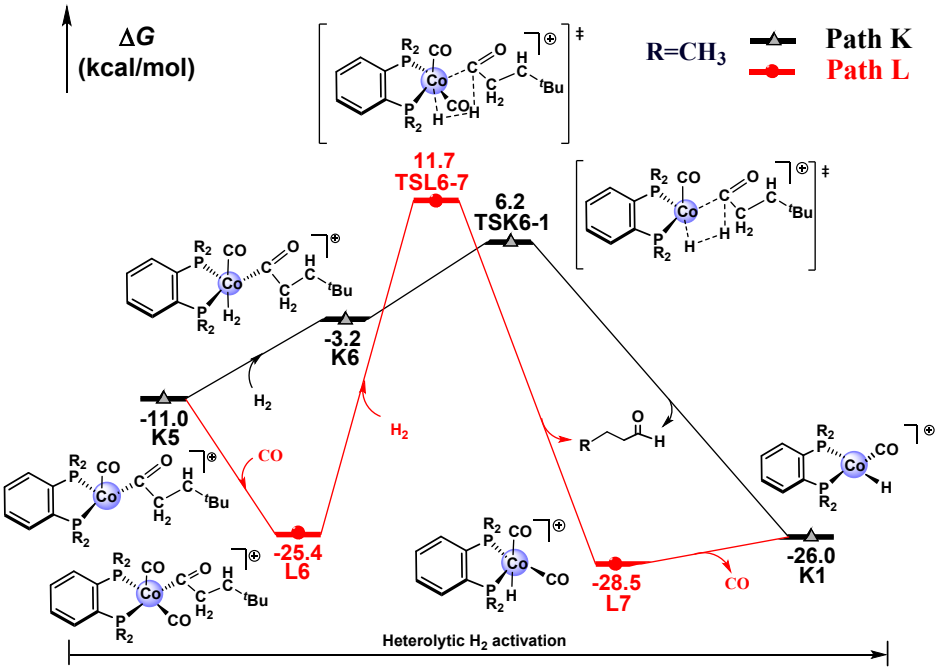


Fig. S13. With -CH_3 as substituent on phosphine, the Gibbs free energy barrier profile of hydrogen activation step in dissociative (black line) and associative mechanism

(red line).

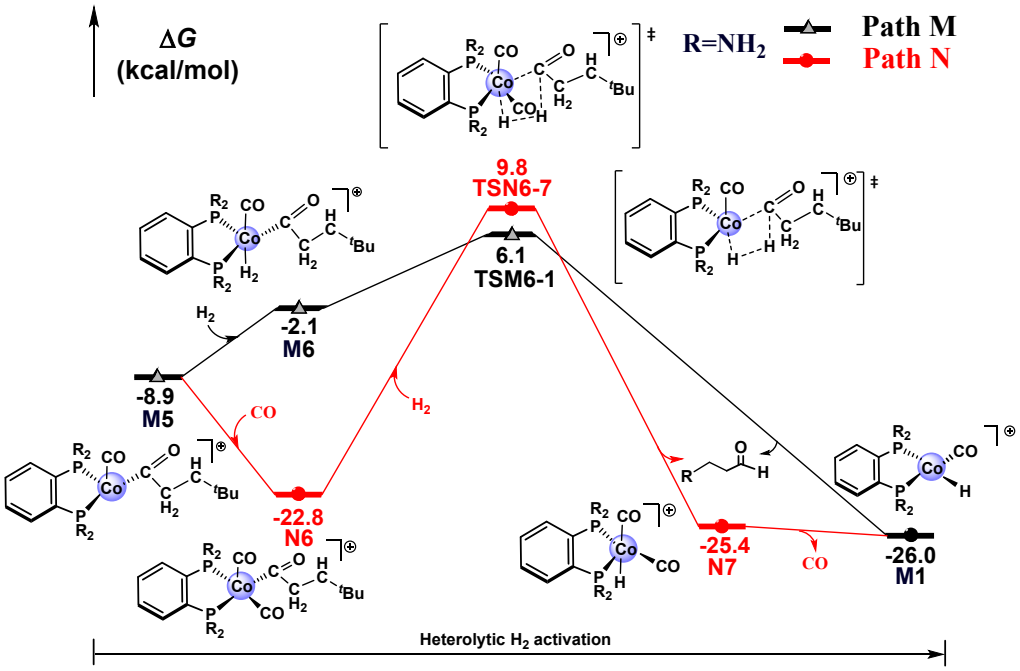


Fig. S14. With -NH_2 as substituent on phosphine, the Gibbs free energy barrier profile of hydrogen activation step in dissociative (black line) and associative mechanism (red line).

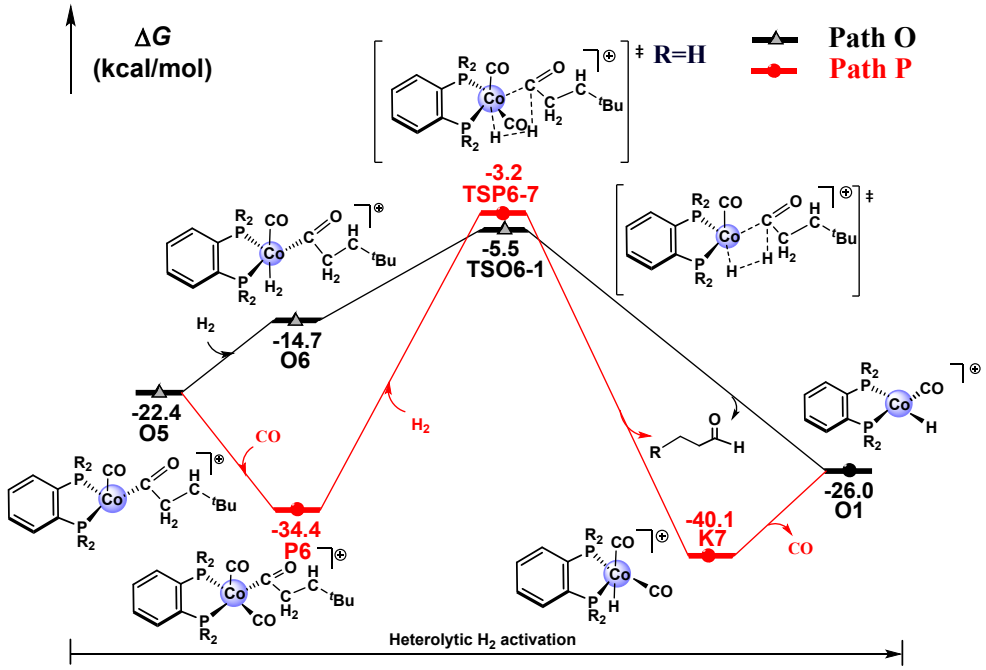


Fig. S15. With -H as substituent on phosphine, the Gibbs free energy barrier profile of hydrogen activation step in dissociative (black line) and associative mechanism (red

line).

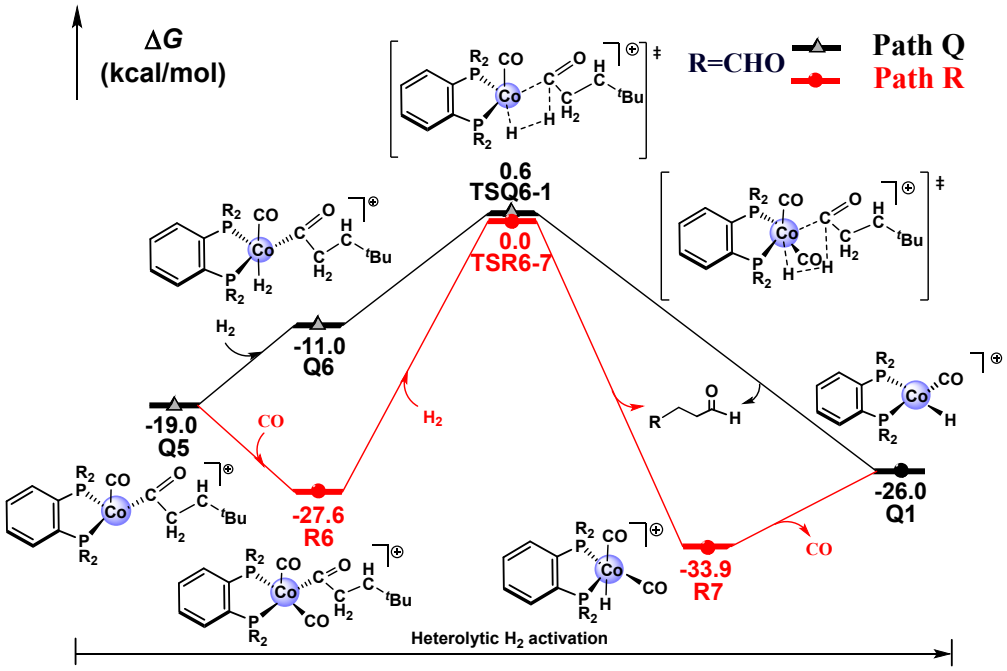


Fig. S16. With -CHO as substituent on phosphine, the Gibbs free energy barrier profile of hydrogen activation step in dissociative (black line) and associative mechanism (red line).

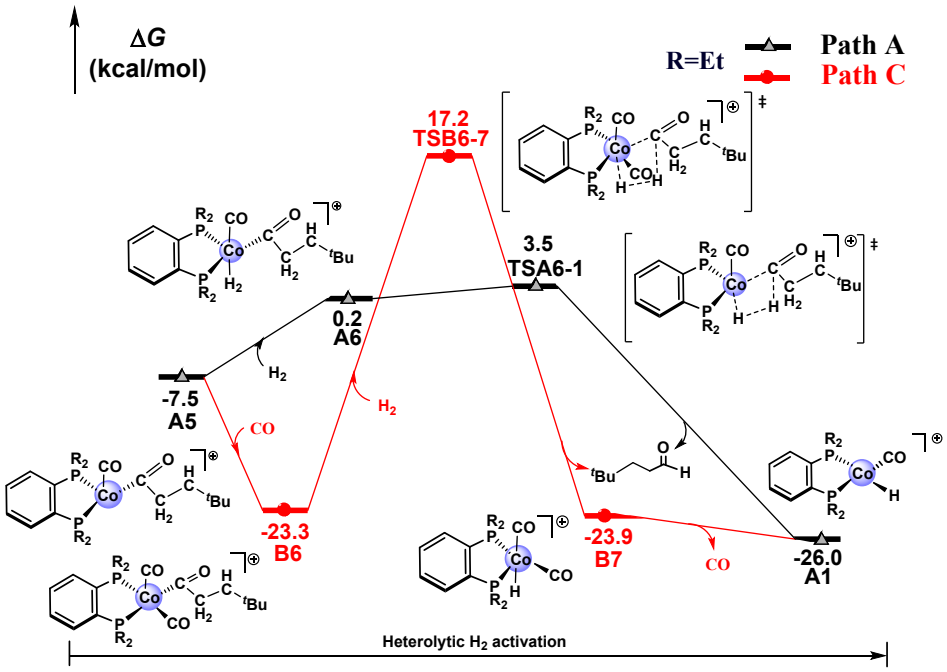


Fig. S17. With -Et as substituent on phosphine, the Gibbs free energy barrier profile of hydrogen activation step in dissociative (black line) and associative mechanism

(red line).

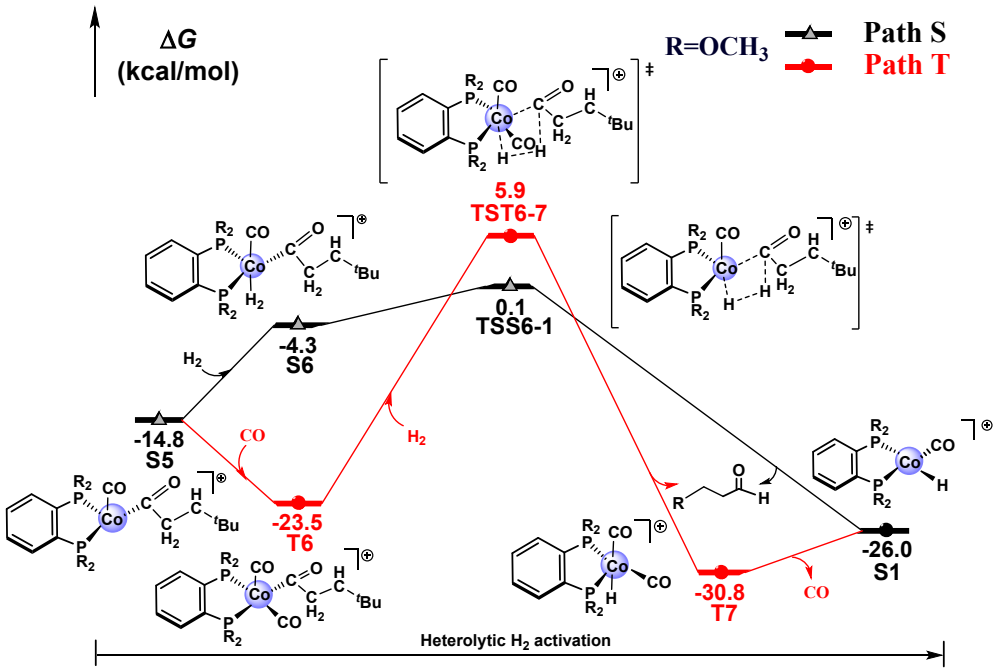


Fig. S18. With -OCH_3 as substituent on phosphine, the Gibbs free energy barrier profile of hydrogen activation step in dissociative (black line) and associative mechanism (red line).

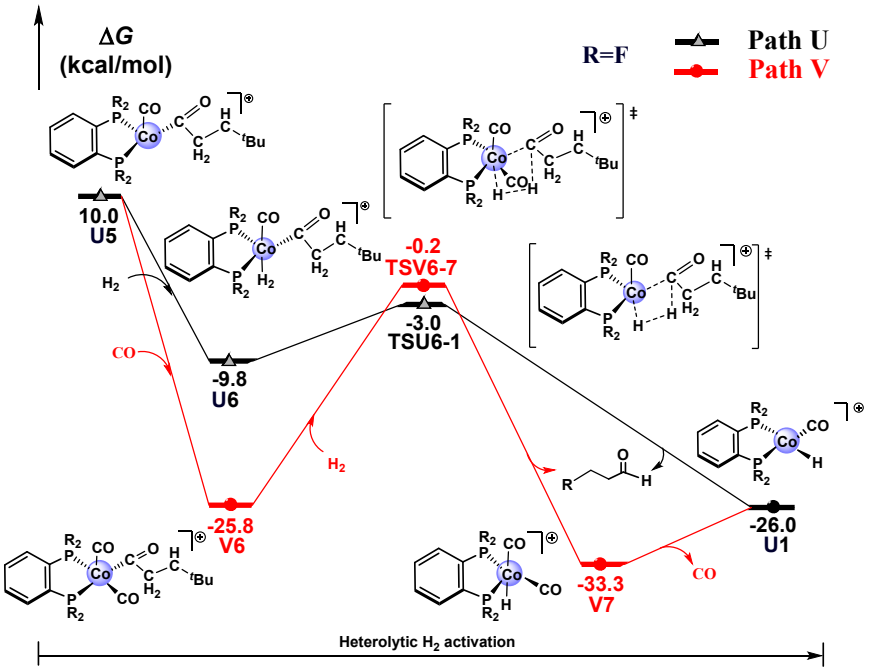


Fig. S19. With -F as substituent on phosphine, the Gibbs free energy barrier profile of

hydrogen activation step in dissociative (black line) and associative mechanism (red line).

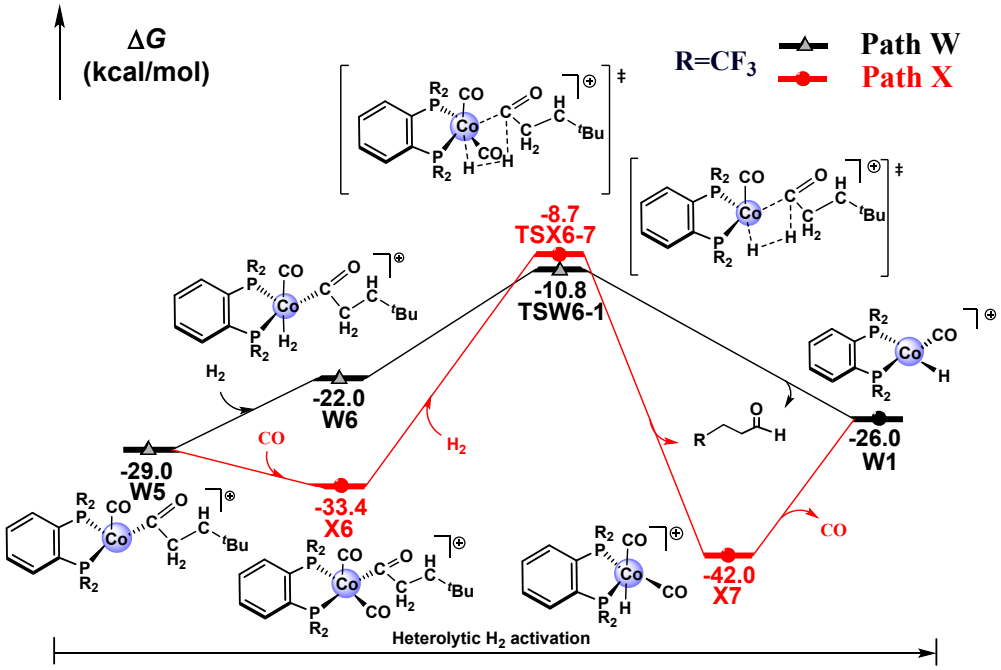


Fig. S20. With -CF_3 as substituent on phosphine, the Gibbs free energy barrier profile of hydrogen activation step in dissociative (black line) and associative mechanism (red line).

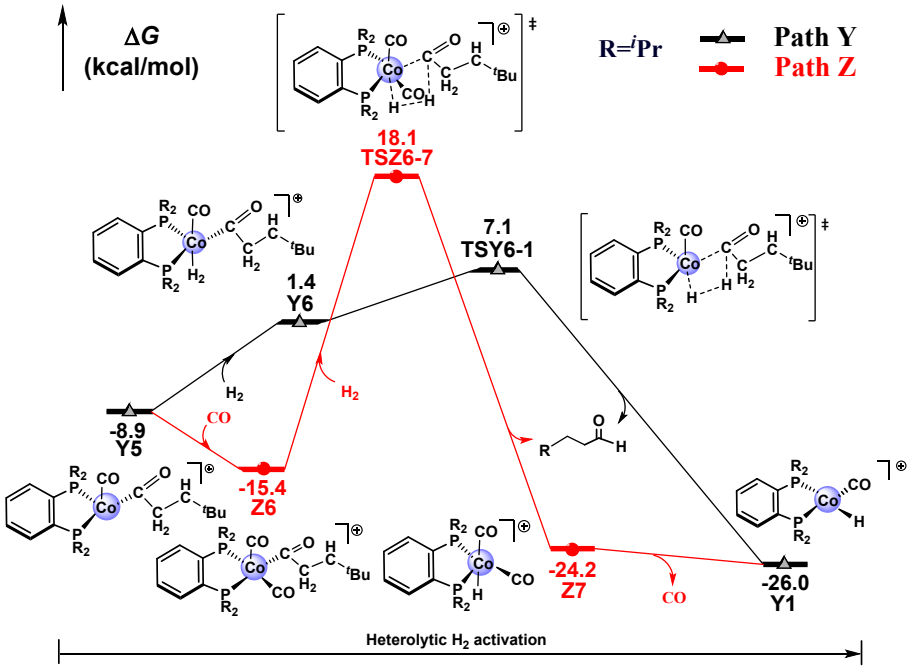


Fig. S21. With -^{i}Pr as substituent on phosphine, the Gibbs free energy barrier profile

of hydrogen activation step in dissociative (black line) and associative mechanism (red line).

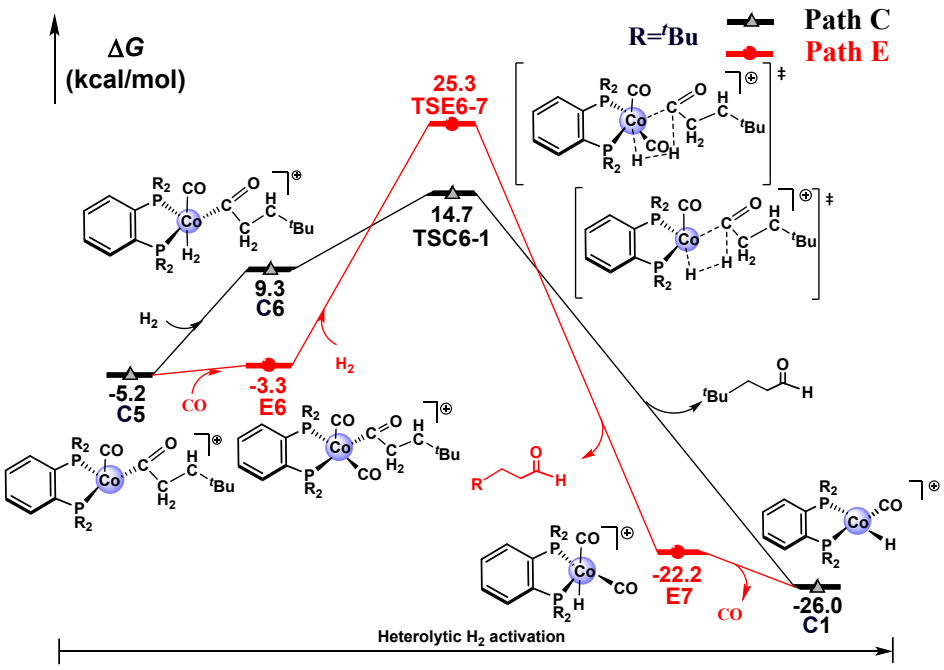
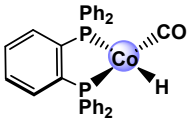
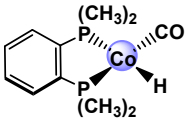
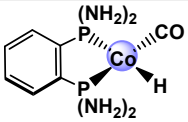
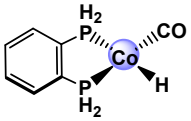
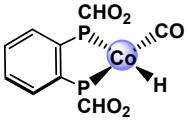
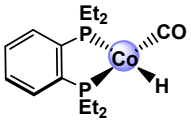
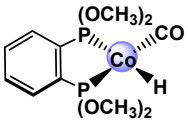
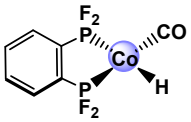
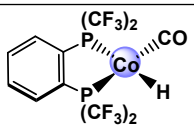
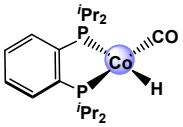
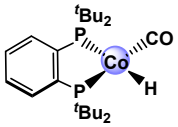


Fig. S22. With -^{t}Bu as substituent on phosphine, the Gibbs free energy barrier profile of hydrogen activation step in dissociative (black line) and associative mechanism (red line).

9. The Gibbs free energy barrier of hydrogen activation step, Mulliken charges of central metal cobalt and the bond length of Co-C

Table S1. The Gibbs free energy barrier of hydrogen activation step, Mulliken charges of central metal cobalt and the bond length of Co-C.

Entry	Catalytic active specie	$\Delta G^{\neq}$(kcal/mol)	Mulliken Charge of Co	Bond length of Co-C (Å)
1		34.6	-0.355	1.923
2		31.6	-0.721	1.991
3		28.9	-0.684	1.996
4		28.9	-0.460	2.052
5		28.2	-0.525	2.076
6		26.8	-0.791	2.013
7		23.6	-1.078	2.032
8		22.8	-0.734	2.107
9		22.6	-0.492	2.107
10		22.5	-0.929	2.015
11		19.9	-0.941	2.063

10. Energies of all the structures

Table S2. The calculated absolute electronic energies (E, in a.u.), thermal free energies (G, in a.u.), and relative Gibbs energies (G, in kcal/mol) (Calculated at 298.15 K and 1 atm).

	E	*G*	Δ*G*
H_2	-1.171273	-1.172611	/
CO	-113.267125	-113.281147	/
3,3-dimethylbutene	-235.779603	-235.643717	/
Linear aldehyde	-350.304656	-350.138786	/
Branched aldehyde	-350.303418	-350.137131	/
Hacac	-345.697573	-345.604466	/
A1	-1489.339230	-1489.020338	/
A2	-1725.135761	-1724.651695	6.7
TSA2-3	-1725.132059	-1724.650985	6.6
A3	-1725.153512	-1724.670522	-3.7
A4	-1838.450529	-1837.961486	-11.2
TSA4-5	-1838.439262	-1837.949429	-2.6
A5	-1838.456538	-1837.959196	-7.5
A6	-1839.622121	-1839.111929	0.2
TSA6-1	-1839.605575	-1839.099962	3.5
B2	-1602.631650	-1602.306615	-5.7
B3	-1838.424019	-1837.938884	1.0
TSB3-4	-1838.405246	-1837.918868	13.3
B6	-1951.760412	-1951.261846	-23.3
TSB6-7	-1952.874172	-1952.362879	17.2
B7	-1602.622228	-1602.294796	-23.9
C2	-1725.132887	-1724.650372	7.1
TSC2-3	-1725.131193	-1724.650009	6.8

C3	-1725.150317	-1724.664144	2.3
C4	-1838.438528	-1837.944809	1.8
TSC4-5	-1838.423092	-1837.930068	10.7
C5	-1838.456619	-1837.962082	-9.0
C6	-1839.621487	-1839.113958	0.7
TSC6-1	-1839.605652	-1839.095188	9.1
D6	-1951.755186	-1951.252212	-20.6
E1	-1803.755547	-1803.209878	/
E2	-2039.529219	-2038.842858	5.1
TSE2-3	-2039.534624	-2038.827419	15.3
E3	-2039.561377	-2038.854494	0.1
E4	-2152.852786	-2152.13678	-2.1
TSE4-5	-2152.847138	-2152.13109	1.9
E5	-2152.863198	-2152.144506	-5.2
E6	-2154.02313	-2153.28667	9.3
TSE6-1	-2154.008055	-2153.274256	14.7
F2	-2039.527558	-2038.826151	14.3
TSF2-3	-2039.527648	-2038.823058	17.0
F3	-2039.552647	-2038.843419	8.7
F4	-2152.834324	-2152.112983	14.8
TSF4-5	-2152.831268	-2152.114195	14.4
F5	-2152.856866	-2152.140422	-1.7
F6	-2154.023036	-2153.286064	11.6
TSF6-1	-2154.00501	-2153.271785	19.1
G6	-2266.14493	-2265.420331	-3.3
TSG6-7	-2267.274302	-2266.53992	-25.3
G7	-1917.035071	-1916.481549	-22.2
H6	-2266.146671	-2265.425169	-5.4
I1	-2098.803539	-2098.395783	/

I5	-2447.924277	-2447.342477	-13.6
I6	-2449.097190	-2448.499722	-5.4
J6	-2561.234120	-2560.648869	-30.1
J7	-2212.091113	-2211.677031	-28.7
TSI6-1	-2449.071175	-2448.475800	4.5
TSJ6-7	-2562.356757	-2561.761639	2.1
K1	-1332.102033	-1331.897256	/
K5	-1681.240446	-1680.857056	-11.0
K6	-1682.407289	-1682.010229	-3.2
L6	-1794.542376	-1794.157281	-25.4
L7	-1445.411102	-1445.194552	-28.5
TSK6-1	-1682.388956	-1681.990833	6.2
TSL6-7	-1795.664178	-1795.263819	11.7
M1	-1396.284324	-1396.120943	/
M5	-1745.404745	-1745.062827	-8.9
M6	-1746.571834	-1746.218620	-2.1
N6	-1858.706353	-1858.362312	-22.8
N7	-1509.571633	-1509.397787	-25.4
TSM6-1	-1746.552085	-1746.199460	6.1
TSN6-7	-1859.828648	-1859.475306	9.8
O1	-1174.826104	-1174.729813	/
O5	-1523.968821	-1523.696489	-22.4
O6	-1525.137343	-1524.850837	-14.7
P6	-1637.265363	-1636.991819	-34.4
P7	-1288.135400	-1288.032544	-40.1
TSO6-1	-1525.115328	-1524.828646	-5.5
TSP6-7	-1638.393758	-1638.107333	-3.2
Q1	-1627.953167	-1627.824292	/
Q5	-1977.087870	-1976.784035	-19.0

QA6	-1978.254926	-1977.938299	-11.0
R6	-2090.380343	-2090.075123	-27.6
R7	-1741.248919	-1741.115812	-33.9
TSQ6-1	-1978.232775	-1977.914064	0.6
TSR6-7	-2091.513796	-2091.195526	0.0
S1	-1632.897847	-1632.672602	/
S5	-1982.019468	-1981.621572	-14.8
S6	-1983.190484	-1982.774475	-4.3
T6	-2095.321510	-2094.916278	-23.5
T7	-1746.189565	-1745.957225	-30.8
TSS6-1	-1983.173716	-1982.761297	0.1
TST6-7	-2096.448315	-2096.034461	5.9
U1	-1571.801121	-1571.732032	/
U5	-1920.936385	-1920.692269	10.0
U6	-1922.105319	-1921.847961	-9.8
V6	-2034.229772	-2033.984108	-25.8
V7	-1685.097918	-1685.022787	-33.3
TSU6-1	-1922.082110	-1921.827661	-3.0
TSV6-7	-2035.360857	-2035.106182	-0.2
W1	-2522.577755	-2522.476661	/
W5	-2871.721809	-2871.450333	-29.0
W6	-2872.900281	-2872.609456	-22.0
X6	-2985.022762	-2984.740814	-33.4
X7	-2635.893159	-2635.782708	-42.0
TSW6-1	-2872.879324	-2872.585455	-10.8
TSX6-7	-2986.154785	-2985.862543	-8.7
Y1	-1646.555188	-1646.122929	/
Y5	-1995.670096	-1995.064835	-8.9
Y6	-1996.835202	-1996.213734	1.4

Z6	-2108.965705	-2108.352336	-15.4
Z7	-1759.835579	-1759.397365	-24.2
TSY6-1	-1996.820371	-1996.199675	7.1
TSZ6-7	-2110.081994	-2109.460811	18.1
A1$_{M06-L}$	-1490.239455	-1489.928086	/
A2$_{M06-L}$	-1726.097676	-1725.626643	0.0
TSA2-3$_{M06-L}$	-1726.095698	-1725.625316	0.4
A3$_{M06-L}$	-1726.110860	-1725.637323	-7.4
A4$_{M06-L}$	-1839.442594	-1838.962165	-19.7
TSA4-5$_{M06-L}$	-1839.423312	-1838.942393	-8.6
A5$_{M06-L}$	-1839.436469	-1838.954114	-15.3
A6$_{M06-L}$	-1840.611187	-1840.113744	-11.1
TSA6-1$_{M06-L}$	-1840.598906	-1840.106168	-6.1
B2$_{M06-L}$	-1603.582670	-1603.265674	-15.6
B3$_{M06-L}$	-1839.415322	-1838.943276	-7.3
TSB3-4$_{M06-L}$	-1839.395178	-1838.921152	7.8
B6$_{M06-L}$	-1952.783865	-1952.296508	-37.3
TSB6-7$_{M06-L}$	-1953.906905	-1953.408457	-0.3
B7$_{M06-L}$	-1603.575858	-1603.256378	-36.5
TSC2-3$_{M06-L}$	-1726.094118	-1725.621981	2.7
C3$_{M06-L}$	-1726.103584	-1725.629493	-2.7
C4$_{M06-L}$	-1839.432497	-1838.950641	-11.7
TSC4-5$_{M06-L}$	-1839.415148	-1838.934088	-2.3
C5$_{M06-L}$	-1839.439783	-1838.957185	-16.6
C6$_{M06-L}$	-1840.612096	-1840.115126	-10.1
TSC6-1$_{M06-L}$	-1840.597388	-1840.102898	-2.9
A1^{IV}	-1489.304262	-1488.987960	22.9
A2^{IV}	-1725.096357	-1724.619822	23.0
A3^{IV}	-1725.135077	-1724.657259	1.6

A4^{IV}	-1838.406406	-1837.924539	12.5
TSA4-5^{IV}	-1838.398826	-1837.913853	20.5
A5^{IV}	-1838.431821	-1837.943269	0.7
A6^{IV}	-1839.610416	-1839.106955	6.0
B2^{IV}	-1602.575300	-1602.257656	24.6
B3^{IV}	-1838.369118	-1837.892985	24.4
B6^{IV}	-1951.706779	-1951.212878	7.8
B7^{IV}	-1602.557546	-1602.237571	10.1
TSC2-3^{IV}	-1725.079756	-1724.601765	38.9
C3^{IV}	-1725.137853	-1724.657807	4.5
C4^{IV}	-1838.411875	-1837.928095	12.2
TSC4-5^{IV}	-1838.411009	-1837.927082	12.6
C5^{IV}	-1838.442130	-1837.952289	-3.7
C6^{IV}	-1839.606538	-1839.104179	7.9
TSC6-1^{IV}	-1839.576992	-1839.076499	23.2
A1^{VI}	-1489.167269	-1488.857156	105.7
A2^{VI}	-1724.962755	-1724.496730	98.8
A3^{VI}	-1725.002482	-1724.529880	80.6
A4^{VI}	-1838.278943	-1837.804460	83.1
A5^{VI}	-1838.307463	-1837.823110	76.2
A6^{VI}	-1839.479700	-1838.988843	103.1
B2^{VI}	-1602.379531	-1602.062698	147.0
B3^{VI}	-1838.230627	-1837.760157	113.4
B6^{VI}	-1951.589975	-1951.100820	77.2
B7^{VI}	-1602.376977	-1602.060870	122.6
C3^{VI}	-1725.006663	-1724.532651	82.0
C4^{VI}	-1838.281231	-1837.806109	102.3
C5^{VI}	-1838.306754	-1837.823872	76.2
C6^{VI}	-1839.478403	-1838.985021	81.2

IM1	-1833.883171	-1833.463883	-37.3
TS1-2	-1835.000108	-1834.566168	0.8
IM2	-1489.30948	-1488.987268	-14.0
IM3	-1602.624131	-1602.297639	-33.5
IM4	-1602.626911	-1602.299083	-35.3
IM5	-1715.899745	-1715.570713	-28.3
IM6	-1602.621729	-1602.29462	-32.7
IM7	-3205.276856	-3204.583281	-26.0

11. Frequencies of transition states

Table S3. Calculated imaginary frequencies of transition states.

In Tetrahydrofuran Solution	
TSA2-3	298.89*i*
TSA4-5	243.84*i*
TSA6-1	1292.94*i*
TSB3-4	154.76*i*
TSB6-7	1340.75*i*
TSC2-3	196.14*i*
TSC4-5	196.14*i*
TSC6-1	1142.56*i*
TSE2-3	227.45*i*
TSE4-5	247.98*i*
TSE6-1	1192.23*i*
TSF2-3	441.56*i*
TSF4-5	180.28*i*
TSF6-1	1151.18*i*
TSG6-7	1367.17*i*
TSI6-1	1239.24*i*
TSJ6-7	1379.60*i*

TSK6-1	1230.80*i*
TSL6-7	1440.91*i*
TSM6-1	1226.81*i*
TSN6-7	1429.54*i*
TSO6-1	1208.20*i*
TSP6-7	1449.59*i*
TSQ6-1	1224.75*i*
TSR6-7	1418.91*i*
TSS6-1	1243.65*i*
TST6-7	1339.07*i*
TSU6-1	1249.33*i*
TSV6-7	1449.67*i*
TSW6-1	1231.91*i*
TSX6-7	1439.31*i*
TSY6-1	1121.82*i*
TSZ6-7	1256.52*i*
TSA2-3$_{\mathbf{M06\text{-}L}}$	179.19*i*
TSA4-5$_{\mathbf{M06\text{-}L}}$	256.48*i*
TSA6-1$_{\mathbf{M06\text{-}L}}$	910.74*i*
TSB3-4$_{\mathbf{M06\text{-}L}}$	234.12*i*
TSB6-7$_{\mathbf{M06\text{-}L}}$	1395.07*i*
TSC2-3$_{\mathbf{M06\text{-}L}}$	501.65*i*
TSC4-5$_{\mathbf{M06\text{-}L}}$	207.77*i*
TSC6-1$_{\mathbf{M06\text{-}L}}$	1022.18*i*
TSA4-5$^{\mathbf{IV}}$	315.02*i*
TSC2-3$^{\mathbf{IV}}$	947.92*i*
TSC4-5$^{\mathbf{IV}}$	-272.20*i*
TSC6-1$^{\mathbf{IV}}$	1359.07*i*
TS1-2	1453.3*i*

12. Cartesian coordinates of all the structures

Table S4: Atomic cartesian coordinates of all intermediates and transition states (presented in Å).

3,3-dimethylbutene

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.352667	0.000796	0.000022
C	-1.117019	-0.462085	1.253277
H	-1.207688	-1.554704	1.282593
H	-0.605014	-0.141020	2.167793
H	-2.129697	-0.041020	1.263780
C	-0.252535	1.528612	-0.000003
H	0.275110	1.896355	0.887550
H	0.274906	1.896337	-0.887683
H	-1.254823	1.972267	0.000112
C	-1.117287	-0.462104	-1.253062
H	-0.605475	-0.141057	-2.167693
H	-1.207967	-1.554724	-1.282338
H	-2.129965	-0.041035	-1.263351
C	1.005455	-0.669082	-0.000113
H	0.963063	-1.760664	-0.000143
C	2.199427	-0.080117	-0.000164
H	3.114663	-0.667561	-0.000233
H	2.320647	1.000707	-0.000126

A1

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.910447	0.845342	-0.000741
C	-3.087700	-0.275943	-0.001059
C	-1.697957	-0.123912	-0.000437
C	-1.137744	1.161120	0.000441
C	-1.971217	2.283752	0.000844
C	-3.352515	2.124290	0.000255
H	-4.989054	0.723252	-0.001271
H	-3.526871	-1.269376	-0.001846
H	-1.541014	3.281796	0.001606
H	-3.997411	2.997701	0.000538
P	0.684165	1.308000	0.001046
P	-0.564130	-1.562557	-0.000862
C	1.114301	2.337604	-1.452386
H	0.541760	3.271379	-1.411803
H	2.173429	2.596610	-1.337009
C	1.113267	2.335017	1.456590
H	2.172500	2.594187	1.342570
H	0.540788	3.268892	1.417182
C	0.883089	1.600133	-2.769294
H	1.459289	0.667667	-2.805923
H	-0.175273	1.357092	-2.910812
H	1.199042	2.221639	-3.612908
C	0.880952	1.595185	2.771955
H	-0.177516	1.351855	2.912172
H	1.457177	0.662684	2.807418

H	1.196161	2.215167	3.616974
C	-1.038623	-2.566817	1.453574
H	-2.111736	-2.779693	1.383154
H	-0.505848	-3.519396	1.359075
C	-0.696703	-1.881839	2.774539
H	0.381119	-1.702380	2.860144
H	-1.216527	-0.923148	2.874354
H	-0.996425	-2.515082	3.615314
C	-1.037281	-2.564516	-1.457297
H	-0.504382	-3.517149	-1.364088
H	-2.110411	-2.777717	-1.388223
C	-0.694270	-1.876973	-2.776629
H	-1.214190	-0.918196	-2.875094
H	0.383611	-1.697121	-2.860817
H	-0.993022	-2.508600	-3.618968
Co	1.526139	-0.797377	-0.000202
H	1.870781	-2.292715	-0.000973
C	3.317044	-0.472177	-0.000052
O	4.446571	-0.320427	0.000012

A2

Coordinates (Angstroms)

	X	Y	Z
C	-4.441576	1.334731	-0.701069
C	-3.241743	1.769689	-0.150558
C	-2.136112	0.913373	-0.119297
C	-2.238479	-0.380940	-0.640315

C	-3.448241	-0.809500	-1.197773
C	-4.543609	0.045916	-1.227504
H	-5.299234	2.000117	-0.722611
H	-3.162568	2.774169	0.257208
H	-3.537621	-1.813108	-1.604633
H	-5.480545	-0.292052	-1.659326
P	-0.769405	-1.472660	-0.534000
P	-0.520360	1.432750	0.562148
C	-1.405529	-2.986396	0.299591
H	-2.107953	-3.466121	-0.392437
H	-0.553127	-3.666060	0.414826
C	-0.504740	-2.048623	-2.258398
H	0.266580	-2.826702	-2.215914
H	-1.426760	-2.530336	-2.604213
C	-2.083744	-2.736495	1.644718
H	-1.391887	-2.321412	2.382998
H	-2.929252	-2.047598	1.547583
H	-2.464181	-3.680783	2.047322
C	-0.093935	-0.925343	-3.206007
H	-0.874438	-0.160554	-3.276592
H	0.829897	-0.440756	-2.873997
H	0.078542	-1.322905	-4.211239
C	-0.065036	2.920255	-0.424695
H	-0.691861	3.753234	-0.085579
H	0.969884	3.164610	-0.159912
C	-0.212005	2.734766	-1.934727
H	0.338600	1.862662	-2.299910
H	-1.262103	2.611200	-2.217124
H	0.175999	3.616208	-2.454895
C	-0.900224	2.109708	2.229537

H	0.064357	2.338229	2.696366
H	-1.429081	3.060278	2.094242
C	-1.723484	1.172518	3.111564
H	-2.710158	0.982141	2.677462
H	-1.230562	0.207893	3.262718
H	-1.870238	1.626799	4.096549
Co	0.888276	-0.298006	0.474680
H	1.772795	0.759713	1.090483
C	0.852666	-1.032815	2.242688
O	1.089952	-1.409036	3.293922
C	3.895382	0.379794	-0.434903
C	4.242878	1.538446	0.507472
H	3.348841	2.108953	0.784638
H	4.713273	1.174639	1.428838
H	4.943038	2.225772	0.019653
C	5.204981	-0.284954	-0.905802
H	5.785808	-0.664295	-0.056880
H	5.000477	-1.122813	-1.581524
H	5.825095	0.443968	-1.440111
C	3.116639	0.914799	-1.637885
H	3.000117	0.161118	-2.424331
H	2.119200	1.235463	-1.312737
H	3.628344	1.777229	-2.078921
C	3.108283	-0.696301	0.300894
H	3.435596	-0.875035	1.324879
C	2.351911	-1.674261	-0.308026
H	2.143027	-2.607870	0.207546
H	2.219821	-1.679099	-1.387420

A3

	Coordinates (Angstroms)		
	X	Y	Z
C	4.515549	0.003743	-1.462260
C	3.410285	-0.833091	-1.360176
C	2.250323	-0.390487	-0.714792
C	2.202119	0.902999	-0.176047
C	3.320864	1.736933	-0.281635
C	4.471821	1.288071	-0.919064
H	5.413470	-0.345150	-1.962934
H	3.454004	-1.834863	-1.779116
H	3.293947	2.742232	0.129909
H	5.335688	1.941102	-0.996655
P	0.635658	1.478225	0.585738
P	0.793274	-1.477878	-0.495401
C	1.133252	2.258530	2.174306
H	1.831663	3.073534	1.950889
H	0.228782	2.717201	2.591102
C	0.158660	2.919175	-0.461002
H	-0.820996	3.255440	-0.100895
H	0.867559	3.735182	-0.276867
C	1.750122	1.280330	3.171004
H	1.032153	0.514030	3.478000
H	2.629816	0.780283	2.751465
H	2.066895	1.814431	4.072554
C	0.106151	2.584656	-1.951471
H	1.108419	2.398353	-2.350013
H	-0.505165	1.698042	-2.151410

H	-0.328503	3.419950	-2.509653
C	0.450561	-2.182551	-2.153332
H	1.350883	-2.701809	-2.501232
H	-0.324426	-2.944691	-2.009521
C	0.001308	-1.135251	-3.168446
H	-0.909587	-0.624096	-2.838698
H	0.776441	-0.378453	-3.331147
H	-0.212124	-1.609653	-4.131477
C	1.434059	-2.912732	0.465395
H	0.557094	-3.502241	0.757490
H	2.033403	-3.534120	-0.210363
C	2.259174	-2.519212	1.690348
H	3.196296	-2.035121	1.398825
H	1.721157	-1.831294	2.349719
H	2.507817	-3.411999	2.272893
Co	-0.814500	-0.296991	0.516259
C	-4.098479	0.394950	-0.449536
C	-4.811729	1.505314	0.331838
H	-5.370956	1.094664	1.181061
H	-4.093381	2.238430	0.721925
H	-5.519450	2.040896	-0.311070
C	-3.343666	1.016618	-1.626742
H	-2.621523	1.763677	-1.273414
H	-2.803274	0.264048	-2.211800
H	-4.037318	1.523399	-2.307022
C	-5.129210	-0.621438	-0.954107
H	-4.655353	-1.410948	-1.548481
H	-5.654134	-1.097183	-0.116941
H	-5.878025	-0.127679	-1.584400
C	-3.113756	-0.316679	0.507019

H	-2.427596	0.547640	0.867534
C	-2.289842	-1.460906	-0.008165
H	-2.284381	-1.589676	-1.093296
H	-2.423646	-2.412956	0.504333
C	-0.809497	-1.010580	2.290418
O	-0.946167	-1.576781	3.271616
H	-3.617228	-0.593154	1.440409

A4

Coordinates (Angstroms)

	X	Y	Z
C	-4.682703	-1.764146	-0.321118
C	-4.112294	-0.497205	-0.293147
C	-2.725093	-0.358913	-0.172825
C	-1.915256	-1.494969	-0.076760
C	-2.496060	-2.767284	-0.108336
C	-3.874336	-2.898840	-0.231791
H	-5.758647	-1.871262	-0.416752
H	-4.745483	0.383363	-0.367609
H	-1.873559	-3.654767	-0.030885
H	-4.322944	-3.886960	-0.256214
P	-0.112155	-1.264504	0.134957
P	-1.914538	1.276117	-0.169942
C	0.233796	-2.075981	1.753251
H	0.196831	-3.159562	1.592156
H	1.263424	-1.825350	2.028078
C	0.635696	-2.365917	-1.128058

H	1.722045	-2.304082	-1.005817
H	0.345113	-3.398005	-0.901246
C	-0.731355	-1.673158	2.867661
H	-0.779202	-0.588585	3.005894
H	-1.745790	-2.029694	2.665610
H	-0.401004	-2.113172	3.813705
C	0.228438	-1.991104	-2.552276
H	-0.844744	-2.140223	-2.710003
H	0.464404	-0.945867	-2.780694
H	0.764277	-2.618987	-3.270895
C	-2.415592	2.027694	-1.769864
H	-3.508510	1.990525	-1.842432
H	-2.130323	3.085986	-1.732846
C	-1.764748	1.330161	-2.962093
H	-0.670671	1.392755	-2.911708
H	-2.045826	0.272720	-3.008397
H	-2.081457	1.803558	-3.896567
C	-2.807601	2.277633	1.082581
H	-2.355941	3.276135	1.057598
H	-3.843915	2.381786	0.739067
C	-2.769027	1.698595	2.494062
H	-3.202887	0.693897	2.527450
H	-1.748427	1.645806	2.885137
H	-3.348944	2.336033	3.168901
Co	0.364621	0.966372	-0.065746
C	0.760542	1.360439	1.784742
C	0.714168	2.650729	-0.672724
O	1.181220	1.556825	2.824744
O	0.958619	3.705814	-1.028853
C	4.616060	-0.524121	-0.088982

C	5.338568	-1.238516	1.062097
H	5.403439	-0.595247	1.948779
H	4.811620	-2.156836	1.351384
H	6.360216	-1.515933	0.774866
C	4.582129	-1.454292	-1.308846
H	4.062731	-2.393250	-1.077102
H	4.076170	-0.989027	-2.162794
H	5.600071	-1.709578	-1.627969
C	5.383570	0.757009	-0.441702
H	4.969139	1.249409	-1.328630
H	5.358238	1.475933	0.387375
H	6.435250	0.530217	-0.655136
C	3.177328	-0.198083	0.393588
H	3.269260	0.372510	1.327940
C	2.303810	0.575447	-0.584948
H	2.141809	0.030247	-1.523067
H	2.810885	1.508596	-0.847242
H	2.710019	-1.151490	0.665765

A5

Coordinates (Angstroms)

	X	Y	Z
C	-4.634478	1.472350	-0.704778
C	-3.503549	1.769770	0.046046
C	-2.372234	0.947531	-0.021268
C	-2.386515	-0.181892	-0.852870
C	-3.529655	-0.472007	-1.607217

C	-4.647538	0.349714	-1.533111
H	-5.508158	2.114114	-0.644697
H	-3.504275	2.640735	0.696567
H	-3.544611	-1.340651	-2.260420
H	-5.531146	0.116043	-2.119185
P	-0.890729	-1.232444	-0.958819
P	-0.892618	1.292802	1.006724
C	-1.489162	-2.949788	-0.709580
H	-2.243968	-3.161749	-1.475799
H	-0.631680	-3.601837	-0.905170
C	-0.421354	-1.177509	-2.736929
H	0.523539	-1.725820	-2.821003
H	-1.170296	-1.734476	-3.311929
C	-2.051668	-3.193786	0.688594
H	-1.278545	-3.077593	1.455101
H	-2.873038	-2.506321	0.918481
H	-2.439562	-4.214796	0.764028
C	-0.278301	0.244095	-3.280250
H	-1.246315	0.754046	-3.316906
H	0.397565	0.848871	-2.666568
H	0.126970	0.218307	-4.296670
C	-0.526762	3.073288	0.705135
H	-1.395855	3.653237	1.037840
H	0.305390	3.339391	1.367795
C	-0.193331	3.402943	-0.747713
H	0.717823	2.897976	-1.082638
H	-1.010060	3.117481	-1.419362
H	-0.031535	4.479979	-0.858194
C	-1.565998	1.301715	2.725939
H	-0.700566	1.357049	3.397323

H	-2.145209	2.221105	2.869857
C	-2.427162	0.081383	3.053317
H	-3.372385	0.106149	2.502578
H	-1.927561	-0.861509	2.807883
H	-2.659391	0.064401	4.122915
Co	0.666857	-0.419342	0.545257
C	0.656613	-1.219493	2.220155
C	2.038668	-1.762602	0.025958
O	0.675689	-1.729579	3.241326
O	1.855812	-2.786879	-0.576955
C	4.021079	0.976804	-0.464888
C	4.146742	2.434082	-0.000323
H	3.210995	2.788161	0.452013
H	4.941770	2.543577	0.747220
H	4.383087	3.095363	-0.842117
C	5.330129	0.548966	-1.140934
H	6.172386	0.616676	-0.441958
H	5.281166	-0.479782	-1.515836
H	5.549588	1.199339	-1.995984
C	2.867363	0.873491	-1.464950
H	2.793711	-0.121023	-1.920249
H	1.913679	1.096313	-0.960992
H	2.977539	1.600140	-2.278275
C	3.737085	0.108403	0.778808
H	2.904321	0.566112	1.341371
C	3.434783	-1.374267	0.535837
H	3.506030	-1.907433	1.495024
H	4.167896	-1.837562	-0.133752
H	4.605203	0.165353	1.446359

A6

	Coordinates (Angstroms)		
	X	Y	Z
C	-4.700675	1.510738	-1.104814
C	-3.532530	1.919289	-0.472762
C	-2.476478	1.019022	-0.286779
C	-2.600591	-0.304994	-0.738015
C	-3.785075	-0.704563	-1.368344
C	-4.827547	0.196062	-1.551979
H	-5.513316	2.216662	-1.246143
H	-3.447854	2.943079	-0.118466
H	-3.895411	-1.726821	-1.720455
H	-5.740374	-0.126234	-2.043510
P	-1.204029	-1.473875	-0.495976
P	-0.957921	1.532363	0.598811
C	-1.954526	-2.911126	0.375934
H	-2.729149	-3.330928	-0.277188
H	-1.161253	-3.663620	0.455892
C	-0.939385	-2.191094	-2.172922
H	-0.237753	-3.021277	-2.039965
H	-1.890546	-2.623155	-2.504636
C	-2.531782	-2.592406	1.751303
H	-1.756299	-2.257884	2.446584
H	-3.302452	-1.816326	1.695325
H	-2.990914	-3.489207	2.180032
C	-0.404938	-1.208033	-3.211621
H	-0.999801	-0.287676	-3.247864

H	0.635496	-0.939264	-3.008637
H	-0.439162	-1.663045	-4.206721
C	-0.485510	3.156853	-0.132778
H	-1.325068	3.845367	0.017488
H	0.345212	3.537376	0.474381
C	-0.095785	3.108634	-1.607665
H	0.846300	2.572918	-1.763299
H	-0.871139	2.628250	-2.214720
H	0.042538	4.125257	-1.989194
C	-1.558149	2.036643	2.269693
H	-0.665961	2.224680	2.878590
H	-2.076827	2.995975	2.158981
C	-2.475985	1.023163	2.950077
H	-3.413550	0.904024	2.398351
H	-2.012340	0.037133	3.043135
H	-2.721483	1.368586	3.959380
Co	0.580826	-0.213961	0.427719
C	0.558597	-0.658764	2.188319
C	2.010021	-1.618786	0.233047
O	0.524927	-0.938945	3.295686
O	1.804192	-2.688270	-0.273673
C	4.655586	0.648182	-0.470419
C	4.799999	2.176209	-0.479246
H	3.828167	2.666612	-0.621325
H	5.225157	2.539567	0.464497
H	5.460779	2.501929	-1.291244
C	6.044342	0.022280	-0.273954
H	6.479485	0.323990	0.686517
H	6.011512	-1.072938	-0.300992
H	6.726747	0.347728	-1.068011

C	4.081709	0.191125	-1.818474
H	3.886124	-0.887850	-1.840981
H	3.148910	0.714595	-2.058396
H	4.789853	0.410111	-2.626318
C	3.736572	0.266005	0.714210
H	2.824598	0.882610	0.669570
C	3.354023	-1.218312	0.827391
H	3.256767	-1.488146	1.888541
H	4.119797	-1.880990	0.410448
H	4.243955	0.567874	1.637670
H	1.399304	0.067317	-1.119544
H	0.802581	0.574309	-1.146051

B2

Coordinates (Angstroms)

	X	Y	Z
C	-3.818081	1.482288	0.324504
C	-2.491263	1.857120	0.503955
C	-1.465205	0.949925	0.221455
C	-1.777821	-0.333055	-0.243773
C	-3.114509	-0.704551	-0.419412
C	-4.129429	0.201892	-0.134831
H	-4.612853	2.187701	0.545790
H	-2.256661	2.853806	0.868182
H	-3.364018	-1.701035	-0.773152
H	-5.166622	-0.088134	-0.271021
P	-0.400631	-1.477178	-0.611785

P	0.295017	1.374559	0.467471
C	-0.737539	-3.010419	0.335249
H	-1.590179	-3.512166	-0.136922
H	0.138513	-3.652861	0.194008
C	-0.605201	-1.922612	-2.375702
H	0.007697	-2.814892	-2.545643
H	-1.651965	-2.196884	-2.548059
C	-1.007097	-2.772404	1.820127
H	-0.174389	-2.257965	2.309878
H	-1.911610	-2.175195	1.971477
H	-1.147051	-3.732543	2.326113
C	-0.173024	-0.785307	-3.298375
H	-0.770057	0.117286	-3.131084
H	0.883984	-0.537229	-3.140930
H	-0.296090	-1.078398	-4.345554
C	0.556055	2.935783	-0.457184
H	-0.140348	3.686447	-0.065985
H	1.571174	3.271860	-0.213317
C	0.388696	2.768813	-1.965255
H	1.099095	2.038997	-2.370252
H	-0.625675	2.441216	-2.217603
H	0.566510	3.723493	-2.470109
C	0.429215	1.880497	2.227912
H	1.490765	2.082372	2.412106
H	-0.106232	2.831287	2.336368
C	-0.107921	0.850184	3.218121
H	-1.174798	0.662364	3.061285
H	0.420355	-0.104890	3.140823
H	0.022536	1.219231	4.240129
Co	1.520701	-0.381137	-0.272802

C	2.202335	-1.157981	1.354768
O	2.690658	-1.737705	2.203327
C	3.073604	0.476338	-0.744161
O	4.048612	0.972251	-1.060291
H	2.062155	-1.609317	-0.994862

B3

	Coordinates (Angstroms)		
	X	Y	Z

C	4.681554	1.395586	-0.878456
C	3.982632	0.194714	-0.854172
C	2.639055	0.164046	-0.463807
C	1.999766	1.355829	-0.100286
C	2.710671	2.561573	-0.124108
C	4.045162	2.580764	-0.510172
H	5.723990	1.408810	-1.181397
H	4.488300	-0.724841	-1.135483
H	2.221067	3.489721	0.158771
H	4.589616	3.519811	-0.525412
P	0.235881	1.344086	0.375577
P	1.714555	-1.412237	-0.365490
C	0.180308	2.185311	2.010032
H	0.482395	3.226966	1.849092
H	-0.872018	2.200740	2.317370
C	-0.517672	2.601270	-0.736063
H	-1.576765	2.671524	-0.468185
H	-0.060019	3.564334	-0.480465

C	1.051107	1.537741	3.082245
H	0.740256	0.511235	3.296236
H	2.105249	1.519911	2.786785
H	0.972548	2.103040	4.016153
C	-0.355047	2.318560	-2.225740
H	0.701377	2.280358	-2.511977
H	-0.824213	1.372721	-2.515438
H	-0.831617	3.116381	-2.804548
C	1.950330	-2.179641	-2.021844
H	3.027537	-2.288073	-2.196111
H	1.534978	-3.193026	-1.961013
C	1.299355	-1.394607	-3.158829
H	0.213952	-1.329273	-3.035296
H	1.696315	-0.375132	-3.216951
H	1.499060	-1.887994	-4.115558
C	2.764108	-2.462177	0.729362
H	2.208034	-3.392538	0.895645
H	3.675316	-2.728118	0.180381
C	3.122888	-1.801691	2.060114
H	3.743417	-0.913031	1.907999
H	2.235817	-1.498907	2.625195
H	3.687884	-2.501891	2.683522
Co	-0.498728	-0.774771	0.217812
C	-0.456848	-1.423451	1.939112
O	-0.464270	-1.929035	2.961075
C	-4.449223	0.459840	-0.389012
C	-5.638073	1.436441	-0.310101
H	-6.180105	1.318158	0.635103
H	-5.302394	2.478032	-0.381918
H	-6.339281	1.250330	-1.132121

C	-3.711419	0.677124	-1.722104
H	-3.308683	1.694648	-1.795779
H	-2.878113	-0.026422	-1.829781
H	-4.395953	0.524737	-2.565019
C	-4.969402	-0.977437	-0.313895
H	-4.153832	-1.707302	-0.363304
H	-5.525835	-1.153589	0.613740
H	-5.644945	-1.177420	-1.153059
C	-3.510767	0.795015	0.748617
H	-3.154352	1.826782	0.744451
C	-3.122981	0.001340	1.751182
H	-2.488929	0.386265	2.546760
H	-3.459167	-1.028185	1.849970
C	-1.328922	-2.154936	-0.620008
O	-1.778149	-3.023909	-1.206802
H	-0.601911	-0.201411	-1.157169

B6

Coordinates (Angstroms)

	X	Y	Z

C	-4.805013	-1.920909	0.487861
C	-4.219041	-0.676230	0.681892
C	-2.876088	-0.473891	0.345665
C	-2.121680	-1.524270	-0.188012
C	-2.720952	-2.774384	-0.382144
C	-4.054545	-2.970324	-0.043853
H	-5.847363	-2.075621	0.748367

H	-4.805275	0.138170	1.099021
H	-2.150671	-3.596393	-0.805628
H	-4.513257	-3.942176	-0.197201
P	-0.378851	-1.215548	-0.672424
P	-2.058568	1.132972	0.616947
C	0.555799	-2.580032	0.129791
H	0.100210	-3.520096	-0.201006
H	1.569844	-2.558505	-0.280511
C	-0.353217	-1.664132	-2.454076
H	0.678969	-1.547781	-2.798398
H	-0.607591	-2.727932	-2.530510
C	0.579691	-2.507923	1.653612
H	1.114247	-1.622152	2.009576
H	-0.432941	-2.489407	2.071096
H	1.093115	-3.385466	2.058919
C	-1.300269	-0.814765	-3.298866
H	-2.343287	-0.961860	-2.999602
H	-1.056222	0.248127	-3.216568
H	-1.211722	-1.096377	-4.352911
C	-3.122199	2.367351	-0.228339
H	-4.144763	2.256996	0.150457
H	-2.768299	3.356286	0.088155
C	-3.085189	2.235141	-1.749114
H	-2.071164	2.377187	-2.141473
H	-3.442328	1.251733	-2.072796
H	-3.727714	2.992936	-2.208034
C	-2.290175	1.490636	2.407653
H	-1.655472	2.355629	2.634152
H	-3.328774	1.806822	2.559000
C	-1.957579	0.310926	3.321820

H	-2.690788	-0.493611	3.209633
H	-0.968576	-0.112883	3.119038
H	-1.971359	0.636398	4.366560
Co	0.100141	1.008424	-0.212769
C	0.260116	2.840050	-0.433889
O	0.356537	3.969898	-0.542154
C	4.857279	-0.654156	0.341283
C	4.968052	-2.084936	0.887551
H	4.205698	-2.275929	1.654018
H	4.836719	-2.825771	0.088821
H	5.950976	-2.254045	1.343057
C	5.933873	-0.439192	-0.730703
H	5.786421	-1.118484	-1.579460
H	5.929689	0.587758	-1.113895
H	6.930798	-0.630121	-0.315888
C	5.067735	0.337852	1.492363
H	5.054249	1.377732	1.145833
H	4.292847	0.224658	2.260683
H	6.039127	0.167958	1.971768
C	3.444480	-0.504743	-0.260773
H	2.714513	-0.743199	0.522724
C	3.106178	0.866477	-0.854953
H	3.208254	1.652611	-0.097114
H	3.319681	-1.261125	-1.047934
C	0.961271	0.999373	1.511851
O	1.479746	1.099849	2.520597
H	3.765675	1.104428	-1.696033
C	1.680203	0.900631	-1.364514
O	1.407671	0.950675	-2.541147

B7

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.162206	1.755170	-0.202161
C	-0.474922	3.113259	-0.324030
H	-1.508997	3.434379	-0.394621
C	0.532171	4.072882	-0.347599
H	0.274210	5.122651	-0.447421
C	1.864685	3.689274	-0.224038
H	2.650660	4.437899	-0.217079
C	2.191328	2.341937	-0.114569
H	3.232804	2.056302	-0.009064
C	1.188672	1.366349	-0.134396
C	-0.522376	-2.200889	1.326622
Co	-0.301607	-1.533301	-0.368454
O	-0.700637	-2.586431	2.383696
P	-1.452627	0.468136	-0.001111
P	1.605770	-0.410522	-0.082688
C	-2.814964	0.914770	-1.150404
H	-3.005668	1.991637	-1.104908
H	-2.453032	0.689475	-2.159682
C	-4.104750	0.148687	-0.851070
H	-4.844533	0.351909	-1.631412
H	-3.946504	-0.934675	-0.818693
H	-4.537973	0.454535	0.106646
C	-2.119626	0.739852	1.695656
H	-2.848050	-0.064742	1.855973

H	-1.287936	0.547426	2.384113
C	-2.748920	2.099550	1.987330
H	-3.183473	2.095981	2.992470
H	-2.004298	2.900237	1.950408
H	-3.549033	2.339103	1.279082
C	2.813556	-0.790391	-1.417907
H	2.335727	-0.469861	-2.349881
H	2.838534	-1.887046	-1.450402
C	4.230600	-0.232570	-1.307915
H	4.860307	-0.703522	-2.069852
H	4.257379	0.845890	-1.484304
H	4.684765	-0.435970	-0.332716
C	2.495347	-0.652782	1.503735
H	3.301402	0.087207	1.564225
H	1.780164	-0.417966	2.300638
C	3.048757	-2.068656	1.660895
H	3.492757	-2.187929	2.653921
H	2.266524	-2.829373	1.552264
H	3.825451	-2.280456	0.919016
C	-1.547712	-2.455341	-1.323606
O	-2.300309	-2.997627	-1.985118
H	0.004794	-0.982329	-1.731359

Branched aldehyde

	Coordinates (Angstroms)		
	X	Y	Z

C	-1.666014	-0.245453	0.321987

O	-2.593865	-0.783910	-0.241824
C	0.856646	-0.208183	-0.009107
C	0.748621	-1.729055	-0.202512
H	0.053306	-2.182331	0.515118
H	0.396124	-1.975892	-1.211378
H	1.725224	-2.206262	-0.060193
C	1.933880	0.329381	-0.961275
H	1.674308	0.129062	-2.007753
H	2.082198	1.408724	-0.848440
H	2.895782	-0.155787	-0.756476
C	1.274561	0.090319	1.438080
H	1.432086	1.161686	1.603054
H	0.533017	-0.259741	2.165157
H	2.219306	-0.418590	1.663488
C	-0.515941	0.440145	-0.376930
C	-0.625661	1.940998	-0.066119
H	0.204893	2.499011	-0.508145
H	-0.627602	2.133604	1.012504
H	-0.675603	0.285392	-1.450886
H	-1.555686	2.347016	-0.478422
H	-1.642984	-0.203532	1.432225

C2

Coordinates (Angstroms)			
	X	Y	Z

C	4.698044	0.969529	-0.066009
C	3.893430	-0.146451	-0.261348

C	2.502494	-0.030779	-0.165572
C	1.917862	1.205115	0.129247
C	2.736657	2.324217	0.322865
C	4.117999	2.205266	0.224116
H	5.777240	0.878064	-0.139826
H	4.346980	-1.109546	-0.480021
H	2.298305	3.291676	0.552650
H	4.746148	3.077498	0.376774
P	0.087047	1.305442	0.264239
P	1.393713	-1.463277	-0.396206
C	-0.151192	2.082917	1.916442
H	0.341363	3.061900	1.886549
H	-1.221568	2.268862	2.040679
C	-0.334002	2.666235	-0.900853
H	-1.399243	2.887074	-0.765212
H	0.218003	3.564208	-0.599819
C	0.390120	1.251701	3.076639
H	-0.131930	0.294626	3.169029
H	1.459818	1.047645	2.961198
H	0.251917	1.792833	4.018182
C	-0.024870	2.306155	-2.352664
H	1.048229	2.144537	-2.499637
H	-0.548190	1.394621	-2.664658
H	-0.336598	3.115190	-3.020684
C	1.851634	-2.148118	-2.034476
H	2.925825	-2.367092	-2.025223
H	1.322218	-3.102392	-2.133478
C	1.501981	-1.208843	-3.186424
H	0.426788	-1.001670	-3.219468
H	2.032361	-0.254644	-3.098562

H	1.783304	-1.662682	-4.141697
C	1.977020	-2.722729	0.809935
H	1.232012	-3.526028	0.798675
H	2.916578	-3.142956	0.431733
C	2.168272	-2.176057	2.224477
H	2.977975	-1.440743	2.259710
H	1.262708	-1.694821	2.606734
H	2.424285	-2.992977	2.906380
Co	-0.732276	-0.785917	-0.222570
H	-0.825521	-2.236383	-0.630033
C	-1.247597	-1.468800	1.458510
O	-1.540662	-2.055071	2.394296
C	-3.960778	0.301111	-0.113467
C	-3.560859	1.176680	1.080752
H	-2.857902	0.656344	1.739276
H	-3.091033	2.108682	0.744134
H	-4.444782	1.442144	1.672182
C	-5.012806	1.062918	-0.947482
H	-4.622066	2.026262	-1.297042
H	-5.318545	0.481079	-1.824449
H	-5.904071	1.260218	-0.340709
C	-4.573509	-1.012703	0.378069
H	-4.981713	-1.602546	-0.449980
H	-3.844446	-1.633003	0.909251
H	-5.395819	-0.800647	1.070120
C	-2.781596	0.091844	-1.047429
H	-2.383637	1.011698	-1.470461
C	-2.422472	-1.082027	-1.639094
H	-1.779411	-1.077657	-2.517649
H	-2.935212	-2.014601	-1.427504

C3

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.502686	1.291206	-0.646530
C	-3.224712	1.779865	-0.402726
C	-2.151896	0.896884	-0.232961
C	-2.372347	-0.485776	-0.304643
C	-3.662937	-0.968205	-0.552386
C	-4.721597	-0.084459	-0.723799
H	-5.329238	1.982845	-0.777700
H	-3.062568	2.852851	-0.342671
H	-3.841556	-2.038574	-0.615676
H	-5.719350	-0.467060	-0.915780
P	-0.957398	-1.626779	-0.064847
P	-0.454878	1.508794	0.089650
C	-1.530982	-2.779713	1.250336
H	-2.413298	-3.312098	0.876124
H	-0.735903	-3.523701	1.379400
C	-0.973798	-2.679910	-1.575398
H	-0.213320	-3.456220	-1.427856
H	-1.943616	-3.187026	-1.642811
C	-1.848809	-2.091908	2.576392
H	-0.969993	-1.596140	2.999647
H	-2.639015	-1.342546	2.459918
H	-2.194453	-2.831022	3.306244
C	-0.690491	-1.882816	-2.847082

H	-1.454214	-1.115874	-3.015464
H	0.285578	-1.388205	-2.797518
H	-0.682853	-2.546101	-3.717895
C	-0.157850	2.734204	-1.247939
H	-0.894899	3.540578	-1.159303
H	0.828119	3.176107	-1.060136
C	-0.211963	2.107513	-2.640685
H	0.526357	1.305011	-2.751444
H	-1.201956	1.690027	-2.852194
H	0.003700	2.863007	-3.402814
C	-0.637365	2.530954	1.610840
H	0.366488	2.865137	1.893338
H	-1.215397	3.426138	1.351817
C	-1.296352	1.784751	2.769387
H	-2.331100	1.515378	2.534939
H	-0.756016	0.867350	3.023360
H	-1.309444	2.419594	3.661249
Co	0.971601	-0.315652	0.157129
C	3.683612	-0.279344	-0.591331
C	2.983638	-1.425369	-1.342844
H	2.252806	-1.965605	-0.711129
H	2.473842	-1.059330	-2.242210
H	3.704734	-2.188306	-1.658850
C	4.709885	0.360591	-1.544612
H	4.219492	0.783119	-2.429891
H	5.271914	1.161634	-1.052269
H	5.431520	-0.392095	-1.885828
C	4.426054	-0.847975	0.622803
H	4.916287	-0.058961	1.202804
H	3.757291	-1.399824	1.292303

H	5.202614	-1.548146	0.293243
C	2.620625	0.775200	-0.218344
H	2.231405	1.200451	-1.157579
C	3.052447	1.887527	0.714196
H	3.977070	2.365311	0.360366
H	3.242034	1.533871	1.733220
C	1.416928	-0.572442	1.922608
O	1.677348	-0.602081	3.036208
H	2.292654	2.672772	0.773152

C4

Coordinates (Angstroms)

	X	Y	Z

C	4.837815	-0.459743	-0.128348
C	3.690459	-1.224451	0.042213
C	2.426931	-0.621214	0.025399
C	2.321451	0.765203	-0.165949
C	3.485944	1.526379	-0.326689
C	4.735483	0.919230	-0.309280
H	5.812241	-0.937830	-0.115703
H	3.783526	-2.295423	0.197920
H	3.414882	2.600399	-0.477834
H	5.631218	1.518473	-0.439979
P	0.661961	1.543966	-0.228897
P	0.920148	-1.611253	0.345264
C	0.784972	2.946635	0.965183
H	1.563926	3.620770	0.589737

H	-0.162117	3.494195	0.900102
C	0.618372	2.451615	-1.846982
H	-0.442862	2.562501	-2.100242
H	1.011109	3.461641	-1.684468
C	1.083658	2.557182	2.409723
H	0.258209	2.003401	2.863905
H	1.993196	1.951576	2.484459
H	1.236822	3.460853	3.008444
C	1.378999	1.785077	-2.994909
H	2.459970	1.857994	-2.846681
H	1.137296	0.724734	-3.111009
H	1.134372	2.285478	-3.937369
C	1.115743	-3.156724	-0.637975
H	2.025475	-3.649642	-0.276435
H	0.277403	-3.805027	-0.355954
C	1.178362	-2.979573	-2.152389
H	0.204745	-2.719300	-2.573535
H	1.902264	-2.210542	-2.443116
H	1.489329	-3.920230	-2.617817
C	1.150864	-2.249051	2.065940
H	0.175548	-2.631595	2.389244
H	1.826141	-3.110554	2.013358
C	1.698338	-1.227639	3.061929
H	2.738687	-0.976097	2.834888
H	1.125470	-0.296727	3.070894
H	1.665111	-1.646369	4.072651
Co	-0.941809	-0.246834	-0.020655
C	-1.282747	-0.050894	1.757738
C	-1.025244	-0.469972	-1.825306
O	-1.448800	0.084961	2.878956

O	-1.122300	-0.523767	-2.961689
C	-3.976849	-0.254523	-0.096267
C	-3.625383	-1.675053	-0.564000
H	-3.424590	-1.711521	-1.641290
H	-2.736981	-2.053851	-0.033282
H	-4.450776	-2.367211	-0.358980
C	-4.395315	-0.327413	1.378833
H	-3.665180	-0.865070	1.991487
H	-4.551455	0.663617	1.817696
H	-5.340172	-0.876554	1.464940
C	-5.190019	0.234410	-0.913342
H	-5.522782	1.226816	-0.588676
H	-4.953558	0.288157	-1.982864
H	-6.035353	-0.453395	-0.791210
C	-2.795691	0.716934	-0.366757
H	-2.807815	0.921614	-1.441976
C	-2.859046	2.079339	0.314833
H	-2.093907	2.748607	-0.092038
H	-2.726427	2.046179	1.400390
H	-3.829550	2.559670	0.122811

C5

Coordinates (Angstroms)			
	X	Y	Z

C	4.535262	1.732722	-0.011560
C	3.295401	1.833211	-0.630760
C	2.259855	0.955872	-0.287297

C	2.480138	-0.029473	0.685160
C	3.732336	-0.122598	1.304413
C	4.753568	0.754034	0.958958
H	5.332745	2.417109	-0.283985
H	3.130672	2.597649	-1.385976
H	3.909656	-0.884829	2.058939
H	5.721565	0.674642	1.443985
P	1.127861	-1.188970	1.118016
P	0.612189	1.079526	-1.076125
C	1.903073	-2.850673	0.916561
H	2.643763	-2.981641	1.714632
H	1.111022	-3.589649	1.086010
C	0.958374	-1.018548	2.947821
H	0.087449	-1.617710	3.238995
H	1.835218	-1.478596	3.418192
C	2.558477	-3.062102	-0.448142
H	1.862599	-2.891158	-1.275341
H	3.412086	-2.390982	-0.585169
H	2.924210	-4.090532	-0.530558
C	0.805431	0.426726	3.421168
H	1.721955	0.997923	3.242879
H	-0.016572	0.942142	2.914622
H	0.600432	0.447651	4.496322
C	0.115999	2.833593	-0.820906
H	0.823346	3.465496	-1.370799
H	-0.859151	2.950564	-1.307809
C	0.050713	3.260817	0.643746
H	-0.673587	2.669587	1.212921
H	1.026467	3.164049	1.131540
H	-0.255667	4.309557	0.712344

C	0.951203	1.018482	-2.880401
H	-0.007098	1.205366	-3.376420
H	1.616812	1.855904	-3.121566
C	1.550785	-0.304173	-3.349027
H	2.470233	-0.549340	-2.805957
H	0.842759	-1.128272	-3.222260
H	1.796230	-0.245242	-4.414319
Co	-0.731313	-0.605483	-0.212010
C	-0.781076	-2.110771	-1.284239
C	-2.319546	0.060816	-1.206236
O	-0.807271	-3.031465	-1.959386
O	-2.330688	0.570751	-2.293926
C	-3.698032	0.628423	0.884508
C	-3.686090	2.116332	0.506536
H	-2.772890	2.391223	-0.035142
H	-4.540979	2.367587	-0.131935
H	-3.738695	2.741663	1.405243
C	-5.004728	0.311048	1.625485
H	-5.870369	0.405549	0.959497
H	-5.002333	-0.701051	2.044107
H	-5.141996	1.012697	2.456108
C	-2.514845	0.344616	1.815361
H	-2.407015	-0.720538	2.053280
H	-1.572766	0.718448	1.379613
H	-2.622617	0.881062	2.764527
C	-3.622605	-0.218468	-0.416713
C	-3.777822	-1.731782	-0.228352
H	-4.767686	-1.963226	0.174071
H	-3.029895	-2.154341	0.453781
H	-4.427778	0.126324	-1.078173

H	-3.688967	-2.248277	-1.190288

C6

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.538849	2.025400	-0.615818
C	-3.237396	2.224115	-0.171589
C	-2.331476	1.157897	-0.125755
C	-2.746976	-0.119425	-0.532050
C	-4.061930	-0.311434	-0.973705
C	-4.951848	0.754923	-1.017498
H	-5.234127	2.858729	-0.648970
H	-2.920705	3.216652	0.138782
H	-4.396053	-1.298111	-1.283366
H	-5.968628	0.597184	-1.363980
P	-1.571288	-1.524221	-0.443649
P	-0.606462	1.398337	0.446224
C	-2.386077	-2.709689	0.712526
H	-3.250964	-3.145609	0.198822
H	-1.668416	-3.521288	0.883608
C	-1.751707	-2.382627	-2.066401
H	-1.091972	-3.257945	-2.027717
H	-2.777540	-2.763908	-2.130189
C	-2.822571	-2.081920	2.035217
H	-1.998926	-1.572668	2.544637
H	-3.621011	-1.349517	1.879673
H	-3.201901	-2.855810	2.709995

C	-1.433295	-1.522190	-3.286968
H	-2.043476	-0.612738	-3.309460
H	-0.379814	-1.225966	-3.321591
H	-1.641544	-2.087020	-4.201440
C	0.011381	2.802831	-0.575484
H	-0.566119	3.698052	-0.315095
H	1.042809	2.983303	-0.250837
C	-0.045585	2.555037	-2.081543
H	0.552695	1.687497	-2.376380
H	-1.073557	2.388204	-2.421282
H	0.346282	3.425329	-2.617686
C	-0.774089	2.175381	2.103820
H	0.241629	2.445267	2.412472
H	-1.338767	3.107527	1.981917
C	-1.434368	1.279478	3.147313
H	-2.434065	0.961678	2.832183
H	-0.835707	0.385681	3.346419
H	-1.538973	1.821266	4.093053
Co	0.536079	-0.653241	0.191375
C	0.633367	-1.496090	1.827755
C	2.311517	0.138264	0.727989
O	0.729390	-2.016607	2.839616
O	2.368214	1.124557	1.413212
C	4.539082	0.282759	-0.549738
C	5.144119	1.378705	0.340213
H	4.386534	2.069661	0.716619
H	5.662011	0.941782	1.202762
H	5.876775	1.958599	-0.233589
C	5.695380	-0.573975	-1.090137
H	6.209069	-1.104719	-0.279289

H	5.358187	-1.311856	-1.824968
H	6.430351	0.071455	-1.584688
C	3.807057	0.940225	-1.729363
H	3.391835	0.198168	-2.421653
H	2.993276	1.592626	-1.387648
H	4.503521	1.562846	-2.302475
C	3.572733	-0.633939	0.280332
C	3.251984	-1.971643	-0.394785
H	4.120122	-2.634445	-0.366167
H	2.954391	-1.854466	-1.441269
H	4.076822	-0.852703	1.233566
H	2.441748	-2.496153	0.129820
H	1.342388	-0.195358	-1.494271
H	0.760380	-0.641543	-1.714683

CAT1

Coordinates (Angstroms)

	X	Y	Z
Co	0.962725	0.000001	0.000033
P	-0.713737	-1.530817	-0.035093
O	2.207746	1.370215	0.040233
C	3.480256	1.232180	0.041368
C	4.140462	-0.000002	-0.000050
H	5.223584	-0.000003	-0.000097
C	4.260014	2.514408	0.108954
H	3.873500	3.221933	-0.631359
H	5.327119	2.355839	-0.060080

H	4.123712	2.966973	1.098347
C	-2.335563	-0.699165	-0.057953
C	-3.548410	-1.389811	-0.143212
H	-3.562362	-2.469257	-0.257191
C	-4.750331	-0.692423	-0.078273
H	-5.690181	-1.231609	-0.142509
P	-0.713740	1.530817	0.035108
C	-2.335566	0.699162	0.057925
C	-3.548417	1.389805	0.143152
H	-3.562376	2.469250	0.257135
C	-4.750335	0.692413	0.078181
H	-5.690188	1.231597	0.142391
O	2.207742	-1.370219	-0.040136
C	3.480251	-1.232185	-0.041391
C	4.260004	-2.514415	-0.109028
H	4.123686	-2.966946	-1.098435
H	5.327112	-2.355854	0.059991
H	3.873498	-3.221962	0.631267
C	-0.749394	-2.728663	-1.426258
H	-1.692345	-3.283273	-1.361685
H	-0.786650	-2.134403	-2.345955
C	0.434680	-3.694628	-1.449281
H	0.469890	-4.308405	-0.542840
H	0.336098	-4.369855	-2.305142
H	1.384896	-3.162304	-1.534705
C	-0.608471	-2.503543	1.518867
H	-0.650442	-1.771511	2.333420
H	0.406194	-2.918313	1.525252
C	-1.648902	-3.602696	1.716148
H	-1.646243	-4.322258	0.890650

H	-1.426010	-4.152015	2.636876
H	-2.656184	-3.186944	1.813604
C	-0.608437	2.503550	-1.518845
H	-0.650393	1.771523	-2.333404
H	0.406230	2.918315	-1.525205
C	-0.749425	2.728660	1.426275
H	-1.692381	3.283260	1.361699
H	-0.786678	2.134397	2.345971
C	-1.648860	3.602709	-1.716140
H	-1.646214	4.322264	-0.890635
H	-1.425947	4.152035	-2.636859
H	-2.656141	3.186961	-1.813619
C	0.434637	3.694639	1.449306
H	1.384862	3.162327	1.534714
H	0.469830	4.308434	0.542876
H	0.336053	4.369850	2.305180

CO

Coordinates (Angstroms)

	X	Y	Z
C	0.000000	0.000000	-0.648593
O	0.000000	0.000000	0.486445

D6

Coordinates (Angstroms)

	X	Y	Z
C	-4.189980	2.684425	-0.285085
C	-2.856710	2.619228	0.100739
C	-2.159850	1.408980	0.010889
C	-2.810631	0.264941	-0.461712
C	-4.151850	0.339312	-0.854929
C	-4.836172	1.545483	-0.768382
H	-4.726939	3.625130	-0.213403
H	-2.356264	3.511642	0.467179
H	-4.662769	-0.545704	-1.224645
H	-5.876425	1.600283	-1.074058
P	-1.880363	-1.306554	-0.491993
P	-0.384355	1.300094	0.438117
C	-2.888724	-2.467630	0.520701
H	-3.763817	-2.763398	-0.069832
H	-2.275744	-3.366072	0.659319
C	-2.069193	-1.945878	-2.203424
H	-1.709414	-2.981829	-2.194151
H	-3.138207	-1.979995	-2.443171
C	-3.330389	-1.894979	1.866948
H	-2.490228	-1.506632	2.451357
H	-4.046823	-1.078335	1.735157
H	-3.814765	-2.676536	2.460410
C	-1.304295	-1.115977	-3.231500
H	-1.654716	-0.078289	-3.247052
H	-0.227836	-1.114179	-3.023712
H	-1.446207	-1.533169	-4.233442
C	0.376075	2.599374	-0.620269
H	0.062819	3.571155	-0.221134

H	1.459856	2.532241	-0.478286
C	-0.003644	2.489130	-2.096278
H	0.168357	1.484735	-2.494151
H	-1.059154	2.733821	-2.250101
H	0.593597	3.189014	-2.689161
C	-0.252725	1.996430	2.133879
H	0.788545	1.863023	2.443782
H	-0.437149	3.074033	2.053931
C	-1.205551	1.371342	3.150006
H	-2.251721	1.491740	2.850924
H	-1.010865	0.304739	3.292667
H	-1.075253	1.858238	4.121605
Co	0.304485	-0.876470	0.158691
C	0.174897	-1.633673	1.966766
C	2.157729	-0.220479	0.596107
O	0.250743	-2.124914	2.988707
O	2.402885	0.068942	1.742927
C	4.546063	0.508343	-0.198737
C	5.280361	-0.205254	0.947994
H	4.714485	-0.167714	1.880819
H	5.464335	-1.258433	0.699477
H	6.254053	0.268568	1.121420
C	5.458220	0.454817	-1.436893
H	5.600376	-0.575484	-1.786586
H	5.063080	1.046228	-2.269389
H	6.445358	0.860118	-1.185909
C	4.309017	1.979472	0.173312
H	3.799026	2.522938	-0.631465
H	3.715525	2.072582	1.087817
H	5.268896	2.480894	0.344926

C	3.208043	-0.225477	-0.527876
C	2.594523	0.173522	-1.874985
H	3.167872	-0.245870	-2.705012
H	2.562881	1.258947	-2.002331
H	3.447923	-1.300579	-0.593011
H	1.566699	-0.196050	-1.980343
C	0.951065	-2.442704	-0.564698
O	1.302948	-3.433611	-1.005685

E1

Coordinates (Angstroms)

	X	Y	Z
C	1.121767	3.919767	0.085356
C	1.697522	2.657044	0.015205
C	0.908058	1.499251	0.014049
C	-0.496043	1.630775	0.064426
C	-1.060002	2.910325	0.148241
C	-0.261709	4.047345	0.161396
H	1.755384	4.801332	0.088213
H	2.777188	2.579503	-0.027428
H	-2.136414	3.026552	0.199105
H	-0.720810	5.028669	0.227305
P	-1.546547	0.122554	-0.012144
P	1.650590	-0.190587	-0.007525
Co	-0.078198	-1.644940	-0.042031
H	1.030371	-2.689097	-0.102939
C	-1.099613	-3.133950	0.010284

O	-1.636294	-4.141565	0.040404
C	-2.347374	0.160860	-1.723369
C	-2.993537	1.494501	-2.119792
C	-1.195340	-0.109058	-2.701887
C	-3.371111	-0.977416	-1.842698
H	-3.820464	1.782531	-1.468332
H	-2.261823	2.307354	-2.136498
H	-3.394633	1.393904	-3.136001
H	-0.687231	-1.063580	-2.498131
H	-1.590634	-0.162119	-3.723563
H	-0.457487	0.696752	-2.671982
H	-3.713132	-1.032516	-2.883253
H	-2.936392	-1.949679	-1.589203
H	-4.253603	-0.821282	-1.216720
C	-2.837098	0.211770	1.373814
C	-3.272686	-1.231675	1.684941
C	-2.187237	0.789554	2.639799
C	-4.083458	1.043383	1.035359
H	-3.697697	-1.743581	0.816522
H	-2.437678	-1.829028	2.067296
H	-4.044477	-1.207068	2.463688
H	-1.830332	1.814653	2.504176
H	-2.938530	0.799392	3.438449
H	-1.354146	0.172541	2.985328
H	-4.746973	1.037550	1.908808
H	-3.848564	2.087633	0.813206
H	-4.647577	0.627969	0.197356
C	2.929478	-0.279224	-1.405235
C	3.151992	-1.759181	-1.762924
C	2.364105	0.428796	-2.645260

C	4.287026	0.353149	-1.058858
H	3.533381	-2.345212	-0.922622
H	2.230860	-2.231631	-2.117224
H	3.892015	-1.811353	-2.570783
H	2.149847	1.486918	-2.466478
H	3.112294	0.371376	-3.444897
H	1.457664	-0.058259	-3.011434
H	4.938531	0.256036	-1.935607
H	4.212668	1.419597	-0.831706
H	4.788548	-0.147309	-0.227445
C	2.445147	-0.409825	1.695589
C	1.269658	-0.574973	2.671349
C	3.294210	-1.688484	1.726105
C	3.284996	0.786030	2.164138
H	0.640586	0.319301	2.684526
H	0.646930	-1.449997	2.431887
H	1.660225	-0.723282	3.685449
H	4.210013	-1.596440	1.136749
H	3.590787	-1.879773	2.764462
H	2.736641	-2.560644	1.370995
H	3.704796	0.546884	3.148956
H	4.119866	1.010191	1.497185
H	2.678540	1.689041	2.279071

E2

Coordinates (Angstroms)		
X	Y	Z

C	-3.993479	1.992970	-1.298218
C	-2.670766	2.279044	-0.990876
C	-1.789302	1.283556	-0.544361
C	-2.246766	-0.045432	-0.454136
C	-3.594752	-0.308258	-0.740952
C	-4.464194	0.693488	-1.149734
H	-4.653417	2.784793	-1.638732
H	-2.330798	3.300755	-1.089399
H	-3.980430	-1.314336	-0.663990
H	-5.501211	0.453706	-1.363052
P	-1.065175	-1.408994	-0.033795
P	-0.089843	1.706666	0.027320
C	-1.882237	-2.391413	1.384933
C	-1.027565	-2.463832	-1.624487
C	-2.383015	-1.381292	2.426739
H	-1.580536	-0.734799	2.788745
H	-3.186200	-0.747804	2.038218
H	-2.776505	-1.931048	3.290249
C	-0.130217	-1.690522	-2.601727
H	-0.583618	-0.731086	-2.868502
H	0.867227	-1.504315	-2.194141
H	-0.013566	-2.268157	-3.526958
C	0.733367	2.694471	-1.384682
C	0.478748	1.906189	-2.677453
H	0.848006	0.879512	-2.601514
H	-0.582585	1.875443	-2.943673
H	1.019363	2.388737	-3.500679
C	-0.402333	2.825688	1.537631
C	-1.106814	1.995506	2.620894
H	-2.023021	1.528212	2.246671

H	-0.468925	1.225240	3.049554
H	-1.388767	2.665761	3.441616
Co	0.980527	-0.306373	0.490389
H	2.109530	0.676420	0.689132
C	1.032861	-0.395926	2.421225
O	1.376775	-0.491484	3.506433
C	4.119292	-0.858018	-0.476858
C	4.861699	0.409322	-0.032673
H	4.195628	1.270535	0.061211
H	5.337306	0.252778	0.943260
H	5.648619	0.662828	-0.751571
C	5.126563	-2.029751	-0.446382
H	5.526469	-2.186996	0.562173
H	4.656397	-2.962375	-0.777040
H	5.969804	-1.813842	-1.113027
C	3.571064	-0.726845	-1.899954
H	3.193484	-1.683911	-2.276325
H	2.756755	0.000569	-1.956672
H	4.362422	-0.396723	-2.581904
C	3.045517	-1.228326	0.536218
H	3.360134	-1.061810	1.566144
C	2.058705	-2.165365	0.317445
H	1.667909	-2.764762	1.130530
H	1.926061	-2.555737	-0.684493
C	0.953866	3.322500	2.060051
H	0.808115	3.788941	3.041933
H	1.678096	2.508696	2.177947
H	1.385894	4.080030	1.398549
C	-1.324683	4.035117	1.295224
H	-1.317155	4.639150	2.211116

H	-1.015462	4.684367	0.478046
H	-2.359489	3.726263	1.125654
C	-3.062554	-3.294739	0.988881
H	-3.420190	-3.793616	1.898106
H	-3.911006	-2.743309	0.580323
H	-2.781221	-4.077903	0.282432
C	-0.821074	-3.285778	2.048644
H	-0.007943	-2.703744	2.487708
H	-1.297047	-3.842365	2.864963
H	-0.392321	-4.017123	1.358607
C	2.247933	2.745049	-1.145413
H	2.715567	3.301163	-1.967049
H	2.515139	3.244171	-0.210232
H	2.678631	1.747720	-1.133581
C	0.267294	4.143629	-1.586187
H	0.557577	4.784627	-0.750121
H	0.772665	4.531629	-2.479074
H	-0.804897	4.245920	-1.761524
C	-2.383240	-2.666787	-2.320682
H	-2.218421	-3.323175	-3.184294
H	-3.127654	-3.147923	-1.682497
H	-2.798044	-1.730321	-2.701610
C	-0.435595	-3.858884	-1.357023
H	-1.133672	-4.502313	-0.815799
H	-0.238260	-4.337299	-2.324103
H	0.502466	-3.844461	-0.802700

E3

	Coordinates (Angstroms)		
	X	Y	Z
C	-4.546984	-0.369048	-1.283500
C	-3.573646	0.575706	-0.982907
C	-2.285108	0.202951	-0.573019
C	-1.982289	-1.174953	-0.477096
C	-2.977118	-2.113151	-0.783738
C	-4.250006	-1.722261	-1.178518
H	-5.535554	-0.043202	-1.592327
H	-3.838320	1.620317	-1.062832
H	-2.760122	-3.171632	-0.720353
H	-5.000812	-2.472736	-1.404868
P	-0.289143	-1.723046	0.003479
P	-1.045001	1.472677	-0.034306
C	-0.433337	-3.063664	1.339171
C	0.440446	-2.425574	-1.595658
C	-1.439351	-2.567732	2.388009
H	-1.130445	-1.617438	2.831884
H	-2.444727	-2.445015	1.973412
H	-1.496833	-3.303439	3.199195
C	-0.446298	-3.411323	-2.366533
H	-0.697244	-4.306872	-1.794809
H	-1.375548	-2.941867	-2.701816
H	0.097555	-3.733572	-3.263552
C	-0.852818	2.751426	-1.430633
C	0.039084	2.126915	-2.513361
H	1.005922	1.795295	-2.127892
H	-0.453115	1.279782	-2.996964
H	0.231292	2.879793	-3.287721

C	-1.860584	2.279476	1.491919
C	-2.386055	1.135748	2.375373
H	-3.206525	0.590764	1.898951
H	-1.604652	0.416870	2.631960
H	-2.764571	1.559094	3.313396
Co	0.862876	0.230621	0.531556
C	4.452504	0.638636	-0.432342
C	5.399860	-0.536331	-0.158825
H	5.794533	-0.498587	0.863671
H	4.886544	-1.497692	-0.289335
H	6.251424	-0.517720	-0.849121
C	3.976946	0.565423	-1.886288
H	3.503894	-0.400756	-2.097235
H	3.262231	1.360036	-2.129543
H	4.826647	0.671561	-2.570721
C	5.189345	1.960910	-0.186239
H	4.553493	2.822408	-0.421210
H	5.503415	2.048432	0.861077
H	6.086847	2.023855	-0.813008
C	3.262064	0.538068	0.556530
C	2.227336	1.638669	0.544884
H	2.153657	2.172329	-0.404475
H	2.284123	2.343849	1.374577
C	0.996748	0.167020	2.402464
O	1.168480	0.248163	3.529316
H	3.651843	0.399586	1.572264
H	2.772548	-0.457914	0.318960
C	-0.859410	-4.457056	0.852432
H	-0.909358	-5.121362	1.724306
H	-1.845780	-4.471244	0.384516

H	-0.133922	-4.889843	0.159173
C	0.945497	-3.217514	2.009113
H	1.320231	-2.280060	2.426934
H	0.854476	-3.933138	2.835097
H	1.700271	-3.606826	1.321332
C	1.800647	-3.074781	-1.301713
H	2.314807	-3.261898	-2.252398
H	2.449939	-2.432764	-0.695477
H	1.694599	-4.036490	-0.792248
C	0.653356	-1.195670	-2.484224
H	1.186244	-1.481929	-3.399215
H	-0.303513	-0.756432	-2.779031
H	1.244503	-0.422768	-1.979581
C	-0.805109	3.072347	2.282705
H	-1.252723	3.395972	3.230373
H	0.079815	2.479992	2.520336
H	-0.474753	3.968972	1.755129
C	-3.031494	3.225584	1.192197
H	-3.433537	3.581921	2.149013
H	-2.722038	4.106601	0.625165
H	-3.852219	2.733509	0.664830
C	-0.145811	3.993144	-0.862390
H	0.740613	3.744393	-0.272733
H	0.178229	4.621294	-1.701088
H	-0.813395	4.598578	-0.243745
C	-2.147030	3.198444	-2.127238
H	-2.889706	3.611083	-1.441267
H	-1.887659	3.988239	-2.843227
H	-2.604269	2.383684	-2.695340

E4

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.827911	3.070686	0.135255
C	-2.449616	2.964594	0.012943
C	-1.806039	1.719126	-0.045740
C	-2.594152	0.551273	0.010523
C	-3.985949	0.676947	0.134351
C	-4.602151	1.918241	0.200956
H	-4.290832	4.051100	0.185559
H	-1.870048	3.875149	-0.028247
H	-4.608173	-0.206247	0.181099
H	-5.680764	1.981656	0.304831
P	-1.808982	-1.113286	-0.067932
P	0.041452	1.609437	-0.060507
C	-2.481383	-2.121917	1.397860
C	-2.399200	-1.859749	-1.713695
C	-2.455291	-1.218185	2.639799
H	-1.472709	-0.773223	2.814303
H	-3.186270	-0.407052	2.569614
H	-2.703867	-1.820932	3.521310
C	-3.890861	-1.651143	-2.018229
H	-4.552765	-2.080540	-1.263374
H	-4.137207	-0.593021	-2.140520
H	-4.112010	-2.148363	-2.970715
C	0.644392	2.536328	-1.627556
C	0.586306	1.527120	-2.782724

H	1.127596	0.603516	-2.559193
H	-0.445185	1.278746	-3.037219
H	1.043187	1.976675	-3.672791
C	0.570640	2.544260	1.514809
C	-0.294236	2.030854	2.677646
H	-1.355344	2.256542	2.537457
H	-0.193088	0.955276	2.831961
H	0.034998	2.522096	3.600883
Co	0.532994	-0.728908	-0.041204
C	5.055066	-0.908544	-0.094068
C	5.973584	-1.590101	0.929696
H	5.855632	-1.143066	1.924938
H	5.749181	-2.660977	1.013388
H	7.027054	-1.490583	0.640740
C	5.282795	-1.546755	-1.470195
H	5.028093	-2.614209	-1.456832
H	4.681920	-1.064918	-2.250180
H	6.335055	-1.457889	-1.766766
C	5.396335	0.586391	-0.153977
H	4.832598	1.100509	-0.941095
H	5.175400	1.081725	0.800556
H	6.462602	0.731855	-0.366014
C	3.592005	-1.115158	0.375118
C	2.533011	-0.408843	-0.464082
H	2.625307	-0.649766	-1.529234
H	2.651585	0.663260	-0.356114
C	0.926004	-1.053128	1.828162
O	1.317219	-1.281559	2.874050
H	3.532629	-0.745471	1.407532
H	3.410128	-2.197235	0.431297

C	-3.907178	-2.673760	1.235218
H	-4.168243	-3.203401	2.159567
H	-4.658082	-1.894604	1.092913
H	-3.989032	-3.392761	0.417651
C	-1.548473	-3.325864	1.624024
H	-0.524181	-3.031777	1.861405
H	-1.925254	-3.901490	2.477667
H	-1.516203	-3.998546	0.762670
C	-2.086667	-3.362061	-1.781372
H	-2.285712	-3.705697	-2.803579
H	-1.041145	-3.590920	-1.564979
H	-2.714816	-3.954796	-1.112364
C	-1.603456	-1.137548	-2.806796
H	-0.520515	-1.257075	-2.685887
H	-1.877698	-1.548679	-3.785747
H	-1.843125	-0.071075	-2.817895
C	2.045157	2.217645	1.813068
H	2.316552	2.675080	2.771781
H	2.225323	1.144008	1.898333
H	2.725760	2.613180	1.055478
C	0.413493	4.073265	1.464053
H	0.832019	4.484652	2.390916
H	0.947834	4.538516	0.634059
H	-0.632269	4.385310	1.426523
C	2.095709	3.033283	-1.493238
H	2.809832	2.233704	-1.291406
H	2.380419	3.482432	-2.452316
H	2.214635	3.805248	-0.730571
C	-0.222956	3.741278	-2.025071
H	-0.227197	4.531281	-1.269470

H	0.199080	4.170134	-2.942266
H	-1.255310	3.457129	-2.245054
C	1.017117	-2.403193	-0.581296
O	1.411300	-3.424475	-0.905070

E5

Coordinates (Angstroms)

	X	Y	Z
C	-4.001759	2.545354	-1.294373
C	-2.712167	2.669060	-0.794778
C	-1.938607	1.546722	-0.464243
C	-2.504384	0.263060	-0.629132
C	-3.800884	0.157576	-1.153481
C	-4.545975	1.280710	-1.487089
H	-4.571700	3.435840	-1.541112
H	-2.302221	3.663059	-0.677130
H	-4.244829	-0.818888	-1.301713
H	-5.546738	1.165146	-1.891607
P	-1.597816	-1.257808	-0.104319
P	-0.193408	1.734165	0.105782
Co	0.591775	-0.474742	0.541134
C	0.988456	-0.493963	2.339568
C	1.565748	-2.202968	0.568498
O	1.229464	-0.620982	3.449232
O	1.390053	-3.206725	1.199490
C	4.959505	-0.562004	-0.558090
C	5.638297	0.642633	0.109136

H	4.998334	1.533488	0.063515
H	5.858582	0.438819	1.164298
H	6.583247	0.883887	-0.391304
C	5.911821	-1.764440	-0.518038
H	6.155262	-2.039623	0.515449
H	5.481348	-2.643400	-1.011375
H	6.850068	-1.526728	-1.032904
C	4.633309	-0.210215	-2.015249
H	5.539830	0.112787	-2.540362
H	4.227083	-1.068315	-2.563129
H	3.905955	0.608645	-2.074261
C	3.674190	-0.867882	0.239872
H	3.088580	0.064121	0.315818
C	2.776974	-1.974455	-0.339727
H	3.308062	-2.928411	-0.423189
H	2.419462	-1.696505	-1.337622
H	3.949520	-1.136497	1.268536
C	0.737038	2.329240	-1.431902
C	2.155399	2.760547	-1.035497
C	0.826767	1.090529	-2.335118
C	0.063526	3.450557	-2.232700
H	2.166331	3.720812	-0.513205
H	2.647959	2.018245	-0.398514
H	2.759486	2.873109	-1.943881
H	-0.168371	0.764219	-2.649657
H	1.400223	1.330990	-3.238834
H	1.331683	0.248126	-1.840684
H	0.713695	3.713016	-3.077097
H	-0.897740	3.133097	-2.646865
H	-0.093853	4.357819	-1.645485

C	-0.151162	3.039905	1.482677
C	-1.276325	2.697861	2.470680
C	1.193833	2.920271	2.222424
C	-0.298366	4.501115	1.030472
H	-2.267772	2.782598	2.014790
H	-1.165696	1.689181	2.880609
H	-1.234179	3.401780	3.310652
H	2.050673	3.147254	1.583622
H	1.201750	3.642657	3.047576
H	1.342918	1.930593	2.658714
H	-0.269888	5.138829	1.922918
H	0.520589	4.817622	0.379504
H	-1.244643	4.704431	0.525055
C	-2.580185	-1.851755	1.410746
C	-1.930970	-3.151045	1.908577
C	-2.429800	-0.763991	2.484482
C	-4.088740	-2.059741	1.210021
H	-2.090558	-3.980680	1.212459
H	-0.853212	-3.037066	2.062885
H	-2.386358	-3.432123	2.866153
H	-2.857215	0.189916	2.159237
H	-2.968021	-1.080690	3.386131
H	-1.389027	-0.600144	2.768146
H	-4.506867	-2.404045	2.164351
H	-4.599299	-1.126904	0.954671
H	-4.334218	-2.811065	0.460398
C	-1.710605	-2.498681	-1.553586
C	-1.537530	-1.736346	-2.875682
C	-0.530908	-3.476815	-1.432576
C	-2.998228	-3.332194	-1.627359

H	-2.344713	-1.024705	-3.070541
H	-0.585060	-1.200223	-2.910108
H	-1.528614	-2.465372	-3.694998
H	-0.503059	-3.997110	-0.472303
H	-0.617999	-4.232786	-2.222635
H	0.425224	-2.965672	-1.578445
H	-2.940338	-3.964668	-2.521740
H	-3.105628	-3.998364	-0.767508
H	-3.903347	-2.727630	-1.720835

E6

Coordinates (Angstroms)

	X	Y	Z

C	-4.273930	1.950824	-1.364860
C	-3.049168	2.264700	-0.790898
C	-2.098357	1.276910	-0.494306
C	-2.425964	-0.077343	-0.735965
C	-3.651404	-0.367774	-1.353747
C	-4.565158	0.627352	-1.674882
H	-4.987190	2.739711	-1.582351
H	-2.831097	3.303697	-0.583326
H	-3.906317	-1.394780	-1.582413
H	-5.504625	0.366032	-2.152159
P	-1.336651	-1.450180	-0.144680
P	-0.417106	1.762698	0.090482
Co	0.731712	-0.293234	0.632473
C	0.592595	-0.378608	2.432118

C	2.161214	-1.704325	1.104184
O	0.547044	-0.517477	3.567861
O	1.951658	-2.873610	1.242914
C	4.779887	-0.301943	-0.790352
C	5.022601	0.966152	-1.620233
H	4.076870	1.398942	-1.971255
H	5.544347	1.731640	-1.032767
H	5.634927	0.744005	-2.502252
C	6.134110	-0.866205	-0.335956
H	6.655813	-0.162116	0.323506
H	6.025175	-1.816177	0.199375
H	6.777852	-1.055724	-1.202913
C	4.072106	-1.343646	-1.667154
H	3.803639	-2.245517	-1.103047
H	3.162731	-0.936253	-2.124310
H	4.729702	-1.658930	-2.485819
C	3.935335	0.099630	0.441765
H	3.051167	0.659404	0.106253
C	3.504499	-1.038310	1.378736
H	3.386989	-0.632745	2.393548
H	4.259162	-1.829062	1.444703
H	4.527113	0.811358	1.029186
H	1.491567	-0.823990	-0.859716
H	1.156133	-0.143392	-1.056698
C	0.317230	2.761314	-1.360447
C	0.573874	1.802629	-2.533222
C	-0.576934	3.883817	-1.915070
C	1.660593	3.353151	-0.906064
H	1.402890	1.114830	-2.344394
H	-0.319382	1.227813	-2.797744

H	0.856398	2.392822	-3.413195
H	-0.924171	4.588110	-1.159381
H	0.011328	4.452613	-2.645904
H	-1.445793	3.481029	-2.442606
H	2.200186	3.724389	-1.785933
H	1.530801	4.196642	-0.222767
H	2.299402	2.608742	-0.417262
C	-0.619459	2.887641	1.616311
C	0.734098	2.955714	2.350107
C	-1.064779	4.335884	1.364034
C	-1.664648	2.223999	2.526737
H	1.175169	1.973691	2.538779
H	1.469021	3.546635	1.797595
H	0.585614	3.441736	3.321860
H	-2.035821	4.408292	0.868672
H	-1.167100	4.830919	2.337845
H	-0.329787	4.904720	0.790033
H	-1.714880	2.777500	3.471914
H	-2.661364	2.239490	2.074726
H	-1.421974	1.187174	2.768516
C	-2.406244	-2.325888	1.159561
C	-1.575835	-3.500289	1.698834
C	-2.650773	-1.312369	2.287679
C	-3.793720	-2.828171	0.729604
H	-1.509380	-4.317079	0.972930
H	-0.556245	-3.196717	1.960595
H	-2.055032	-3.898730	2.601806
H	-3.149361	-0.406801	1.926248
H	-3.303468	-1.771513	3.040286
H	-1.731825	-1.027394	2.797852

H	-4.237769	-3.350880	1.586267
H	-4.465228	-2.002959	0.477296
H	-3.773928	-3.531862	-0.101206
C	-1.024712	-2.584345	-1.650587
C	-0.789312	-1.691944	-2.877937
C	0.261958	-3.383079	-1.379704
C	-2.128315	-3.595742	-1.990779
H	-1.694518	-1.157394	-3.182541
H	0.003043	-0.958716	-2.707886
H	-0.474660	-2.323946	-3.717833
H	0.220229	-3.943415	-0.443268
H	0.411624	-4.099752	-2.196988
H	1.146285	-2.741995	-1.344990
H	-1.843163	-4.112919	-2.915603
H	-2.238037	-4.359406	-1.216160
H	-3.100877	-3.131965	-2.170148

F2

Coordinates (Angstroms)

	X	Y	Z
C	4.730907	0.569767	-1.214495
C	3.873406	-0.413063	-0.734833
C	2.538684	-0.121582	-0.423188
C	2.079357	1.206607	-0.559742
C	2.946809	2.177594	-1.076710
C	4.259533	1.864631	-1.408159
H	5.760941	0.319807	-1.448884

H	4.251392	-1.421562	-0.615879
H	2.596428	3.193796	-1.217871
H	4.915418	2.633464	-1.804687
P	0.391820	1.650685	0.024301
P	1.345784	-1.443375	0.060730
C	0.681443	2.730092	1.551345
C	-0.512162	2.599256	-1.341669
C	1.286008	1.811741	2.621259
H	0.619961	0.983576	2.878790
H	2.248392	1.401771	2.300444
H	1.460363	2.393188	3.534467
C	-2.009650	2.399116	-1.047601
H	-2.258147	1.333423	-0.982981
H	-2.324161	2.879806	-0.117198
H	-2.602804	2.830758	-1.863482
C	1.131387	-2.503773	-1.492095
C	2.431327	-2.934683	-2.184026
H	3.003420	-2.075697	-2.545078
H	3.077076	-3.544640	-1.548990
H	2.166103	-3.539181	-3.060326
C	2.057297	-2.433274	1.510258
C	2.687809	-1.446740	2.502053
H	3.522544	-0.889386	2.065566
H	1.952217	-0.736109	2.885577
H	3.074462	-2.012952	3.357617
Co	-0.674290	-0.358872	0.403058
H	-1.195239	-1.766065	0.593227
C	-1.521812	-0.222948	2.007150
O	-1.995309	-0.304520	3.045313
C	-4.985667	-0.625202	-0.199107

C	-4.723096	0.668481	0.591099
H	-3.666916	0.752821	0.869272
H	-4.982299	1.555523	0.000186
H	-5.318835	0.687237	1.511535
C	-6.477839	-0.683362	-0.574902
H	-6.767456	0.177013	-1.190272
H	-6.706069	-1.595808	-1.137632
H	-7.099184	-0.675788	0.328821
C	-4.628480	-1.841064	0.659635
H	-4.860016	-2.778485	0.140701
H	-3.562657	-1.852878	0.915888
H	-5.199842	-1.824986	1.594757
C	-4.183066	-0.568990	-1.480790
H	-4.404746	0.297449	-2.107718
C	-3.277192	-1.447405	-1.915062
H	-2.787532	-1.310328	-2.876255
H	-3.011770	-2.343803	-1.359198
C	1.659912	3.897520	1.350167
H	1.707793	4.463208	2.289055
H	2.672263	3.544304	1.134742
H	1.357511	4.591521	0.564527
C	-0.667332	3.266544	2.055256
H	-1.412735	2.473443	2.177384
H	-0.515998	3.731068	3.037057
H	-1.084932	4.029490	1.392510
C	-0.197595	1.932774	-2.688278
H	-0.762567	2.448789	-3.473945
H	0.864277	1.992445	-2.946179
H	-0.501267	0.883238	-2.705201
C	-0.205188	4.096788	-1.453599

H	0.849332	4.292097	-1.668760
H	-0.790359	4.505128	-2.286868
H	-0.486327	4.652793	-0.555977
C	0.893978	-3.146938	2.220658
H	1.299150	-3.702605	3.075141
H	0.157655	-2.434667	2.603108
H	0.375613	-3.860038	1.574648
C	3.109874	-3.478086	1.112453
H	3.472201	-3.960534	2.028574
H	2.700505	-4.263901	0.473077
H	3.977723	-3.037597	0.614922
C	0.350095	-1.614589	-2.467787
H	0.111950	-2.183941	-3.374630
H	-0.599551	-1.279913	-2.031126
H	0.935151	-0.739689	-2.766617
C	0.283948	-3.741827	-1.164080
H	0.031971	-4.247872	-2.103914
H	0.820933	-4.460795	-0.539535
H	-0.653245	-3.476187	-0.664197

F3

Coordinates (Angstroms)

	X	Y	Z

C	-4.284707	1.866179	-0.352084
C	-2.935581	2.193517	-0.375574
C	-1.929821	1.223703	-0.239199
C	-2.318121	-0.130415	-0.103466

C	-3.686546	-0.437493	-0.065369
C	-4.664302	0.540676	-0.180905
H	-5.031953	2.647245	-0.453765
H	-2.669909	3.234902	-0.487435
H	-4.002999	-1.465111	0.050914
H	-5.713702	0.265105	-0.141864
P	-1.069744	-1.489631	-0.027001
P	-0.158189	1.752639	-0.074039
C	-1.492771	-2.576722	1.477273
C	-1.356828	-2.454781	-1.641300
C	-1.749816	-1.630154	2.658930
H	-0.902807	-0.963452	2.840309
H	-2.643381	-1.016790	2.507979
H	-1.897287	-2.224267	3.568880
C	-2.817859	-2.785807	-1.981175
H	-3.323969	-3.363716	-1.205632
H	-3.403227	-1.884854	-2.183963
H	-2.825281	-3.389310	-2.897947
C	0.271557	2.731022	-1.644302
C	1.610477	3.450632	-1.419706
H	1.515837	4.289130	-0.723976
H	2.389365	2.778448	-1.048248
H	1.956561	3.857327	-2.377945
C	-0.183052	2.885250	1.464380
C	-1.002488	2.157845	2.542500
H	-2.062461	2.080461	2.283983
H	-0.620749	1.150012	2.729249
H	-0.925491	2.717419	3.482713
Co	1.085325	-0.340902	0.193872
C	3.809609	-1.221699	-0.561623

C	2.761766	-2.170954	-1.158548
H	1.994375	-2.439792	-0.417892
H	2.275422	-1.734123	-2.039206
H	3.222462	-3.114393	-1.473537
C	4.898156	-0.975064	-1.628056
H	4.471463	-0.526707	-2.533184
H	5.685739	-0.311237	-1.256307
H	5.365354	-1.926290	-1.910035
C	4.445736	-1.885084	0.665075
H	5.249492	-1.273835	1.087990
H	3.706035	-2.068669	1.452877
H	4.877693	-2.852648	0.385560
C	3.166894	0.129403	-0.236245
H	2.777172	0.611118	-1.142791
C	3.937515	1.076267	0.641925
H	4.937715	1.253628	0.219089
H	4.085978	0.683299	1.652825
C	1.559879	-0.517429	1.943980
O	1.883190	-0.550151	3.043465
H	3.444240	2.045293	0.724521
C	1.255534	3.029343	1.983873
H	1.715736	2.060156	2.185961
H	1.897658	3.577450	1.289961
H	1.237046	3.590188	2.926512
C	-0.755405	4.295649	1.269887
H	-1.799096	4.296345	0.947473
H	-0.718776	4.814401	2.236344
H	-0.166076	4.886476	0.563877
C	0.446892	1.689148	-2.759357
H	1.187154	0.921173	-2.510431

H	-0.499817	1.195130	-2.989906
H	0.787908	2.192465	-3.672599
C	-0.763376	3.751754	-2.138849
H	-1.685949	3.267789	-2.470924
H	-1.012183	4.509651	-1.392767
H	-0.340407	4.272198	-3.007486
C	-2.689572	-3.530463	1.347304
H	-2.791180	-4.077353	2.293242
H	-3.637177	-3.013940	1.178807
H	-2.548365	-4.274321	0.559432
C	-0.253030	-3.436910	1.790796
H	0.652635	-2.838445	1.918554
H	-0.425325	-3.977566	2.729538
H	-0.057591	-4.181220	1.014045
C	-0.824380	-1.557275	-2.765535
H	-0.915949	-2.080924	-3.725122
H	-1.405304	-0.633059	-2.837341
H	0.229791	-1.298444	-2.626832
C	-0.547430	-3.760615	-1.614538
H	0.499014	-3.604582	-1.338492
H	-0.978863	-4.498522	-0.932711
H	-0.560454	-4.199932	-2.619507

F4

Coordinates (Angstroms)

	X	Y	Z
C	4.626167	-1.188404	-0.313283

C	3.365072	-1.736641	-0.123876
C	2.214650	-0.936467	-0.041646
C	2.353335	0.465942	-0.145753
C	3.634140	0.996252	-0.363068
C	4.760443	0.188561	-0.445200
H	5.493681	-1.838283	-0.373249
H	3.280599	-2.813744	-0.062847
H	3.761075	2.064345	-0.484012
H	5.734687	0.636623	-0.614245
P	0.914645	1.617116	0.027367
P	0.563144	-1.747670	0.080252
C	1.316117	2.576139	1.630513
C	1.000261	2.792993	-1.483372
C	1.350215	1.561802	2.780482
H	0.416880	1.016254	2.895630
H	2.163611	0.841180	2.653367
H	1.527687	2.098266	3.720518
C	1.925849	4.014796	-1.384653
H	1.596058	4.722808	-0.620102
H	2.970409	3.753535	-1.201019
H	1.888995	4.538569	-2.348330
C	0.472982	-2.910453	-1.445273
C	1.143814	-2.191282	-2.627677
H	0.841537	-1.146210	-2.727657
H	2.234129	-2.210152	-2.544554
H	0.866233	-2.703748	-3.556389
C	0.565429	-2.775457	1.684273
C	1.686839	-3.815982	1.848327
H	1.507380	-4.345575	2.792254
H	1.724438	-4.565261	1.061277

H	2.667541	-3.340110	1.934704
Co	-1.108877	0.024651	-0.048411
C	-1.593356	0.231752	1.682165
C	-1.227952	0.089795	-1.873097
O	-1.917313	0.439158	2.759194
O	-1.390481	0.181268	-3.000123
C	-4.251880	0.025188	-0.123728
C	-3.911553	-1.271513	-0.864815
H	-3.737770	-1.097805	-1.933216
H	-3.008848	-1.726878	-0.436306
H	-4.725986	-1.999991	-0.775344
C	-4.614867	-0.336971	1.322353
H	-3.859051	-0.976923	1.789280
H	-4.761320	0.545583	1.953480
H	-5.553961	-0.902146	1.329493
C	-5.495371	0.656853	-0.786641
H	-5.844175	1.537498	-0.236940
H	-5.286631	0.958384	-1.820192
H	-6.316941	-0.068614	-0.807770
C	-3.091406	1.039614	-0.267793
H	-3.051641	1.319175	-1.322639
C	-3.201947	2.339106	0.512255
H	-2.331022	2.972245	0.331525
H	-3.308268	2.206389	1.591781
H	-4.080667	2.901268	0.167639
C	2.665012	3.312508	1.692761
H	2.728430	3.801856	2.672897
H	3.508550	2.620383	1.628401
H	2.786806	4.087538	0.939033
C	0.177208	3.577611	1.864468

H	0.329268	4.077200	2.829025
H	0.146641	4.353041	1.093002
H	-0.799004	3.084579	1.899773
C	-0.417379	3.344596	-1.719515
H	-1.171859	2.565872	-1.837088
H	-0.735757	3.996313	-0.900488
H	-0.418200	3.945883	-2.636882
C	1.457327	1.967130	-2.698949
H	1.227711	2.522205	-3.616409
H	2.536200	1.788992	-2.675890
H	0.972421	0.992615	-2.775950
C	0.723128	-1.818982	2.871641
H	0.733722	-2.409341	3.795768
H	1.666338	-1.268452	2.821581
H	-0.096466	-1.110453	2.958691
C	-0.801987	-3.471759	1.767915
H	-0.916218	-3.923464	2.760804
H	-1.631416	-2.767034	1.627632
H	-0.896836	-4.272727	1.028348
C	-1.006836	-3.170925	-1.779203
H	-1.057150	-3.896415	-2.599771
H	-1.559545	-3.592121	-0.934799
H	-1.532456	-2.277333	-2.114391
C	1.132604	-4.290735	-1.302981
H	0.601525	-4.928559	-0.591473
H	1.079763	-4.784576	-2.281313
H	2.187749	-4.243763	-1.026153

F5

	Coordinates (Angstroms)		
	X	Y	Z
C	-4.146887	2.241434	-1.323085
C	-2.806329	2.425823	-1.012192
C	-1.988344	1.366434	-0.588774
C	-2.556569	0.073674	-0.501068
C	-3.914146	-0.090149	-0.813938
C	-4.709065	0.975488	-1.213298
H	-4.747574	3.087888	-1.641620
H	-2.398286	3.423225	-1.096942
H	-4.364190	-1.071806	-0.753527
H	-5.757814	0.812430	-1.441382
P	-1.537014	-1.392203	-0.032995
P	-0.255846	1.705152	-0.019502
Co	0.622856	-0.456755	0.566951
C	0.707059	-0.636117	2.418397
C	2.644386	-0.028944	0.706146
O	0.823951	-0.684192	3.554959
O	3.111003	0.975927	1.148051
C	4.767050	-0.931324	-0.475003
C	4.451877	-0.085129	-1.716635
H	3.744815	-0.587820	-2.386842
H	4.037724	0.893221	-1.449273
H	5.371589	0.092465	-2.285475
C	5.763425	-0.179952	0.420237
H	5.376319	0.788140	0.746133
H	6.010088	-0.767376	1.313398
H	6.694943	-0.003418	-0.129908

C	5.434635	-2.242706	-0.923438
H	5.599774	-2.920541	-0.077268
H	4.846169	-2.772088	-1.679849
H	6.411024	-2.019032	-1.367542
C	3.464584	-1.280320	0.319544
C	2.587053	-2.344073	-0.340757
H	3.089495	-3.313761	-0.349229
H	2.333100	-2.091516	-1.374872
H	3.766024	-1.662202	1.307806
H	1.655235	-2.508487	0.220378
C	0.671167	2.504844	-1.473736
C	1.106581	1.332010	-2.367274
C	-0.128158	3.486500	-2.339858
C	1.927829	3.223688	-0.957479
H	1.603746	0.540403	-1.791780
H	0.253104	0.892334	-2.888391
H	1.813550	1.687097	-3.126976
H	-0.492902	4.348415	-1.774246
H	0.536860	3.868713	-3.124748
H	-0.975179	3.005038	-2.836315
H	2.544278	3.501579	-1.821559
H	1.686004	4.147617	-0.425194
H	2.534438	2.596643	-0.302276
C	-0.490298	2.914326	1.428947
C	-1.587054	2.319835	2.327247
C	0.813559	2.961672	2.242813
C	-0.884248	4.348933	1.052922
H	-2.569290	2.324131	1.845545
H	-1.353899	1.293155	2.623252
H	-1.658513	2.919289	3.242912

H	1.637393	3.425391	1.697257
H	0.637170	3.556855	3.147426
H	1.138105	1.967134	2.556226
H	-0.935007	4.942672	1.974545
H	-0.154084	4.828479	0.396577
H	-1.869059	4.407409	0.583704
C	-1.493905	-2.445296	-1.612458
C	-0.597012	-1.675249	-2.591177
C	-0.845393	-3.802494	-1.300189
C	-2.838189	-2.681379	-2.316375
H	-1.040041	-0.708875	-2.849900
H	0.405274	-1.504207	-2.185738
H	-0.488637	-2.249942	-3.519141
H	-1.519795	-4.463114	-0.748254
H	-0.603108	-4.301982	-2.246356
H	0.085582	-3.704640	-0.731956
H	-2.660926	-3.349109	-3.169204
H	-3.585426	-3.156981	-1.678703
H	-3.258393	-1.753800	-2.714679
C	-2.441193	-2.312847	1.364457
C	-1.441393	-3.294943	2.003678
C	-2.838070	-1.262864	2.412533
C	-3.687689	-3.120325	0.974624
H	-1.189402	-4.124391	1.338784
H	-0.509517	-2.810516	2.305157
H	-1.895385	-3.723522	2.905447
H	-3.554569	-0.534196	2.020364
H	-3.305817	-1.768733	3.265983
H	-1.969430	-0.718763	2.793197
H	-4.078934	-3.600534	1.880270

H	-4.492802	-2.502231	0.570898
H	-3.459257	-3.915162	0.260723

F6

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.513359	1.669428	-1.203841
C	-3.263274	2.067113	-0.748401
C	-2.268611	1.140336	-0.398911
C	-2.571354	-0.235468	-0.512189
C	-3.832435	-0.620202	-0.992802
C	-4.797659	0.315365	-1.337840
H	-5.253963	2.417688	-1.468526
H	-3.058547	3.126411	-0.683451
H	-4.066806	-1.670426	-1.115462
H	-5.761999	-0.014436	-1.712030
P	-1.352124	-1.526573	-0.029548
P	-0.562772	1.722851	0.042488
Co	0.768575	-0.404347	0.350443
C	1.003569	-0.653092	2.142165
C	2.737878	0.229224	0.625625
O	1.265524	-0.798050	3.246750
O	2.967674	1.350987	0.969120
C	4.917106	-0.452938	-0.578312
C	5.685277	0.796120	-0.122818
H	5.047481	1.681874	-0.074980
H	6.131685	0.646259	0.867622

H	6.497220	1.003957	-0.829417
C	5.924750	-1.609125	-0.695469
H	6.342914	-1.874943	0.282775
H	5.477953	-2.506849	-1.134370
H	6.755248	-1.305960	-1.343225
C	4.300578	-0.187046	-1.959625
H	3.739498	-1.049104	-2.338542
H	3.631453	0.680854	-1.944742
H	5.093145	0.029790	-2.684774
C	3.824567	-0.854347	0.473718
C	3.249077	-2.255832	0.257567
H	3.968859	-3.014917	0.572531
H	3.002656	-2.445610	-0.790626
H	4.312188	-0.836289	1.459858
H	2.341627	-2.422471	0.851325
H	1.582806	-0.357328	-1.318261
H	0.844309	-0.503568	-1.486315
C	-0.766465	2.882330	1.537400
C	-1.893887	3.924124	1.466211
C	-1.073144	1.998168	2.752891
C	0.576863	3.589582	1.776637
H	-1.845135	4.570460	0.589109
H	-2.880596	3.453663	1.502167
H	-1.813158	4.569429	2.350281
H	-0.256959	1.310873	2.982367
H	-1.213225	2.639225	3.632055
H	-1.993781	1.425517	2.613072
H	0.541721	4.088503	2.753311
H	1.412695	2.883728	1.785067
H	0.779361	4.358817	1.025799

C	-0.030238	2.732413	-1.495593
C	-0.462499	1.956624	-2.749872
C	-0.571903	4.164626	-1.607774
C	1.505520	2.807042	-1.494980
H	-0.095020	0.926964	-2.742578
H	-1.548777	1.930767	-2.875376
H	-0.034769	2.447929	-3.632515
H	-0.223852	4.809282	-0.796967
H	-0.197882	4.595767	-2.545253
H	-1.662684	4.210287	-1.650302
H	1.833070	3.385416	-2.368235
H	1.908403	3.290387	-0.602526
H	1.952417	1.814205	-1.571262
C	-2.137742	-2.382402	1.476794
C	-2.269716	-1.324651	2.581540
C	-3.546844	-2.964493	1.280184
C	-1.189678	-3.500575	1.937965
H	-1.322424	-0.855205	2.845410
H	-2.975116	-0.538688	2.293666
H	-2.659556	-1.805590	3.486677
H	-3.601653	-3.741158	0.519244
H	-3.855797	-3.417583	2.230509
H	-4.278327	-2.187132	1.043811
H	-1.547898	-3.903343	2.893081
H	-1.154801	-4.328845	1.224142
H	-0.165714	-3.143448	2.095732
C	-1.205108	-2.744714	-1.494471
C	-2.248044	-3.866890	-1.587456
C	-1.255486	-1.943005	-2.803892
C	0.182420	-3.400525	-1.377025

H	-2.181526	-4.569569	-0.753050
H	-3.273194	-3.495461	-1.656410
H	-2.049240	-4.435804	-2.504572
H	-0.528382	-1.126509	-2.826536
H	-1.011382	-2.615461	-3.635194
H	-2.245414	-1.518567	-2.993350
H	0.308824	-4.127018	-2.189039
H	0.984151	-2.663036	-1.467474
H	0.313276	-3.937181	-0.431836

G6

Coordinates (Angstroms)

	X	Y	Z
C	-4.241238	2.691728	-0.632649
C	-3.880103	1.353328	-0.583186
C	-2.563409	0.950475	-0.314961
C	-1.571029	1.935233	-0.129839
C	-1.964628	3.282266	-0.158568
C	-3.277088	3.663637	-0.398900
H	-5.270985	2.966499	-0.838450
H	-4.651455	0.611325	-0.730911
H	-1.232303	4.061396	-0.018433
H	-3.535497	4.717845	-0.415732
P	0.221215	1.496151	0.074469
P	-2.183700	-0.836558	-0.105072
Co	0.158982	-0.986148	0.299476
C	0.132349	-2.778886	0.817469

O	0.227759	-3.885840	1.073334
C	5.182122	-0.833528	-0.400552
C	5.461479	-0.616571	-1.894039
H	5.180161	-1.498578	-2.482897
H	4.896542	0.241780	-2.280061
H	6.526319	-0.422215	-2.069146
C	5.613817	0.423805	0.367613
H	5.066869	1.309091	0.021605
H	5.457163	0.329293	1.448122
H	6.682266	0.614094	0.210762
C	5.981864	-2.044676	0.096750
H	5.839460	-2.210139	1.171358
H	5.680355	-2.959628	-0.428718
H	7.054467	-1.896438	-0.075773
C	3.668905	-1.092658	-0.245776
H	3.405798	-1.932547	-0.898134
C	3.191732	-1.395439	1.172477
H	3.287282	-2.467727	1.394787
H	3.126755	-0.219619	-0.627809
C	0.822621	-1.575564	-1.446744
O	1.207889	-2.109693	-2.376498
H	3.780810	-0.873727	1.934917
C	1.742684	-1.068423	1.467898
O	1.337685	-0.914705	2.597926
C	-3.117813	-1.312565	1.485317
C	-3.169896	-2.837680	1.654403
C	-2.307389	-0.707427	2.639855
C	-4.550698	-0.765952	1.589310
H	-3.831187	-3.317129	0.928557
H	-2.188005	-3.309660	1.589628

H	-3.566331	-3.058302	2.652487
H	-2.263537	0.382158	2.563967
H	-2.799031	-0.952674	3.589281
H	-1.284427	-1.096048	2.686157
H	-4.993080	-1.160083	2.512558
H	-4.570411	0.324365	1.662051
H	-5.194607	-1.074273	0.762307
C	-2.874032	-1.758337	-1.615667
C	-2.444477	-0.970380	-2.862068
C	-2.236326	-3.159237	-1.663908
C	-4.398727	-1.948826	-1.658175
H	-2.927524	0.010034	-2.916360
H	-1.361553	-0.821508	-2.901345
H	-2.729833	-1.536485	-3.756809
H	-2.472093	-3.761744	-0.782661
H	-2.629315	-3.688991	-2.539618
H	-1.150773	-3.123562	-1.776512
H	-4.641535	-2.496976	-2.576821
H	-4.773661	-2.540505	-0.820214
H	-4.950708	-1.008094	-1.699926
C	0.836841	2.445989	1.610789
C	-0.032240	1.969997	2.785447
C	2.322283	2.085721	1.866682
C	0.745870	3.981740	1.572518
H	-1.082488	2.242776	2.638125
H	0.040282	0.893057	2.942842
H	0.312073	2.467358	3.700428
H	2.987106	2.864589	1.486376
H	2.495065	1.998810	2.944782
H	2.640332	1.149705	1.409961

H	1.294489	4.364416	2.442170
H	1.203854	4.420617	0.682583
H	-0.279531	4.344902	1.667745
C	1.047265	2.248208	-1.494600
C	2.534172	2.539228	-1.244678
C	0.949089	1.210896	-2.619397
C	0.401306	3.543232	-2.012316
H	2.684126	3.415041	-0.609071
H	3.059736	1.694217	-0.798802
H	3.009433	2.748591	-2.210865
H	-0.060950	0.803105	-2.729567
H	1.215449	1.687222	-3.570323
H	1.661240	0.398599	-2.462785
H	0.987918	3.876295	-2.877297
H	-0.625870	3.392295	-2.353666
H	0.417584	4.355202	-1.282794

G7

Coordinates (Angstroms)

	X	Y	Z

C	-0.570551	1.666526	0.091601
C	-1.149984	2.933440	0.242885
H	-2.211188	3.023202	0.434247
C	-0.398978	4.098050	0.131235
H	-0.881925	5.062579	0.253373
C	0.958026	4.020916	-0.160810
H	1.547318	4.923913	-0.285413

C	1.562648	2.775234	-0.274228
H	2.626293	2.724549	-0.478863
C	0.825689	1.594004	-0.120701
C	0.041994	-2.423380	1.451853
Co	0.051685	-1.567107	-0.169102
O	0.025268	-3.058332	2.399677
P	-1.616944	0.138977	0.029619
P	1.702399	-0.012994	-0.050192
C	-0.813551	-2.834700	-1.161802
O	-1.302872	-3.612812	-1.836180
H	0.184929	-0.922464	-1.487881
C	-2.669528	0.398360	-1.538425
C	-1.748209	0.282668	-2.763656
C	-3.732633	-0.709158	-1.608134
C	-3.365011	1.766696	-1.646031
H	-0.899375	0.972098	-2.700119
H	-1.367207	-0.730543	-2.911278
H	-2.324083	0.549455	-3.658283
H	-4.539111	-0.551555	-0.886151
H	-4.182173	-0.703975	-2.608364
H	-3.311769	-1.706056	-1.441688
H	-4.043156	1.733699	-2.507905
H	-3.963135	2.026860	-0.772009
H	-2.646926	2.570741	-1.828963
C	-2.728002	0.096547	1.572642
C	-3.272828	-1.337253	1.715164
C	-1.832394	0.406847	2.779678
C	-3.927714	1.053902	1.600455
H	-3.979964	-1.594645	0.922948
H	-2.480909	-2.090140	1.716288

H	-3.805050	-1.417460	2.670759
H	-1.436436	1.426804	2.747580
H	-2.422763	0.303252	3.697989
H	-0.991700	-0.286857	2.852414
H	-4.441125	0.922557	2.561229
H	-3.638674	2.105695	1.533879
H	-4.654010	0.834684	0.814663
C	2.808747	-0.228481	-1.577007
C	2.082658	0.349489	-2.801255
C	4.197358	0.419387	-1.500197
C	2.981058	-1.747866	-1.766210
H	1.111553	-0.122656	-2.973965
H	1.934884	1.430891	-2.720815
H	2.698545	0.158503	-3.687886
H	4.818868	-0.012274	-0.712501
H	4.709342	0.237173	-2.452902
H	4.148448	1.503259	-1.361288
H	3.521624	-1.934274	-2.701861
H	3.554368	-2.203272	-0.953220
H	2.010487	-2.256421	-1.831476
C	2.722857	0.068123	1.548892
C	1.741834	0.184334	2.723408
C	3.514705	-1.241304	1.680312
C	3.676854	1.270017	1.655740
H	1.079248	1.049642	2.625147
H	1.133094	-0.711391	2.848806
H	2.318077	0.309909	3.647527
H	4.330529	-1.305393	0.954998
H	3.957725	-1.290060	2.682143
H	2.876829	-2.124593	1.559044

H	4.248463	1.155077	2.584751
H	4.393795	1.342695	0.838811
H	3.129502	2.213691	1.730143

H_2

	Coordinates (Angstroms)		
	X	Y	Z

H	0.000000	0.000000	0.370920
H	0.000000	0.000000	-0.370920

H6

	Coordinates (Angstroms)		
	X	Y	Z

C	-3.856335	3.069782	-0.794664
C	-2.491962	2.956951	-0.568435
C	-2.669819	0.551250	-0.398161
C	-4.048765	0.686181	-0.622519
C	-4.642814	1.924306	-0.818262
H	-4.300153	4.049275	-0.942969
H	-1.906562	3.864710	-0.540504
H	-4.679001	-0.191183	-0.645537
H	-5.713165	1.990156	-0.986452
P	-1.936841	-1.116984	-0.115167
P	-0.063104	1.653355	0.014963

C	-2.954230	-1.912673	1.289039
C	-2.215691	-2.069507	-1.743810
C	-3.131113	-0.863572	2.397600
H	-2.175941	-0.484599	2.769406
H	-3.731830	-0.009743	2.070357
H	-3.644539	-1.331336	3.246109
C	-1.150288	-1.555414	-2.718542
H	-1.257189	-0.483697	-2.899128
H	-0.135119	-1.755427	-2.360136
H	-1.265158	-2.066345	-3.682283
C	0.775753	2.452058	-1.488566
C	0.255958	3.817523	-1.967625
H	-0.755465	3.748544	-2.376086
H	0.277107	4.593504	-1.202974
H	0.908158	4.147124	-2.786218
C	0.124600	2.765106	1.562852
C	-1.031040	2.418878	2.514317
H	-1.998322	2.760749	2.135114
H	-1.102045	1.344735	2.702790
H	-0.855099	2.909634	3.478966
Co	0.445046	-0.736109	0.358272
C	0.391877	-0.839820	2.346337
C	2.574448	-0.546245	0.550517
O	0.505855	-0.970275	3.469879
O	2.948974	-0.110616	1.601817
C	5.032801	-0.803641	-0.316433
C	5.570368	-1.384108	1.002190
H	5.094118	-0.933142	1.875085
H	5.412897	-2.469350	1.045328
H	6.649068	-1.202733	1.076273

C	5.827767	-1.453210	-1.463242
H	5.626587	-2.529378	-1.534262
H	5.603388	-0.996947	-2.432762
H	6.901190	-1.326376	-1.281604
C	5.274972	0.711373	-0.351438
H	4.932355	1.155341	-1.292901
H	4.773393	1.222609	0.476331
H	6.348752	0.915015	-0.265150
C	3.522529	-1.165968	-0.497098
C	2.989848	-1.004707	-1.918881
H	3.448763	-1.733072	-2.591017
H	3.177482	-0.003883	-2.317824
H	3.436831	-2.236561	-0.247157
H	1.909865	-1.181110	-1.947392
C	0.864939	-2.526697	0.181431
O	1.121900	-3.638452	0.142173
C	-1.873025	1.713681	-0.363847
C	-4.347508	-2.436613	0.902417
H	-4.309431	-3.229296	0.152718
H	-4.805286	-2.866034	1.802210
H	-5.020493	-1.652520	0.550278
C	-2.153050	-3.101004	1.851902
H	-2.002172	-3.893334	1.114527
H	-1.175095	-2.806709	2.239917
H	-2.711830	-3.535356	2.689433
C	-3.586107	-1.858570	-2.404705
H	-3.738395	-0.820736	-2.712767
H	-3.622256	-2.476003	-3.310984
H	-4.421382	-2.162418	-1.769403
C	-2.000231	-3.577606	-1.542038

H	-1.980878	-4.054546	-2.529372
H	-1.051973	-3.812394	-1.054705
H	-2.805252	-4.046824	-0.971601
C	1.451462	2.432087	2.260352
H	1.508073	1.395041	2.583249
H	2.320213	2.626199	1.626191
H	1.542033	3.065321	3.151385
C	0.120298	4.281708	1.319967
H	-0.785552	4.652256	0.837050
H	0.180964	4.772238	2.299550
H	0.990890	4.606939	0.744637
C	0.566708	1.481422	-2.657377
H	-0.481274	1.479351	-2.974304
H	1.170313	1.807915	-3.513196
H	0.856377	0.459097	-2.415964
C	2.268835	2.579321	-1.159483
H	2.683339	1.655481	-0.751567
H	2.822906	2.818859	-2.075130
H	2.457821	3.381415	-0.439565

Hacac

	Coordinates (Angstroms)		
	X	Y	Z

O	1.268928	1.258264	-0.003232
C	1.246720	0.012213	-0.005806
C	0.007960	-0.728444	-0.005349
H	0.030714	-1.811877	-0.008590

C	2.538263	-0.763737	0.003069
H	2.541405	-1.517104	-0.791831
H	2.641505	-1.296094	0.956161
H	3.385431	-0.086876	-0.123828
O	-1.287378	1.240330	0.003822
C	-1.196805	-0.081328	-0.000054
C	-2.517054	-0.777008	0.000895
H	-3.098774	-0.471543	-0.875819
H	-2.394056	-1.861681	-0.010692
H	-3.088287	-0.489389	0.890523
H	-0.344846	1.575631	0.002825

I1

Coordinates (Angstroms)

	X	Y	Z

C	1.049169	1.368105	3.786329
C	1.658787	1.100571	2.562564
C	0.877355	0.773001	1.454929
C	-0.523050	0.724660	1.574387
C	-1.124715	0.986871	2.804732
C	-0.336724	1.306572	3.908262
H	1.659208	1.630656	4.645034
H	2.739469	1.159153	2.471012
H	-2.205469	0.954405	2.905074
H	-0.809139	1.516768	4.862569
P	-1.457192	0.312263	0.057527
P	1.571307	0.339798	-0.183449

Co	-0.048893	0.681001	-1.692158
H	1.074551	0.797681	-2.718068
C	-1.178654	0.897543	-3.101971
O	-1.850102	1.020816	-4.013714
C	-3.079689	1.109854	0.176769
C	-4.139233	0.522886	0.877278
C	-3.253248	2.350874	-0.444254
C	-5.359414	1.185616	0.965785
H	-4.014495	-0.448184	1.348348
C	-4.474301	3.011754	-0.347848
H	-2.434763	2.795054	-1.006924
C	-5.525495	2.428981	0.357407
H	-6.182651	0.729045	1.506573
H	-4.607556	3.975324	-0.829859
H	-6.479950	2.941749	0.428638
C	-1.736495	-1.484964	0.086255
C	-1.253043	-2.308661	1.104782
C	-2.375452	-2.053659	-1.023483
C	-1.400051	-3.690580	1.008827
H	-0.749955	-1.880102	1.966054
C	-2.528442	-3.432808	-1.109022
H	-2.755619	-1.418011	-1.819961
C	-2.034567	-4.253145	-0.095209
H	-1.013798	-4.327495	1.798658
H	-3.026075	-3.868084	-1.970230
H	-2.145210	-5.330778	-0.168415
C	3.159338	1.204897	-0.324736
C	4.343854	0.661191	0.181997
C	3.175871	2.460451	-0.940508
C	5.534073	1.376047	0.078189

H	4.344098	-0.319381	0.648915
C	4.366982	3.172620	-1.036873
H	2.261364	2.877676	-1.354029
C	5.545835	2.630257	-0.528351
H	6.452891	0.949204	0.468207
H	4.376407	4.145837	-1.517701
H	6.477227	3.182077	-0.612374
C	1.896247	-1.448067	-0.101475
C	2.206341	-2.097598	1.097597
C	1.761911	-2.192718	-1.278616
C	2.382272	-3.477810	1.115374
H	2.295746	-1.535393	2.022570
C	1.930369	-3.573971	-1.253891
H	1.522512	-1.695932	-2.215500
C	2.238723	-4.216690	-0.057452
H	2.620510	-3.977868	2.049168
H	1.816411	-4.145509	-2.169774
H	2.366167	-5.294845	-0.037796

I5

Coordinates (Angstroms)

	X	Y	Z

C	2.844305	3.762816	-1.416980
C	1.530944	3.442971	-1.082744
C	1.195293	2.133833	-0.731154
C	2.194693	1.142694	-0.713035
C	3.508467	1.472138	-1.049530

C	3.830417	2.779908	-1.402245
H	3.094916	4.782494	-1.692672
H	0.766610	4.213782	-1.110650
H	4.280402	0.708423	-1.042417
H	4.853357	3.028967	-1.666887
P	1.701410	-0.541490	-0.201649
P	-0.501618	1.628172	-0.252780
Co	-0.529168	-0.679822	-0.682192
C	-0.813924	-0.681576	-2.513425
C	-0.665843	-2.585134	-0.622298
O	-0.938373	-0.708445	-3.646998
O	-0.113360	-3.533009	-1.092759
C	-4.417426	-3.288510	0.275867
C	-5.416130	-4.080937	-0.579820
H	-5.538581	-3.624800	-1.569989
H	-5.080897	-5.115135	-0.723692
H	-6.401090	-4.110028	-0.099382
C	-4.277902	-3.964643	1.646290
H	-3.843082	-4.967248	1.550026
H	-3.643235	-3.382511	2.325071
H	-5.258792	-4.068743	2.124845
C	-4.944807	-1.857726	0.455193
H	-4.299578	-1.253664	1.104781
H	-5.033205	-1.344132	-0.510649
H	-5.939177	-1.873598	0.916416
C	-3.067236	-3.291243	-0.472658
H	-3.197045	-2.780769	-1.437123
C	-1.904649	-2.631251	0.281752
H	-1.616085	-3.186410	1.181184
H	-2.193587	-1.619300	0.611648

H	-2.778470	-4.325054	-0.696300
C	-1.613018	2.779823	-1.124283
C	-2.649534	3.443588	-0.462840
C	-1.465749	2.933968	-2.509114
C	-3.523344	4.258754	-1.180370
H	-2.778586	3.332516	0.609612
C	-2.334811	3.754948	-3.218391
H	-0.658115	2.428612	-3.032489
C	-3.366593	4.417782	-2.554376
H	-4.325590	4.773244	-0.659998
H	-2.205145	3.878657	-4.289197
H	-4.045637	5.057887	-3.109507
C	-0.625126	2.023544	1.522368
C	-0.178308	3.243833	2.041395
C	-1.124014	1.047016	2.389509
C	-0.226442	3.477159	3.411400
H	0.213764	4.008729	1.376927
C	-1.174867	1.283497	3.760422
H	-1.463115	0.090519	1.998896
C	-0.721968	2.497063	4.271171
H	0.127501	4.422960	3.810304
H	-1.555537	0.517175	4.428512
H	-0.752584	2.680384	5.341034
C	2.941913	-1.685099	-0.865740
C	4.111232	-1.991600	-0.160992
C	2.711610	-2.260806	-2.119302
C	5.046788	-2.860245	-0.714786
H	4.290010	-1.555004	0.817396
C	3.652059	-3.126224	-2.669936
H	1.793075	-2.044357	-2.657033

C	4.818001	-3.425983	-1.968013
H	5.953890	-3.096464	-0.166705
H	3.469590	-3.575500	-3.641307
H	5.547155	-4.108323	-2.394802
C	1.900619	-0.563804	1.612441
C	2.369499	0.537185	2.333305
C	1.477169	-1.709273	2.298976
C	2.403401	0.495772	3.725250
H	2.695926	1.435066	1.817908
C	1.521553	-1.749580	3.688403
H	1.120502	-2.576817	1.748268
C	1.978306	-0.643200	4.403644
H	2.758253	1.360207	4.277970
H	1.196388	-2.643237	4.212572
H	2.002836	-0.670690	5.488975

I6

Coordinates (Angstroms)

	X	Y	Z

C	2.974073	-2.135051	-3.237267
C	1.879884	-2.398353	-2.418744
C	1.405488	-1.419212	-1.542964
C	2.040931	-0.164524	-1.490811
C	3.142754	0.086647	-2.313293
C	3.607092	-0.895421	-3.182394
H	3.330556	-2.898680	-3.921569
H	1.390757	-3.366295	-2.471166

H	3.634214	1.054309	-2.279769
H	4.460375	-0.689265	-3.821032
P	1.385403	1.098408	-0.336164
P	-0.005413	-1.706208	-0.409912
Co	-0.786387	0.448291	0.144549
C	-1.005469	0.166234	1.972363
C	-1.521536	2.208957	0.381483
O	-1.093599	0.005688	3.097601
O	-1.113956	3.244071	0.822059
C	-5.403822	1.768730	0.699924
C	-6.257805	2.153557	1.917003
H	-5.915772	1.634810	2.821132
H	-6.208239	3.232308	2.108473
H	-7.309459	1.889654	1.754407
C	-5.906896	2.531093	-0.532240
H	-5.781822	3.613438	-0.405001
H	-5.372778	2.233024	-1.442218
H	-6.972424	2.333273	-0.698717
C	-5.530256	0.256792	0.463496
H	-4.981323	-0.072540	-0.427157
H	-5.154852	-0.310165	1.325040
H	-6.580521	-0.019766	0.314086
C	-3.944303	2.154907	1.021882
H	-3.610618	1.560470	1.884142
C	-2.945411	1.969187	-0.129066
H	-3.110037	2.689847	-0.938647
H	-3.038977	0.966772	-0.572530
H	-3.906120	3.206010	1.331649
H	-1.284939	1.100304	-2.276761
H	-1.009503	0.419962	-2.413615

C	0.717791	-2.585260	1.018211
C	-0.155218	-3.078357	1.996976
C	2.096196	-2.707073	1.203450
C	0.346889	-3.684556	3.142576
H	-1.231116	-2.991907	1.862224
C	2.595898	-3.305066	2.358899
H	2.787720	-2.337871	0.453207
C	1.724850	-3.793850	3.327812
H	-0.338263	-4.066143	3.893507
H	3.669484	-3.389640	2.497393
H	2.117481	-4.259443	4.226741
C	-1.097898	-2.920005	-1.216269
C	-2.224834	-2.440649	-1.892746
C	-0.854516	-4.297965	-1.170904
C	-3.091904	-3.324858	-2.528495
H	-2.427325	-1.373356	-1.921068
C	-1.724653	-5.179422	-1.805237
H	0.008602	-4.682916	-0.635484
C	-2.841750	-4.694413	-2.483905
H	-3.965735	-2.944796	-3.048883
H	-1.532445	-6.247269	-1.765108
H	-3.521222	-5.386133	-2.972674
C	2.452070	1.043985	1.140073
C	1.976225	1.658427	2.305221
C	3.694883	0.405503	1.155096
C	2.733424	1.628512	3.471979
H	1.019148	2.174250	2.295040
C	4.444227	0.368272	2.328176
H	4.080209	-0.070709	0.259011
C	3.964406	0.975480	3.486202

H	2.357427	2.108820	4.370056
H	5.405008	-0.137454	2.335554
H	4.549706	0.941894	4.400235
C	1.726782	2.693424	-1.154346
C	2.400466	3.729433	-0.504261
C	1.242140	2.894260	-2.453708
C	2.585817	4.952597	-1.146359
H	2.785542	3.591105	0.501295
C	1.434148	4.114222	-3.091715
H	0.729661	2.092417	-2.977447
C	2.103111	5.147851	-2.436802
H	3.110855	5.752820	-0.633458
H	1.060623	4.257841	-4.101259
H	2.249519	6.101873	-2.934389

J6

Coordinates (Angstroms)

	X	Y	Z
C	2.888484	0.863136	3.854116
C	3.016828	0.128389	2.677920
C	2.016693	0.190675	1.708616
C	0.882110	0.994812	1.917865
C	0.769568	1.738574	3.093575
C	1.770335	1.667053	4.059575
H	3.663612	0.806036	4.611860
H	3.892874	-0.493606	2.522023
H	-0.105064	2.357555	3.269582

H	1.670744	2.235399	4.978931
P	-0.361340	1.033511	0.570959
P	2.101320	-0.688856	0.111424
Co	-0.089488	-0.956399	-0.550412
C	0.141406	-2.330933	-1.767493
O	0.283580	-3.197371	-2.492661
C	-5.651363	-1.603150	-0.945958
C	-6.855148	-1.044103	-1.717462
H	-6.968731	0.033642	-1.546895
H	-6.742211	-1.205171	-2.796691
H	-7.783961	-1.533827	-1.400470
C	-5.557550	-3.113538	-1.203221
H	-5.384181	-3.321917	-2.266408
H	-4.746824	-3.580308	-0.631399
H	-6.489775	-3.611683	-0.911107
C	-5.858908	-1.346825	0.552645
H	-5.048230	-1.768477	1.158795
H	-5.911755	-0.272073	0.762850
H	-6.795235	-1.804054	0.895116
C	-4.387404	-0.880639	-1.460994
H	-4.530503	0.202709	-1.356738
C	-3.089932	-1.262927	-0.753771
H	-3.107148	-0.968706	0.302426
H	-4.280456	-1.080749	-2.534268
C	-0.649406	-2.054656	0.947205
O	-1.001669	-2.673574	1.834127
H	-2.920256	-2.349084	-0.762906
C	-1.847505	-0.658750	-1.368136
O	-1.830849	-0.016854	-2.390331
C	3.248699	-2.085336	0.302471

C	4.634102	-1.890569	0.239335
C	2.739346	-3.369999	0.517813
C	5.496648	-2.969065	0.407091
H	5.039374	-0.899355	0.056092
C	3.606399	-4.445869	0.686355
H	1.666641	-3.540065	0.547584
C	4.983530	-4.245484	0.632398
H	6.569653	-2.812499	0.356232
H	3.203976	-5.440543	0.851171
H	5.659730	-5.085594	0.758774
C	2.913705	0.474062	-1.033529
C	3.482953	1.675425	-0.604602
C	2.888759	0.166654	-2.399336
C	4.016609	2.562990	-1.536004
H	3.499872	1.931855	0.450293
C	3.430078	1.052144	-3.324553
H	2.437733	-0.760799	-2.744425
C	3.989804	2.254226	-2.893360
H	4.448105	3.499842	-1.197348
H	3.405043	0.809258	-4.382548
H	4.399441	2.952291	-3.617295
C	-1.974280	1.315503	1.360353
C	-2.931211	2.108413	0.718690
C	-2.311477	0.638439	2.538974
C	-4.206076	2.237935	1.263841
H	-2.686705	2.627592	-0.203473
C	-3.586671	0.773243	3.078830
H	-1.580433	0.017588	3.049529
C	-4.533690	1.574947	2.444066
H	-4.942236	2.859773	0.763802

H	-3.838097	0.253411	3.998122
H	-5.527241	1.680404	2.868976
C	0.016554	2.521932	-0.403731
C	0.148918	3.770371	0.215511
C	0.229259	2.400990	-1.778814
C	0.503646	4.883280	-0.537782
H	-0.023509	3.876118	1.282727
C	0.582180	3.519273	-2.529549
H	0.114159	1.439835	-2.267507
C	0.724339	4.756992	-1.909493
H	0.610305	5.849635	-0.054695
H	0.751694	3.417362	-3.596838
H	1.005591	5.627867	-2.494320

J7

Coordinates (Angstroms)

	X	Y	Z
C	0.598261	-0.307897	1.618913
C	1.254356	-0.384588	2.851138
H	2.340072	-0.397883	2.887187
C	0.520869	-0.437968	4.031247
H	1.036722	-0.502608	4.984035
C	-0.872521	-0.400522	3.992362
H	-1.443410	-0.432165	4.915000
C	-1.534599	-0.324186	2.772499
H	-2.620313	-0.293762	2.745091
C	-0.804072	-0.300055	1.581414

C	-0.003888	0.876159	-2.584251
Co	-0.109897	-0.674378	-1.586347
O	0.084105	1.806641	-3.231532
P	1.518102	-0.161256	0.045751
P	-1.643498	-0.165605	-0.034540
C	0.887569	-1.804021	-2.611619
O	1.531581	-2.539081	-3.194670
H	-0.300887	-1.946013	-0.816713
C	-2.355163	1.514627	0.029362
C	-3.687600	1.760924	0.372051
C	-1.483910	2.591331	-0.170728
C	-4.143017	3.072197	0.490925
H	-4.375006	0.940205	0.549558
C	-1.939861	3.898225	-0.040357
H	-0.436993	2.416487	-0.402728
C	-3.273234	4.140022	0.284626
H	-5.181216	3.256519	0.749577
H	-1.250801	4.723608	-0.191030
H	-3.633409	5.159733	0.382263
C	-3.032612	-1.339659	-0.066635
C	-3.063533	-2.460518	0.767822
C	-4.012672	-1.183198	-1.054327
C	-4.081404	-3.400490	0.630942
H	-2.297182	-2.609331	1.522226
C	-5.027954	-2.125861	-1.185216
H	-3.989475	-0.323824	-1.719655
C	-5.064899	-3.233934	-0.341293
H	-4.103007	-4.265140	1.287287
H	-5.788284	-1.994545	-1.949011
H	-5.856343	-3.970087	-0.444589

C	2.184648	1.535565	0.013852
C	2.893120	1.921263	-1.132592
C	1.958654	2.470568	1.027772
C	3.381219	3.216984	-1.254864
H	3.068901	1.203152	-1.930858
C	2.437639	3.772729	0.894387
H	1.403695	2.195395	1.919185
C	3.150295	4.146587	-0.241495
H	3.934278	3.502691	-2.144398
H	2.253258	4.494284	1.684473
H	3.524179	5.161252	-0.340108
C	2.951668	-1.269817	0.243383
C	4.243123	-0.798459	0.496525
C	2.726026	-2.648456	0.141691
C	5.296334	-1.699298	0.639786
H	4.432501	0.266995	0.583440
C	3.779403	-3.543433	0.292526
H	1.724058	-3.025332	-0.048882
C	5.067265	-3.068803	0.537028
H	6.297753	-1.326412	0.832413
H	3.595825	-4.610438	0.211546
H	5.890699	-3.768221	0.646268

K1

Coordinates (Angstroms)

	X	Y	Z

C	3.966123	-0.195038	0.025644

C	2.974284	0.779914	0.027289
C	1.628224	0.404536	0.004971
C	1.284029	-0.953402	-0.014632
C	2.285571	-1.928502	-0.017824
C	3.622705	-1.547341	0.001999
H	5.011305	0.097779	0.042741
H	3.248766	1.831469	0.044391
H	2.023444	-2.983007	-0.033171
H	4.399917	-2.305152	0.000752
P	-0.488739	-1.380331	-0.013139
P	0.281198	1.643090	-0.003372
Co	-1.672258	0.607629	-0.028803
H	-2.236687	2.050883	0.153316
C	-3.374608	-0.002439	0.002822
O	-4.458200	-0.353946	0.036269
C	-0.766970	-2.379225	1.486191
H	-1.809404	-2.712661	1.501487
H	-0.109726	-3.254572	1.499467
H	-0.578862	-1.771700	2.375893
C	-0.754345	-2.529365	-1.401805
H	-0.095561	-3.399379	-1.317377
H	-1.796080	-2.864842	-1.387519
H	-0.562314	-2.019099	-2.349826
C	0.615703	2.727134	1.420300
H	1.634202	3.124628	1.368433
H	-0.100377	3.553748	1.409839
H	0.492600	2.166697	2.351376
C	0.594747	2.675626	-1.471062
H	-0.120833	3.502873	-1.482996
H	1.614031	3.073998	-1.445478

H	0.462498	2.081154	-2.379467

K5

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.627963	1.348542	-0.918324
C	-3.567143	1.671218	-0.080026
C	-2.434472	0.851691	-0.025525
C	-2.376130	-0.302330	-0.822460
C	-3.448889	-0.619423	-1.662985
C	-4.569385	0.201952	-1.710555
H	-5.502231	1.991327	-0.954757
H	-3.622432	2.566646	0.533371
H	-3.408620	-1.511233	-2.283102
H	-5.397551	-0.050652	-2.365560
P	-0.882549	-1.356816	-0.739721
P	-1.028498	1.244614	1.084493
Co	0.580830	-0.415801	0.760988
C	0.369368	-1.320340	2.367644
C	2.035466	-1.626610	0.234285
O	0.137860	-1.911478	3.316101
O	2.008167	-2.747599	-0.196199
C	3.316637	1.293819	-0.964834
C	3.240396	2.815873	-0.780525
H	2.317448	3.110015	-0.264578
H	4.087052	3.185104	-0.189215
H	3.259595	3.327755	-1.749513

C	4.617904	0.942872	-1.697969
H	5.494786	1.233134	-1.106331
H	4.693320	-0.128992	-1.912570
H	4.669980	1.472690	-2.656202
C	2.119109	0.827061	-1.798932
H	2.171634	-0.244604	-2.021508
H	1.170017	1.024721	-1.274887
H	2.076304	1.358486	-2.756869
C	3.296086	0.655545	0.440338
H	2.404928	1.038795	0.974980
C	3.341146	-0.878588	0.529219
H	3.564809	-1.162139	1.567455
H	4.132307	-1.306530	-0.095713
H	4.151605	1.043168	1.005699
C	-0.568225	2.962726	0.654726
H	0.206336	3.308233	1.347134
H	-0.175047	3.001992	-0.365159
H	-1.429819	3.634797	0.729705
C	-1.803866	1.419673	2.732359
H	-2.567519	2.204274	2.731971
H	-2.267326	0.472036	3.023472
H	-1.032836	1.672729	3.466934
C	-1.477475	-3.002778	-0.219220
H	-2.216599	-3.403681	-0.920126
H	-0.618543	-3.679910	-0.175193
H	-1.921888	-2.931737	0.778092
C	-0.391134	-1.593244	-2.482839
H	-1.193534	-2.073672	-3.052016
H	-0.158009	-0.627517	-2.939644
H	0.498317	-2.228914	-2.519593

K6

	Coordinates (Angstroms)		
	X	Y	Z
C	-5.107959	1.246536	-0.649874
C	-3.868278	1.778658	-0.315254
C	-2.750973	0.943760	-0.199818
C	-2.885545	-0.435087	-0.424282
C	-4.137648	-0.959588	-0.761646
C	-5.243175	-0.123993	-0.872247
H	-5.970589	1.900082	-0.736208
H	-3.771432	2.847279	-0.141742
H	-4.249166	-2.025872	-0.940392
H	-6.211512	-0.540148	-1.132686
P	-1.403276	-1.501439	-0.278195
P	-1.114418	1.620152	0.266809
Co	0.413764	-0.130029	0.284106
C	0.367702	-0.347637	2.097269
C	1.797018	-1.561838	0.271255
O	0.234062	-0.534884	3.216147
O	1.598786	-2.694203	-0.079945
C	4.468822	0.646047	-0.659647
C	4.632132	2.163829	-0.821628
H	3.670213	2.645966	-1.039579
H	5.036620	2.618511	0.091109
H	5.318056	2.398127	-1.644153
C	5.842221	0.033237	-0.349377

H	6.236672	0.410364	0.602371
H	5.806288	-1.060518	-0.290498
H	6.560149	0.292896	-1.136253
C	3.927801	0.057808	-1.968855
H	3.719179	-1.015740	-1.882553
H	3.006962	0.563939	-2.280457
H	4.659344	0.184075	-2.775819
C	3.491829	0.399708	0.512946
H	2.577579	0.985572	0.318395
C	3.138271	-1.070954	0.799658
H	3.054206	-1.223427	1.884881
H	3.912180	-1.762606	0.451502
H	3.932870	0.838676	1.415051
H	1.121295	-0.143504	-1.386449
H	0.581320	0.413937	-1.441528
C	-1.422022	2.478340	1.851309
H	-0.490158	2.929569	2.207023
H	-2.176952	3.262751	1.735130
H	-1.772688	1.759714	2.598214
C	-0.812351	2.990124	-0.905292
H	0.138170	3.470988	-0.651949
H	-0.744141	2.598215	-1.924569
H	-1.609988	3.738794	-0.860215
C	-1.893703	-2.819273	0.887745
H	-2.119555	-2.383286	1.865488
H	-2.770445	-3.367346	0.528959
H	-1.056872	-3.515744	0.999285
C	-1.312546	-2.361231	-1.887706
H	-1.114976	-1.636158	-2.683087
H	-0.488089	-3.079842	-1.855129

H	-2.243137	-2.893145	-2.111155

L6

	Coordinates (Angstroms)		
	X	Y	Z

C	-5.313020	-1.638702	0.143166
C	-4.696326	-0.393098	0.122643
C	-3.303791	-0.303535	0.033981
C	-2.533254	-1.470259	-0.041288
C	-3.160329	-2.719755	-0.018736
C	-4.544935	-2.801653	0.075607
H	-6.394221	-1.706029	0.213270
H	-5.298651	0.510045	0.171672
H	-2.569225	-3.629713	-0.075943
H	-5.028299	-3.773353	0.093308
P	-0.715022	-1.313839	-0.179313
P	-2.439481	1.304292	0.018887
Co	-0.187044	0.912273	-0.165206
C	0.275672	2.640821	-0.622207
O	0.561043	3.713212	-0.879305
C	5.225695	-0.606027	0.142896
C	6.366811	-1.051307	-0.782384
H	6.096642	-1.958923	-1.336572
H	6.609130	-0.270466	-1.513647
H	7.275814	-1.267250	-0.208046
C	5.656295	0.665500	0.887536
H	5.814039	1.496916	0.188897

H	4.910539	0.981055	1.626579
H	6.597534	0.497167	1.424523
C	4.940012	-1.723611	1.156546
H	4.178206	-1.428796	1.887812
H	4.593636	-2.635283	0.653169
H	5.847969	-1.976694	1.717160
C	3.987599	-0.332657	-0.738406
H	3.731197	-1.253273	-1.278880
C	2.752002	0.158850	0.011027
H	2.449142	-0.532936	0.807106
H	4.253298	0.409441	-1.501288
C	0.225516	1.076074	1.712578
O	0.504149	1.155143	2.812986
H	2.932103	1.120688	0.511968
C	1.541870	0.377032	-0.863079
O	1.535583	0.285191	-2.068838
C	-3.021660	2.176977	1.512778
H	-4.103729	2.340290	1.479395
H	-2.776295	1.592610	2.404461
H	-2.517611	3.146642	1.578139
C	-3.184960	2.239487	-1.360158
H	-4.273025	2.294361	-1.254095
H	-2.776044	3.255407	-1.362870
H	-2.936049	1.758528	-2.310587
C	-0.060029	-2.307199	1.204408
H	1.033677	-2.304565	1.171328
H	-0.389507	-1.883651	2.157473
H	-0.414308	-3.340547	1.133416
C	-0.276376	-2.277364	-1.664769
H	-0.741583	-3.267126	-1.625181

H	-0.612802	-1.752743	-2.562934
H	0.809190	-2.395779	-1.714276

L7

	Coordinates (Angstroms)		
	X	Y	Z

C	-1.467213	-0.926539	0.031090
C	-2.520425	-1.842310	0.112123
H	-2.313149	-2.899194	0.256210
C	-3.837571	-1.408679	0.010545
H	-4.648379	-2.128084	0.071072
C	-4.114935	-0.054253	-0.168060
H	-5.142942	0.285265	-0.248127
C	-3.075747	0.866468	-0.243158
H	-3.303128	1.920448	-0.376879
C	-1.748335	0.436090	-0.147352
C	2.155416	0.745798	1.386927
Co	1.518360	0.469217	-0.318728
O	2.543440	0.881685	2.448496
P	0.276262	-1.461124	0.183368
P	-0.377347	1.640664	-0.195201
C	2.911684	-0.382383	-1.127833
O	3.726532	-0.955952	-1.679281
H	0.947013	0.388642	-1.707184
C	0.362808	-2.249145	1.830155
H	-0.350516	-3.075566	1.913652
H	1.375118	-2.634023	1.991294

H	0.142777	-1.508056	2.604592
C	0.448127	-2.856165	-0.982064
H	0.343375	-2.490049	-2.007566
H	1.443499	-3.297828	-0.865955
H	-0.301146	-3.631715	-0.794619
C	-0.623959	2.665377	1.295264
H	0.148797	3.439847	1.333197
H	-1.608314	3.143461	1.269679
H	-0.551243	2.045161	2.193478
C	-0.731226	2.778223	-1.571751
H	-1.676658	3.305720	-1.412565
H	0.076774	3.514116	-1.635898
H	-0.772844	2.219150	-2.510246

Linear aldehyde

Coordinates (Angstroms)

	X	Y	Z
C	-2.581715	-0.382094	0.108864
O	-3.531630	0.214564	-0.348528
C	-0.135235	-0.448905	-0.371169
C	-1.250597	0.233153	0.436985
H	-1.301932	1.307971	0.242692
H	-2.651676	-1.473492	0.307495
H	-1.080169	0.077514	1.511146
H	-0.205185	-1.535443	-0.219378
H	-0.319207	-0.270745	-1.439286
C	1.307099	-0.004858	-0.042357

C	1.486901	1.496858	-0.299499
H	0.865674	2.103418	0.369258
H	2.530404	1.792212	-0.136178
H	1.222759	1.754963	-1.332602
C	1.658773	-0.323133	1.417018
H	1.488077	-1.383288	1.642275
H	2.715468	-0.104760	1.612782
H	1.066709	0.273323	2.120419
C	2.253179	-0.786887	-0.964531
H	2.040965	-0.577023	-2.020091
H	3.298817	-0.517799	-0.772668
H	2.151899	-1.868170	-0.809510

M1

Coordinates (Angstroms)

	X	Y	Z
C	-3.986964	-0.030964	-0.000002
C	-2.959479	0.906662	-0.000081
C	-1.629589	0.478462	-0.000058
C	-1.333535	-0.891264	0.000013
C	-2.370685	-1.826936	0.000069
C	-3.692990	-1.394546	0.000068
H	-5.020459	0.301095	0.000017
H	-3.194835	1.968461	-0.000123
H	-2.152011	-2.891811	0.000124
H	-4.497816	-2.123010	0.000124
P	0.429552	-1.354818	0.000041

P	-0.210035	1.620110	0.000005
Co	1.689872	0.515504	-0.000081
H	2.265413	1.936920	-0.000665
C	3.394992	-0.137443	0.000099
O	4.472272	-0.507588	0.000200
N	0.579044	-2.227238	-1.429872
H	1.535179	-2.453065	-1.686725
H	-0.041020	-3.019766	-1.577435
N	0.578898	-2.228955	1.428845
H	-0.040825	-3.021912	1.575444
H	1.535032	-2.454314	1.686073
N	-0.413496	2.466576	-1.432906
H	-1.319476	2.890940	-1.612852
H	0.350010	3.094309	-1.664934
N	-0.412838	2.465174	1.433883
H	0.350493	3.093163	1.665826
H	-1.318906	2.888991	1.614728

M5

Coordinates (Angstroms)

	X	Y	Z
C	-4.894687	0.984682	-0.539090
C	-3.734602	1.535237	-0.004862
C	-2.533489	0.820746	-0.046804
C	-2.507980	-0.453715	-0.631948
C	-3.676310	-0.999367	-1.169990
C	-4.866164	-0.281666	-1.122201

H	-5.825014	1.542809	-0.499432
H	-3.774576	2.523437	0.446593
H	-3.660495	-1.986405	-1.625525
H	-5.772836	-0.709850	-1.538119
P	-0.913067	-1.327403	-0.683364
P	-0.968578	1.499236	0.613300
Co	0.575751	-0.234071	0.630460
C	0.282660	-0.739196	2.395970
C	1.871535	-1.676881	0.500395
O	0.033012	-1.104244	3.445769
O	1.722974	-2.862744	0.333072
C	3.534414	0.972653	-0.904513
C	3.496918	2.506088	-0.860941
H	2.535543	2.867667	-0.472433
H	4.287630	2.902752	-0.212652
H	3.634961	2.932619	-1.861048
C	4.897234	0.520381	-1.447869
H	5.713358	0.848396	-0.792931
H	4.957891	-0.569354	-1.547497
H	5.070804	0.949613	-2.441613
C	2.428124	0.468588	-1.839718
H	2.446669	-0.623303	-1.942981
H	1.428474	0.774596	-1.486892
H	2.544847	0.892951	-2.843458
C	3.345047	0.461511	0.542159
H	2.459735	0.960696	0.986769
C	3.243890	-1.056010	0.751423
H	3.431567	-1.280291	1.811374
H	3.994230	-1.609790	0.176063
H	4.185367	0.829654	1.142205

N	-1.435012	2.049259	2.140315
H	-0.659310	2.282577	2.752174
H	-2.158965	2.761895	2.188837
N	-0.654755	2.720408	-0.510119
H	-1.380619	3.418911	-0.653237
H	0.257652	3.156595	-0.424000
N	-1.245350	-2.845568	-0.043717
H	-1.884231	-3.447185	-0.557528
H	-0.383328	-3.335246	0.194574
N	-0.560784	-1.302163	-2.331887
H	0.379038	-1.611821	-2.561312
H	-1.245119	-1.725452	-2.954339

M6

Coordinates (Angstroms)

	X	Y	Z
C	-5.282275	0.798231	-0.621458
C	-4.102663	1.486533	-0.362565
C	-2.893719	0.793382	-0.246010
C	-2.878336	-0.600813	-0.391012
C	-4.068967	-1.285841	-0.651643
C	-5.265855	-0.588882	-0.766973
H	-6.217496	1.342226	-0.710496
H	-4.130649	2.567522	-0.249720
H	-4.063942	-2.367239	-0.765852
H	-6.188104	-1.124904	-0.968870
P	-1.280737	-1.454372	-0.201940

P	-1.320398	1.662695	0.084078
Co	0.396649	0.069684	0.253658
C	0.266233	-0.008669	2.102869
C	1.820348	-1.327634	0.317609
O	0.075220	-0.111949	3.221864
O	1.694705	-2.430401	-0.150633
C	4.630649	0.502000	-0.612744
C	4.843466	1.947626	-1.081815
H	3.916813	2.372369	-1.488927
H	5.174290	2.589301	-0.255685
H	5.605784	1.993332	-1.868266
C	5.968188	-0.057898	-0.107270
H	6.354356	0.538532	0.728239
H	5.876073	-1.095748	0.233293
H	6.717956	-0.041611	-0.907065
C	4.148585	-0.343553	-1.799293
H	3.992944	-1.392708	-1.524385
H	3.211682	0.042098	-2.218647
H	4.895351	-0.324502	-2.601738
C	3.602968	0.522383	0.543855
H	2.747752	1.152956	0.253411
C	3.094041	-0.853670	1.008063
H	2.839807	-0.807087	2.074924
H	3.856045	-1.632520	0.896175
H	4.067982	1.029663	1.396952
H	1.351820	0.286632	-1.391503
H	0.722034	0.689065	-1.555490
N	-1.665417	2.450094	1.537626
H	-0.859726	2.876557	1.985028
H	-2.465153	3.078511	1.555963

N	-1.229078	2.684871	-1.260445
H	-2.021535	3.302639	-1.423844
H	-0.353969	3.194186	-1.339779
N	-1.604900	-2.492292	1.094321
H	-2.364894	-3.157927	0.974289
H	-0.776844	-2.961314	1.450404
N	-1.085084	-2.236606	-1.686138
H	-0.153875	-2.637465	-1.769823
H	-1.791027	-2.921721	-1.946503

N6

Coordinates (Angstroms)

	X	Y	Z

C	-5.082715	-1.694110	0.587961
C	-4.471991	-0.446389	0.645622
C	-3.128762	-0.312737	0.284310
C	-2.399699	-1.432669	-0.129279
C	-3.021903	-2.683411	-0.191552
C	-4.359156	-2.810339	0.167624
H	-6.126159	-1.798440	0.868396
H	-5.045048	0.419094	0.969231
H	-2.466594	-3.558780	-0.519964
H	-4.840553	-3.781920	0.119834
P	-0.649501	-1.188551	-0.587834
P	-2.260108	1.282920	0.291641
Co	-0.072991	0.995949	-0.297449
C	0.324704	2.793315	-0.460472

O	0.568603	3.905110	-0.508849
C	4.664868	-0.874768	0.480697
C	4.706310	-2.218996	1.221655
H	3.995126	-2.232982	2.057142
H	4.453384	-3.048182	0.548891
H	5.706152	-2.410598	1.628492
C	5.677283	-0.909041	-0.671290
H	5.419981	-1.688526	-1.398919
H	5.727050	0.047734	-1.203497
H	6.682763	-1.123301	-0.290022
C	5.027192	0.251739	1.457058
H	5.092180	1.222979	0.952997
H	4.285414	0.334239	2.261677
H	6.002117	0.059826	1.920520
C	3.228638	-0.691909	-0.055581
H	2.538908	-0.795261	0.791612
C	2.944106	0.642599	-0.756802
H	3.026847	1.467812	-0.039621
H	3.009758	-1.511342	-0.754471
C	0.542881	0.809027	1.543169
O	0.865990	0.687253	2.625552
H	3.647310	0.810994	-1.579205
C	1.545560	0.667054	-1.332786
O	1.329964	0.586245	-2.523853
N	-2.472164	1.823433	1.871501
H	-1.908420	2.631942	2.117051
H	-3.425549	1.924452	2.211799
N	-3.108930	2.135427	-0.888775
H	-4.117010	2.210868	-0.773420
H	-2.703249	3.031534	-1.142387

N	0.095453	-2.269739	0.464444
H	-0.291230	-3.210927	0.479840
H	1.105659	-2.310098	0.371526
N	-0.522175	-1.659035	-2.188810
H	-1.258358	-2.219582	-2.604420
H	-0.141206	-0.953358	-2.812360

N7

Coordinates (Angstroms)

	X	Y	Z
C	-1.515326	-0.877371	0.046679
C	-2.607268	-1.747001	0.117318
H	-2.452276	-2.809730	0.287615
C	-3.900537	-1.258334	-0.033957
H	-4.743646	-1.940157	0.019271
C	-4.114036	0.100201	-0.263247
H	-5.123216	0.479081	-0.391290
C	-3.034183	0.973216	-0.333189
H	-3.207830	2.029286	-0.523062
C	-1.733840	0.488633	-0.171117
C	2.159234	0.680425	1.378465
Co	1.540702	0.400636	-0.340329
O	2.517601	0.825530	2.447959
P	0.205621	-1.454441	0.223420
P	-0.304242	1.613543	-0.193423
C	2.912717	-0.489726	-1.153590
O	3.712373	-1.078041	-1.710768

H	0.958506	0.342452	-1.727234
N	0.228801	-1.936979	1.842778
H	-0.452747	-2.637200	2.126452
H	1.151541	-2.173162	2.195476
N	0.262643	-2.725850	-0.885975
H	1.198111	-3.078665	-1.063989
H	-0.384933	-3.496938	-0.740952
N	-0.494878	2.376983	1.296794
H	0.238361	3.041938	1.527597
H	-1.412262	2.780755	1.473376
N	-0.550359	2.669070	-1.473967
H	-1.127004	3.487201	-1.302693
H	0.273964	2.888705	-2.020752

O1

Coordinates (Angstroms)

	X	Y	Z
C	3.951707	0.398685	-0.000290
C	2.826413	1.214840	-0.000080
C	1.552985	0.640302	0.000123
C	1.411103	-0.754712	0.000083
C	2.547932	-1.567699	-0.000146
C	3.812299	-0.989249	-0.000340
H	4.940356	0.846134	-0.000434
H	2.939071	2.294663	-0.000067
H	2.444148	-2.648508	-0.000176
H	4.693676	-1.622794	-0.000522

P	-0.278004	-1.450221	0.000390
P	0.039311	1.657961	0.000268
Co	-1.787318	0.372018	-0.000067
H	-2.539433	1.728121	-0.001324
C	-3.463569	-0.335872	-0.000225
O	-4.533702	-0.720596	-0.000337
H	-0.291213	-2.350825	-1.075664
H	-0.291136	-2.350059	1.077093
H	0.189584	2.535070	-1.082153
H	0.189323	2.534609	1.083104

O5

Coordinates (Angstroms)

	X	Y	Z

C	5.090006	-1.422650	0.010148
C	3.883150	-1.609781	0.672276
C	2.773853	-0.816543	0.358491
C	2.886211	0.174964	-0.630561
C	4.107214	0.354868	-1.290615
C	5.202168	-0.439208	-0.972492
H	5.944655	-2.043756	0.260010
H	3.801400	-2.376876	1.437240
H	4.199418	1.119066	-2.057175
H	6.144670	-0.292246	-1.490678
P	1.423270	1.201943	-1.039421
P	1.173014	-1.064719	1.220300
Co	-0.386178	0.535988	0.335008

C	-0.403588	1.784718	1.738809
C	-1.865244	1.569178	-0.614149
O	-0.350514	2.539675	2.590827
O	-1.691847	2.348717	-1.497797
C	-3.443236	-1.398456	-0.358076
C	-3.450866	-2.675344	0.494588
H	-2.506507	-2.787996	1.043089
H	-4.265759	-2.656515	1.228101
H	-3.582253	-3.564065	-0.133172
C	-4.753177	-1.312635	-1.152627
H	-5.617665	-1.264987	-0.479575
H	-4.781685	-0.431328	-1.803761
H	-4.872417	-2.195672	-1.790873
C	-2.259122	-1.460921	-1.331630
H	-2.246354	-0.615228	-2.029752
H	-1.298512	-1.487191	-0.786513
H	-2.299894	-2.375403	-1.934615
C	-3.324565	-0.201687	0.610701
H	-2.469265	-0.374817	1.288262
C	-3.213250	1.197421	-0.003687
H	-3.335561	1.947453	0.790944
H	-3.985708	1.390257	-0.755756
H	-4.206922	-0.199262	1.261280
H	0.976278	-2.450038	1.077369
H	1.559286	-1.051137	2.571329
H	1.362420	1.097394	-2.439669
H	1.924498	2.511622	-0.945793

O6

	Coordinates (Angstroms)		
	X	Y	Z
C	-5.505768	1.156039	-0.367353
C	-4.301270	1.662823	0.104656
C	-3.135642	0.891294	0.033983
C	-3.188000	-0.399522	-0.516796
C	-4.407371	-0.900063	-0.986493
C	-5.559246	-0.126538	-0.913090
H	-6.405253	1.761211	-0.311282
H	-4.265683	2.662071	0.529443
H	-4.453018	-1.897392	-1.414516
H	-6.499630	-0.522707	-1.283382
P	-1.647001	-1.384321	-0.619338
P	-1.537774	1.549446	0.648432
Co	0.181467	-0.085369	0.259707
C	0.113829	-0.720472	2.011940
C	1.654646	-1.467966	-0.101172
O	-0.041307	-1.111892	3.071290
O	1.433500	-2.437954	-0.760162
C	4.361869	0.775365	-0.511099
C	4.531759	2.298061	-0.420819
H	3.578210	2.814640	-0.589305
H	4.907419	2.596928	0.565579
H	5.244651	2.656214	-1.172763
C	5.725173	0.110308	-0.272596
H	6.108575	0.342038	0.728538
H	5.675021	-0.980243	-0.371911
H	6.457606	0.470034	-1.004789

C	3.859496	0.407386	-1.913046
H	3.676884	-0.668837	-2.018885
H	2.934935	0.939414	-2.163707
H	4.606431	0.684118	-2.666248
C	3.365563	0.345799	0.591083
H	2.463249	0.973264	0.523828
C	2.966289	-1.139465	0.593861
H	2.804385	-1.475619	1.626903
H	3.741660	-1.786344	0.170842
H	3.818010	0.582689	1.560403
H	1.036498	0.449489	-1.394439
H	0.460339	0.951206	-1.380518
H	-1.520347	2.844416	0.101994
H	-1.844602	1.888217	1.977701
H	-1.666250	-1.826098	-1.953407
H	-2.012584	-2.590147	0.004038

P6

Coordinates (Angstroms)

	X	Y	Z
C	-5.324410	-1.537169	0.330103
C	-4.687541	-0.324016	0.563489
C	-3.336525	-0.171621	0.237816
C	-2.629834	-1.244448	-0.323965
C	-3.277295	-2.461632	-0.555395
C	-4.620675	-2.604315	-0.228624
H	-6.373910	-1.652054	0.581957

H	-5.239642	0.504113	0.997847
H	-2.734185	-3.293887	-0.992861
H	-5.121623	-3.549993	-0.409666
P	-0.868087	-1.002042	-0.740798
P	-2.449909	1.402461	0.514702
Co	-0.228020	1.150351	-0.181552
C	0.236545	2.969027	-0.172820
O	0.510662	4.070818	-0.118363
C	4.158195	-1.347409	0.288017
C	4.021480	-2.822430	0.692700
H	3.232807	-2.955906	1.444113
H	3.774063	-3.449888	-0.172553
H	4.957980	-3.197422	1.121962
C	5.280922	-1.212010	-0.749045
H	5.038026	-1.756354	-1.669991
H	5.469265	-0.164923	-1.012467
H	6.217373	-1.622648	-0.353182
C	4.501084	-0.517455	1.532071
H	4.687675	0.534299	1.286623
H	3.691642	-0.555038	2.271947
H	5.408270	-0.904900	2.010223
C	2.801801	-0.908272	-0.305875
H	2.027409	-1.098550	0.448571
C	2.722101	0.558441	-0.757026
H	2.911311	1.234081	0.084727
H	2.567347	-1.550240	-1.165867
C	0.453029	0.750917	1.609971
O	0.786495	0.505385	2.667911
H	3.448791	0.764651	-1.549354
C	1.351230	0.882013	-1.301004

O	1.086027	1.048861	-2.462797
H	-2.738215	1.712809	1.852866
H	-3.259075	2.352673	-0.127512
H	-0.228027	-2.087093	-0.123611
H	-0.776921	-1.387754	-2.086911

P7

Coordinates (Angstroms)

	X	Y	Z
C	1.614575	0.700976	0.296837
C	2.762228	1.460872	0.540985
H	2.672220	2.459427	0.958496
C	4.018711	0.941876	0.248939
H	4.905464	1.538035	0.439755
C	4.142657	-0.338649	-0.288670
H	5.124089	-0.740917	-0.518615
C	3.009033	-1.104707	-0.533545
H	3.108323	-2.100888	-0.954593
C	1.743342	-0.587569	-0.243419
C	-2.262416	-0.914797	1.233708
Co	-1.551916	-0.258551	-0.365503
O	-2.673969	-1.296792	2.220264
P	-0.061323	1.340384	0.657606
P	0.247772	-1.581434	-0.548166
C	-2.827341	0.932282	-0.930744
O	-3.552092	1.718490	-1.314872
H	-0.954072	0.157455	-1.676171

H	-0.008417	1.594618	2.039233
H	0.002252	2.660416	0.183866
H	0.493725	-2.221365	-1.769145
H	0.365187	-2.665439	0.336480

Q1

	Coordinates (Angstroms)		
	X	Y	Z

C	3.534457	1.834721	-0.496635
C	3.042386	0.540872	-0.349110
C	1.668101	0.335255	-0.222980
C	0.785892	1.432573	-0.230258
C	1.291354	2.726655	-0.368885
C	2.663109	2.921371	-0.507869
H	4.602621	1.994435	-0.600198
H	3.728533	-0.300925	-0.330605
H	0.619631	3.580465	-0.367240
H	3.053822	3.927376	-0.620444
P	-0.989270	1.091271	-0.051611
P	0.947561	-1.317689	-0.043560
Co	-1.287580	-1.196632	0.069674
H	-1.216172	-2.706548	0.150557
C	-3.101459	-1.478560	0.126220
O	-4.210788	-1.719931	0.157242
C	-1.880614	1.959640	-1.450960
H	-1.252138	2.352100	-2.271820
C	-1.577709	2.133098	1.400508

H	-2.658934	2.363647	1.386174
C	1.634347	-2.397384	-1.420223
H	2.143327	-1.863491	-2.243816
C	1.766589	-2.109612	1.454327
H	1.651160	-3.207037	1.506840
O	-3.079230	2.054467	-1.424422
O	-0.833244	2.482832	2.272871
O	1.510052	-3.590416	-1.372443
O	2.333174	-1.455256	2.283266

Q5

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.534016	1.199073	-1.365847
C	-3.412661	1.735158	-0.740974
C	-2.332857	0.909781	-0.412534
C	-2.385495	-0.463045	-0.718403
C	-3.516989	-0.989905	-1.347334
C	-4.586507	-0.159916	-1.667487
H	-5.369849	1.844331	-1.616265
H	-3.378994	2.795454	-0.503666
H	-3.563965	-2.048493	-1.587064
H	-5.463218	-0.576590	-2.152489
P	-0.978106	-1.518309	-0.266913
P	-0.860055	1.588748	0.412616
Co	0.667775	-0.196129	0.823694
C	0.374996	-0.562224	2.642244

C	2.190722	-1.592026	0.725520
O	0.136418	-0.832502	3.722000
O	2.016155	-2.756626	0.570467
C	3.639354	0.823947	-1.112825
C	3.618764	2.342724	-1.332163
H	2.696002	2.789785	-0.940970
H	4.464218	2.827492	-0.829716
H	3.679502	2.581868	-2.399974
C	4.936285	0.249953	-1.699706
H	5.814955	0.668728	-1.195035
H	4.980633	-0.841573	-1.610886
H	5.013063	0.493668	-2.765494
C	2.440613	0.202245	-1.839150
H	2.417884	-0.890466	-1.745945
H	1.485118	0.612046	-1.468200
H	2.476390	0.428564	-2.910878
C	3.587667	0.572353	0.411901
H	2.736065	1.128070	0.844006
C	3.529240	-0.882962	0.886960
H	3.696658	-0.914649	1.972449
H	4.292860	-1.513463	0.419006
H	4.478592	1.022966	0.863247
C	-0.371930	3.093647	-0.570468
H	-0.630436	3.085524	-1.646135
C	-1.516998	2.408874	1.962207
H	-1.001576	3.345952	2.245763
C	-1.698948	-2.950050	0.685340
H	-2.616641	-2.721043	1.261104
C	-0.443595	-2.353354	-1.851939
H	-0.015247	-3.365115	-1.727606

O	0.220405	4.000852	-0.041042
O	-2.397630	1.918127	2.617220
O	-1.168798	-4.030825	0.691154
O	-0.525975	-1.801498	-2.917621

Q6

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.995041	1.360961	-0.629420
C	-3.737319	1.870269	-0.321776
C	-2.650572	1.005783	-0.163205
C	-2.835718	-0.382571	-0.314252
C	-4.103684	-0.881250	-0.625027
C	-5.177572	-0.010776	-0.783354
H	-5.832878	2.039799	-0.750907
H	-3.607080	2.942300	-0.206748
H	-4.253654	-1.950445	-0.746282
H	-6.158458	-0.406423	-1.026078
P	-1.426926	-1.503565	-0.051056
P	-1.000105	1.640897	0.252774
Co	0.563887	-0.186648	0.310694
C	0.650779	-0.294053	2.188118
C	2.009740	-1.672546	0.204188
O	0.612529	-0.357421	3.323852
O	1.738390	-2.750400	-0.220786
C	4.643112	0.533912	-0.726352
C	4.797290	2.055362	-0.861963

H	3.829321	2.538517	-1.048277
H	5.221609	2.493808	0.049586
H	5.462743	2.306745	-1.695826
C	6.026045	-0.081507	-0.468340
H	6.450601	0.284084	0.474655
H	5.993682	-1.176199	-0.423453
H	6.717452	0.189620	-1.274596
C	4.062052	-0.030029	-2.028266
H	3.881843	-1.110507	-1.968398
H	3.118341	0.462942	-2.287956
H	4.756584	0.136699	-2.859780
C	3.704326	0.266350	0.471583
H	2.786765	0.860820	0.327708
C	3.350727	-1.206953	0.741326
H	3.260523	-1.378931	1.822780
H	4.112836	-1.901849	0.375172
H	4.176748	0.675249	1.371263
H	1.169465	-0.255731	-1.584991
H	0.611506	0.260788	-1.612398
C	-1.197638	2.610017	1.835203
H	-2.155781	2.493129	2.376446
C	-0.693039	3.062697	-0.930315
H	-0.008098	3.838561	-0.538364
C	-2.017642	-2.713400	1.235702
H	-2.817141	-2.353101	1.911599
C	-1.358204	-2.612647	-1.558486
H	-1.109039	-3.669356	-1.348027
O	-0.295698	3.305331	2.229465
O	-1.162595	3.094923	-2.035465
O	-1.523576	-3.808461	1.329221

O	-1.530701	-2.186313	-2.669265

R6

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.793709	2.007063	-0.811413
C	-4.276841	0.717432	-0.737840
C	-2.948130	0.523955	-0.353380
C	-2.136428	1.630546	-0.049963
C	-2.663360	2.921925	-0.130324
C	-3.990201	3.104544	-0.508035
H	-5.827247	2.156120	-1.106210
H	-4.903351	-0.135908	-0.981876
H	-2.042340	3.782131	0.106788
H	-4.398268	4.108155	-0.567700
P	-0.408370	1.345549	0.439053
P	-2.225809	-1.131327	-0.223156
Co	0.026544	-0.969997	0.445196
C	0.226378	-2.770291	1.031800
O	0.358584	-3.845926	1.367315
C	4.803501	0.355384	-0.689456
C	4.995082	1.685098	-1.433167
H	4.202464	1.843648	-2.175027
H	4.979344	2.532607	-0.737459
H	5.955854	1.699475	-1.960875
C	5.933941	0.183198	0.333542
H	5.895541	0.965287	1.101685

H	5.886126	-0.789618	0.836212
H	6.909457	0.248231	-0.162226
C	4.841546	-0.796548	-1.702126
H	4.751384	-1.775472	-1.216935
H	4.034788	-0.705671	-2.440062
H	5.792283	-0.792259	-2.247893
C	3.431288	0.423285	0.015544
H	2.662474	0.578643	-0.752087
C	3.068586	-0.808776	0.860058
H	3.054281	-1.717540	0.249012
H	3.406914	1.307907	0.663839
C	0.725796	-1.156208	-1.365363
O	1.062449	-1.253171	-2.445293
H	3.777580	-0.941122	1.683562
C	1.699242	-0.638581	1.468923
O	1.457516	-0.342692	2.605499
C	-3.346358	-2.167599	0.851251
H	-4.125630	-1.640610	1.431829
C	-2.535392	-1.937500	-1.889008
H	-2.675108	-3.034495	-1.861712
C	0.572146	2.458039	-0.702584
H	0.267365	2.414901	-1.765278
C	-0.219752	2.219821	2.089066
H	0.767781	2.678214	2.274214
O	-2.533416	-1.293105	-2.902548
O	-3.179083	-3.359873	0.885006
O	1.467679	3.156078	-0.304068
O	-1.121194	2.246844	2.882125

R7

	Coordinates (Angstroms)		
	X	Y	Z
C	0.870413	1.525875	0.030248
C	1.394484	2.819915	0.065592
H	0.731603	3.676352	0.144493
C	2.770420	3.015236	-0.013171
H	3.171218	4.023267	0.010101
C	3.631475	1.926134	-0.123040
H	4.702956	2.084360	-0.185746
C	3.122086	0.631711	-0.156896
H	3.797969	-0.215049	-0.241668
C	1.742201	0.428581	-0.085311
C	-1.675341	-1.627636	1.475200
Co	-1.176052	-1.150055	-0.269137
O	-1.999533	-1.898109	2.527685
P	-0.913664	1.213341	0.140479
P	1.066906	-1.247946	-0.143213
C	-2.788653	-1.140803	-1.153934
O	-3.747743	-1.128458	-1.760346
H	-0.724957	-0.823589	-1.666506
C	-1.506596	2.066312	1.690656
H	-0.734977	2.307178	2.445614
C	-1.685669	2.311396	-1.167278
H	-2.711555	2.655865	-0.940931
C	1.852934	-2.070593	-1.629594
H	2.037461	-1.396701	-2.488143
C	1.895285	-2.168445	1.273069

H	1.876803	-3.270021	1.193566
O	-2.677231	2.309336	1.838213
O	-1.110423	2.573401	-2.188498
O	2.384846	-1.580699	2.198312
O	2.096338	-3.247620	-1.639907

S1

	Coordinates (Angstroms)		
	X	Y	Z

C	-3.983173	-0.615556	0.170474
C	-3.096885	0.454161	0.125832
C	-1.722853	0.205534	0.049340
C	-1.246532	-1.113413	0.019611
C	-2.144610	-2.184206	0.063627
C	-3.508913	-1.929444	0.139505
H	-5.050416	-0.428252	0.233382
H	-3.470459	1.473270	0.155195
H	-1.780543	-3.206899	0.042677
H	-4.211031	-2.756477	0.175764
P	0.553975	-1.350291	-0.089215
P	-0.496679	1.549066	0.009155
Co	1.521174	0.681989	0.031453
H	1.925152	2.159786	0.109459
C	3.325985	0.307754	0.105085
O	4.449527	0.146672	0.167031
O	0.803120	-2.239905	-1.410007
O	0.920382	-2.460409	1.018987

O	-0.903508	2.504366	-1.213750
O	-0.888789	2.526652	1.220838
C	0.806482	-1.526535	-2.654820
H	1.592319	-0.762086	-2.660528
H	1.018657	-2.261716	-3.430587
H	-0.170367	-1.071025	-2.847943
C	1.156962	-1.968363	2.347109
H	1.445699	-2.830773	2.947516
H	1.972866	-1.234746	2.349037
H	0.248963	-1.522254	2.766674
C	-0.484835	2.099038	-2.525874
H	0.601895	1.960560	-2.561334
H	-0.998808	1.181637	-2.829899
H	-0.763893	2.908549	-3.199622
C	-0.471576	2.117430	2.531710
H	0.614495	1.968694	2.563514
H	-0.742443	2.927366	3.208122
H	-0.989409	1.201654	2.835850

S5

Coordinates (Angstroms)

	X	Y	Z
C	-5.104098	0.826552	-0.500905
C	-3.927394	1.498258	-0.181486
C	-2.709001	0.821770	-0.249605
C	-2.673197	-0.530463	-0.630588
C	-3.858003	-1.195539	-0.953134

C	-5.069488	-0.513615	-0.886606
H	-6.054180	1.348411	-0.443968
H	-3.955920	2.538875	0.127235
H	-3.833716	-2.243241	-1.238641
H	-5.992803	-1.030952	-1.127944
P	-1.052790	-1.363564	-0.668512
P	-1.129230	1.620435	0.153571
Co	0.296973	-0.143858	0.697217
C	-0.288672	-0.575908	2.421463
C	1.641276	-1.495237	0.612720
O	-0.644704	-0.892537	3.455892
O	1.827452	-2.591454	1.042711
C	4.986521	0.353295	-0.273912
C	6.353851	0.146135	0.392052
H	6.295999	0.315011	1.474413
H	6.723415	-0.873320	0.228684
H	7.094908	0.843026	-0.016958
C	5.107077	0.067231	-1.776374
H	5.371837	-0.981374	-1.959773
H	4.171152	0.276586	-2.308614
H	5.886231	0.694525	-2.224688
C	4.542156	1.806806	-0.055205
H	3.584606	2.025139	-0.544659
H	4.436174	2.030322	1.013843
H	5.281209	2.501917	-0.470352
C	3.996142	-0.624402	0.393264
H	3.890090	-0.349858	1.450805
C	2.605817	-0.676070	-0.253311
H	2.613323	-1.171163	-1.231581
H	2.220829	0.344265	-0.428301

H	4.409675	-1.639240	0.368950
O	-1.518605	2.848257	1.143450
O	-0.840029	2.405790	-1.230345
O	-1.382294	-2.917259	-0.396313
O	-0.654875	-1.536090	-2.225480
C	-1.589017	2.581843	2.549369
H	-0.607729	2.286618	2.937912
H	-1.897700	3.513288	3.024606
H	-2.330868	1.806146	2.768212
C	0.453310	2.987949	-1.428443
H	0.563939	3.154526	-2.500386
H	0.526558	3.941078	-0.897898
H	1.248619	2.315898	-1.082763
C	-1.611121	-3.336003	0.956752
H	-0.680480	-3.291941	1.528884
H	-2.391708	-2.732597	1.432692
H	-1.949919	-4.370606	0.899818
C	-0.190876	-0.383392	-2.936038
H	0.169064	-0.743902	-3.899748
H	-1.003318	0.331935	-3.094634
H	0.635466	0.102828	-2.405299

S6

Coordinates (Angstroms)		
X	Y	Z

C	4.814238	-1.391936	-1.186728
C	3.644675	-1.885333	-0.619491

C	2.592977	-1.010038	-0.331177
C	2.717592	0.358770	-0.614891
C	3.895981	0.844952	-1.187595
C	4.940386	-0.030128	-1.466207
H	5.630420	-2.070058	-1.415609
H	3.545510	-2.945501	-0.404844
H	3.993770	1.901085	-1.418933
H	5.855820	0.348731	-1.909780
P	1.297662	1.450026	-0.276963
P	1.066441	-1.595552	0.472854
Co	-0.547391	0.109282	0.319158
C	-0.593780	0.325863	2.164034
C	-2.004269	1.520490	0.202412
O	-0.559188	0.439774	3.297429
O	-1.836906	2.607139	-0.268727
C	-4.648146	-0.709283	-0.603951
C	-4.787348	-2.228425	-0.770957
H	-3.823975	-2.692297	-1.018548
H	-5.158581	-2.695802	0.149208
H	-5.491170	-2.469074	-1.576256
C	-6.026343	-0.123146	-0.264656
H	-6.401984	-0.521692	0.685740
H	-6.007315	0.970008	-0.188597
H	-6.750241	-0.381393	-1.046376
C	-4.146676	-0.103837	-1.921056
H	-3.975300	0.976492	-1.840943
H	-3.213478	-0.576915	-2.248429
H	-4.885372	-0.256391	-2.716697
C	-3.654835	-0.448521	0.552461
H	-2.733840	-1.022675	0.354018

C	-3.310465	1.029840	0.810156
H	-3.179548	1.199408	1.887322
H	-4.105103	1.708052	0.483386
H	-4.079073	-0.875745	1.467526
H	-1.360327	-0.073659	-1.352991
H	-0.811504	-0.614178	-1.395580
O	1.515392	-2.016476	1.974160
O	0.844068	-3.101136	-0.079735
O	1.959545	2.444311	0.815159
O	1.242251	2.424296	-1.579165
C	2.412293	-1.177450	2.714398
H	2.218524	-0.111766	2.549333
H	2.251016	-1.408323	3.767792
H	3.447553	-1.398275	2.439422
C	0.151762	-3.275306	-1.320813
H	0.143991	-4.347451	-1.517988
H	-0.880267	-2.915820	-1.244796
H	0.669636	-2.763970	-2.139766
C	1.129659	3.459271	1.399833
H	0.891934	4.230482	0.662897
H	0.202621	3.033252	1.798247
H	1.706670	3.894679	2.216160
C	0.456453	2.006200	-2.699421
H	0.572197	2.777972	-3.461430
H	0.819037	1.053330	-3.101843
H	-0.599820	1.924605	-2.428330

T6

	Coordinates (Angstroms)		
	X	Y	Z
C	4.703477	2.068841	0.469502
C	4.202078	0.778923	0.601274
C	2.856641	0.533512	0.310989
C	2.024457	1.574765	-0.110638
C	2.533756	2.870763	-0.239869
C	3.871571	3.110953	0.052788
H	5.747644	2.266293	0.690135
H	4.850457	-0.029539	0.926111
H	1.892244	3.682594	-0.570017
H	4.273448	4.114117	-0.048252
P	0.297196	1.185626	-0.547788
P	2.118260	-1.119710	0.463150
Co	-0.063275	-1.045830	-0.189566
C	-0.204576	-2.901547	-0.430524
O	-0.274803	-4.029935	-0.546945
C	-4.797539	0.672048	0.355354
C	-4.991358	2.152610	0.712190
H	-4.192445	2.506225	1.376986
H	-4.982944	2.781176	-0.186735
H	-5.948490	2.309055	1.223663
C	-5.905096	0.233555	-0.611145
H	-5.836491	0.773399	-1.563643
H	-5.854067	-0.840463	-0.825292
H	-6.892726	0.435065	-0.179609
C	-4.869051	-0.162962	1.640913
H	-4.730879	-1.233028	1.447105
H	-4.103822	0.153936	2.360301

H	-5.846862	-0.042942	2.122555
C	-3.406978	0.538428	-0.299958
H	-2.654818	0.808613	0.449951
C	-3.073549	-0.844350	-0.876570
H	-3.218416	-1.628612	-0.123653
H	-3.317091	1.276606	-1.106946
C	-0.889894	-1.095988	1.546938
O	-1.429879	-1.227414	2.539848
H	-3.698708	-1.070617	-1.746335
C	-1.633497	-0.905095	-1.310843
O	-1.253013	-0.952409	-2.455427
O	2.531693	-1.652584	1.927388
O	3.060981	-2.112508	-0.392845
O	-0.576980	2.343432	0.154104
O	0.123139	1.707265	-2.059274
C	2.253702	-0.823691	3.066487
H	2.177513	-1.491757	3.924103
H	3.069924	-0.111963	3.217084
H	1.313186	-0.271912	2.956199
C	2.937382	-2.035211	-1.821046
H	3.497481	-2.878536	-2.224063
H	1.889109	-2.114945	-2.137370
H	3.365536	-1.098856	-2.193092
C	-0.634007	2.425372	1.582563
H	-1.172437	1.573755	2.008862
H	0.369717	2.488866	2.015657
H	-1.181879	3.339405	1.811216
C	0.971853	1.133454	-3.067179
H	0.517465	1.381748	-4.025797
H	1.972342	1.572085	-3.003864

H	1.027263	0.045818	-2.969534

T7

Coordinates (Angstroms)

	X	Y	Z
C	-1.381352	1.028197	-0.104372
C	-2.377094	1.999810	-0.228972
H	-2.109827	3.036188	-0.414124
C	-3.714022	1.632704	-0.108752
H	-4.489913	2.386109	-0.201520
C	-4.061389	0.302556	0.131709
H	-5.106512	0.025551	0.226724
C	-3.075572	-0.671616	0.250931
H	-3.348383	-1.706086	0.437381
C	-1.731742	-0.305951	0.136364
C	2.339002	-1.017460	-1.228265
Co	1.508148	-0.546155	0.350314
O	2.917074	-1.285144	-2.170439
P	0.390621	1.426184	-0.257045
P	-0.427723	-1.564463	0.233056
C	2.901467	0.318261	1.185176
O	3.717002	0.889898	1.732088
H	0.843129	-0.387441	1.693404
O	-0.733779	-2.582479	-0.979495
O	-0.856788	-2.580772	1.399033
O	0.532112	2.208232	-1.666844
O	0.615783	2.724512	0.680949

C	0.221945	1.492611	-2.866528
H	0.551717	2.121832	-3.693401
H	0.751450	0.535008	-2.915544
H	-0.856563	1.322133	-2.945311
C	0.320593	2.635834	2.080181
H	0.608902	3.593649	2.512813
H	-0.749179	2.469133	2.242045
H	0.890380	1.835716	2.563437
C	-0.669456	-2.109673	-2.328874
H	-1.189847	-1.153799	-2.446454
H	0.367759	-2.019584	-2.660785
H	-1.167144	-2.863705	-2.938893
C	-0.814341	-2.161922	2.768823
H	-1.295145	-2.957561	3.337992
H	0.221015	-2.044106	3.103397
H	-1.364780	-1.226760	2.913352

TSA2-3

	Coordinates (Angstroms)		
	X	Y	Z

C	4.808917	-0.491304	-0.317123
C	3.658695	-1.227973	-0.058786
C	2.408029	-0.600982	-0.062882
C	2.318089	0.769733	-0.336112
C	3.480362	1.505049	-0.592830
C	4.719865	0.876222	-0.581008
H	5.777465	-0.981510	-0.311587

H	3.734789	-2.292395	0.147038
H	3.418140	2.569761	-0.802598
H	5.619815	1.449597	-0.781307
P	0.652230	1.531519	-0.384476
P	0.859872	-1.510799	0.300080
C	0.783844	3.060317	0.621160
H	1.498746	3.723380	0.119483
H	-0.197328	3.546112	0.572463
C	0.486116	2.151795	-2.104741
H	-0.380391	2.823433	-2.110298
H	1.370301	2.750393	-2.354302
C	1.200328	2.822322	2.070337
H	0.455124	2.235382	2.614472
H	2.161407	2.300966	2.132727
H	1.305781	3.781735	2.586627
C	0.292080	1.014404	-3.104607
H	1.154986	0.339763	-3.116059
H	-0.600662	0.425541	-2.858681
H	0.162686	1.413151	-4.115762
C	0.941558	-3.003805	-0.767881
H	1.798625	-3.606262	-0.446331
H	0.040948	-3.590839	-0.552375
C	1.043845	-2.683302	-2.257840
H	0.224947	-2.039811	-2.596829
H	1.986770	-2.176750	-2.488156
H	1.007673	-3.607583	-2.843118
C	1.098883	-2.180716	2.000888
H	0.115016	-2.535401	2.330668
H	1.754166	-3.056898	1.940136
C	1.671159	-1.164250	2.989444

H	2.717068	-0.937891	2.760913
H	1.120153	-0.218386	2.982660
H	1.626322	-1.567886	4.005776
Co	-0.857000	-0.062224	0.039920
C	-4.173614	0.057593	-0.269988
C	-4.202296	1.571307	-0.026183
H	-3.525234	1.856159	0.787067
H	-3.905232	2.122651	-0.926771
H	-5.214768	1.890842	0.246046
C	-5.250833	-0.292430	-1.319362
H	-5.102178	0.269616	-2.248838
H	-5.234691	-1.361747	-1.560202
H	-6.245148	-0.046502	-0.930189
C	-4.501865	-0.690219	1.025274
H	-4.643519	-1.761825	0.847859
H	-3.724214	-0.572309	1.784717
H	-5.433791	-0.298859	1.447888
C	-2.857523	-0.395553	-0.901920
H	-2.717253	-0.011582	-1.913245
C	-2.178204	-1.569968	-0.592354
H	-1.627058	-2.075936	-1.379447
H	-2.464273	-2.180404	0.259944
C	-1.283607	0.215042	1.866793
O	-1.569562	0.410988	2.955117
H	-1.804180	1.043939	-0.364933

TSA4-5

Coordinates (Angstroms)

	X	Y	Z
C	4.950383	1.051455	-0.631576
C	4.159465	-0.088105	-0.540565
C	2.785931	0.027247	-0.301053
C	2.209717	1.296592	-0.155051
C	3.012625	2.438773	-0.249526
C	4.376872	2.315142	-0.485467
H	6.015950	0.955876	-0.815788
H	4.612262	-1.069703	-0.653438
H	2.571106	3.425587	-0.135738
H	4.995715	3.204350	-0.555747
P	0.409242	1.416803	0.147847
P	1.713860	-1.448364	-0.149341
C	0.244609	2.442436	1.666058
H	0.521052	3.471919	1.410120
H	-0.822347	2.450111	1.918921
C	-0.200504	2.518375	-1.191871
H	-1.273983	2.663033	-1.018392
H	0.277881	3.498115	-1.078782
C	1.077898	1.947502	2.847136
H	0.842198	0.912644	3.113693
H	2.149356	2.002851	2.630409
H	0.878993	2.568288	3.726248
C	0.055121	1.950389	-2.587101
H	1.128114	1.867696	-2.788993
H	-0.389683	0.956371	-2.711822
H	-0.379589	2.608088	-3.346286
C	1.983278	-2.403821	-1.692410
H	3.058669	-2.566608	-1.828302

H	1.519420	-3.384421	-1.531471
C	1.374057	-1.714887	-2.911549
H	0.290999	-1.585377	-2.793651
H	1.823072	-0.730010	-3.080127
H	1.540394	-2.316866	-3.810254
C	2.486534	-2.472087	1.166674
H	1.812360	-3.321116	1.328771
H	3.427910	-2.874187	0.773790
C	2.731017	-1.717622	2.471980
H	3.447737	-0.901579	2.334677
H	1.808258	-1.291896	2.877923
H	3.138624	-2.401698	3.222967
Co	-0.424902	-0.730586	0.073000
C	-0.783736	-1.008472	1.930447
C	-1.391284	-2.104610	-0.449875
O	-1.056732	-1.196695	3.019983
O	-1.858956	-3.147543	-0.663098
C	-4.702659	0.546807	-0.120523
C	-5.514540	0.879927	1.139065
H	-5.759760	-0.028417	1.703215
H	-4.955067	1.549791	1.804139
H	-6.456107	1.377005	0.876861
C	-4.392424	1.846869	-0.875389
H	-3.778482	2.519717	-0.262173
H	-3.858959	1.657322	-1.814374
H	-5.318503	2.377666	-1.126402
C	-5.525924	-0.389828	-1.014108
H	-5.024013	-0.598907	-1.965848
H	-5.715812	-1.347412	-0.513651
H	-6.495704	0.063408	-1.251332

C	-3.391144	-0.135285	0.339508
H	-3.651156	-1.043324	0.901414
C	-2.420511	-0.489810	-0.779198
H	-1.996324	0.390526	-1.267906
H	-2.890981	-1.066937	-1.576622
H	-2.890939	0.539311	1.046634

TSA6-1

	Coordinates (Angstroms)		
	X	Y	Z

C	4.760099	1.951187	-0.631946
C	4.323093	0.666680	-0.329001
C	2.957370	0.411376	-0.167240
C	2.031582	1.453231	-0.306268
C	2.479589	2.742549	-0.611903
C	3.837695	2.987947	-0.776675
H	5.820635	2.145503	-0.758316
H	5.046371	-0.137618	-0.223722
H	1.767691	3.557286	-0.714063
H	4.180103	3.990676	-1.013057
P	0.260770	1.099894	-0.005752
P	2.322044	-1.269082	0.170144
C	-0.182301	2.234188	1.368292
H	0.015799	3.261689	1.041444
H	-1.263128	2.143305	1.520318
C	-0.636954	1.796209	-1.446093
H	-1.705756	1.735201	-1.209723

H	-0.385470	2.861688	-1.507936
C	0.574063	1.914287	2.655664
H	0.385074	0.886976	2.981911
H	1.653147	2.047836	2.524758
H	0.248369	2.584524	3.457344
C	-0.332209	1.093066	-2.765400
H	0.741690	1.092990	-2.981922
H	-0.681614	0.056504	-2.759292
H	-0.840416	1.605600	-3.588205
C	2.929664	-2.288422	-1.235817
H	4.002792	-2.456300	-1.086749
H	2.436349	-3.263002	-1.147093
C	2.677920	-1.668397	-2.610235
H	1.621843	-1.432557	-2.776797
H	3.249479	-0.744160	-2.739259
H	2.987381	-2.369042	-3.391777
C	3.255318	-1.877698	1.624461
H	3.075979	-2.958090	1.674719
H	4.325677	-1.730051	1.440275
C	2.817876	-1.196596	2.918924
H	2.989302	-0.115559	2.879623
H	1.753059	-1.370527	3.113780
H	3.382429	-1.596365	3.766983
Co	0.097933	-1.115164	0.491181
C	-0.479027	-2.022612	-1.139110
O	-0.807203	-2.714803	-1.980842
C	-5.206758	0.310424	-0.246074
C	-6.372250	1.058665	0.416420
H	-6.821217	0.460255	1.218405
H	-6.035459	2.007486	0.852461

H	-7.157312	1.284798	-0.314997
C	-4.645993	1.178915	-1.382279
H	-4.252734	2.127843	-0.995505
H	-3.841525	0.675515	-1.932765
H	-5.432672	1.416789	-2.108153
C	-5.721240	-1.017284	-0.818474
H	-4.939342	-1.553973	-1.369150
H	-6.086592	-1.677008	-0.021545
H	-6.549819	-0.841637	-1.514875
C	-4.133933	0.066033	0.837216
H	-4.599501	-0.428682	1.698193
C	-2.933466	-0.759450	0.381425
H	-3.197812	-1.811960	0.203245
H	-3.776421	1.039804	1.197607
H	-2.530862	-0.391807	-0.569289
C	-1.800825	-0.779961	1.376256
O	-1.864825	-0.351292	2.501304
H	-0.909532	-1.952734	1.357637
H	0.117956	-2.501208	1.231185

TSB3-4

Coordinates (Angstroms)			
	X	Y	Z

C	4.450094	0.088937	-1.696374
C	3.332256	-0.727617	-1.583789
C	2.225426	-0.312533	-0.831606
C	2.249270	0.931767	-0.188382

C	3.381321	1.747405	-0.311004
C	4.474318	1.330321	-1.059784
H	5.303761	-0.240372	-2.280820
H	3.321700	-1.692152	-2.084078
H	3.409375	2.713916	0.185672
H	5.347307	1.969944	-1.146831
P	0.798365	1.450920	0.800392
P	0.750609	-1.385655	-0.708757
C	1.527993	1.898220	2.439950
H	2.031001	2.868773	2.359690
H	0.682699	2.034471	3.125308
C	0.381587	3.098720	0.076129
H	-0.484595	3.480002	0.631046
H	1.210283	3.788431	0.276598
C	2.496351	0.850594	2.991278
H	2.070262	-0.157820	2.980735
H	3.422679	0.822010	2.409372
H	2.755608	1.088517	4.027968
C	0.090731	3.047914	-1.423664
H	0.988208	2.776571	-1.989164
H	-0.687881	2.317553	-1.667944
H	-0.245220	4.028441	-1.776796
C	0.263350	-1.686720	-2.460873
H	1.003688	-2.358757	-2.910133
H	-0.686595	-2.233463	-2.433509
C	0.127484	-0.414474	-3.293013
H	-0.536625	0.312050	-2.815570
H	1.099539	0.064944	-3.446126
H	-0.290870	-0.654185	-4.275804
C	1.435172	-3.021527	-0.205411

H	0.596572	-3.727052	-0.170610
H	2.094976	-3.362896	-1.011748
C	2.184898	-3.010577	1.123894
H	2.622602	-3.996633	1.309357
H	2.998614	-2.277888	1.121198
H	1.521678	-2.784328	1.963378
Co	-0.843744	-0.424344	0.616240
C	-0.463295	-1.030508	2.291858
O	-0.323156	-1.344841	3.381429
C	-3.792205	0.764830	-0.618918
C	-4.544929	2.111529	-0.708991
H	-4.823088	2.477938	0.285919
H	-3.932757	2.878523	-1.197772
H	-5.463256	1.986393	-1.293223
C	-3.374632	0.348185	-2.034340
H	-2.678324	1.075762	-2.467567
H	-2.888381	-0.633596	-2.035367
H	-4.253135	0.294259	-2.687475
C	-4.745911	-0.273279	-0.019865
H	-4.275544	-1.250424	0.123173
H	-5.145807	0.055634	0.945418
H	-5.593578	-0.419200	-0.698314
C	-2.582796	1.070693	0.264125
H	-2.061638	1.974330	-0.040258
C	-2.431564	0.690089	1.586465
H	-1.873640	1.323479	2.270433
H	-3.120649	-0.016315	2.041632
C	-2.018572	-2.122612	0.243310
O	-2.261352	-3.220780	0.066386
H	-1.214527	0.200293	-0.709306

TSB6-7

	Coordinates (Angstroms)		
	X	Y	Z
C	3.050762	0.614034	0.103294
C	4.291766	1.258465	0.188899
H	4.359785	2.334728	0.072313
C	5.453854	0.531358	0.417352
H	6.407450	1.045092	0.488628
C	5.388665	-0.852267	0.558171
H	6.291369	-1.424982	0.747704
C	4.166630	-1.504568	0.442222
H	4.138189	-2.584797	0.539673
C	2.987674	-0.787996	0.199471
C	-0.643050	-0.022163	1.546183
C	-1.886057	-1.205020	-0.951792
Co	-0.293158	0.189821	-0.246139
O	-0.786222	-0.208883	2.663122
O	-1.659047	-2.378454	-0.864390
P	1.520852	1.587041	-0.142148
P	1.377216	-1.634511	-0.046522
H	-3.931252	-1.499421	0.732540
C	1.888776	2.574509	-1.651257
H	2.805181	3.148586	-1.475843
H	2.110212	1.848833	-2.441710
C	0.754655	3.503116	-2.077894
H	1.076493	4.115530	-2.926163

H	-0.127133	2.938075	-2.398666
H	0.459258	4.183883	-1.271972
C	1.397216	2.795853	1.247109
H	0.417582	3.271456	1.120116
H	1.324399	2.193197	2.160128
C	2.471246	3.870244	1.402859
H	2.152483	4.585980	2.167785
H	3.425237	3.446495	1.727366
H	2.633665	4.427978	0.475011
C	1.547324	-2.549763	-1.639481
H	1.676514	-1.777936	-2.408186
H	0.559723	-2.991845	-1.810033
C	2.636318	-3.612048	-1.757545
H	2.555348	-4.110850	-2.729490
H	3.637404	-3.175449	-1.691163
H	2.543294	-4.381463	-0.983643
C	1.379930	-2.909564	1.285803
H	2.280056	-3.526265	1.193706
H	1.469845	-2.364585	2.232950
C	0.138109	-3.799124	1.298705
H	0.225640	-4.540441	2.100120
H	-0.773580	-3.220079	1.472002
H	0.016511	-4.337529	0.353713
C	-3.268101	-0.623738	-1.112218
C	-3.949677	-0.508381	0.261692
H	-3.211660	0.343060	-1.620417
H	-3.825385	-1.318519	-1.749458
H	-3.359577	0.156032	0.907755
C	-5.406441	0.004284	0.240497
C	-5.469331	1.451648	-0.263662

H	-6.501931	1.819562	-0.243161
H	-4.867455	2.116027	0.368259
H	-5.110444	1.544499	-1.295420
C	-6.289616	-0.890506	-0.639253
H	-6.045157	-0.790522	-1.703194
H	-6.183342	-1.947199	-0.364020
H	-7.345162	-0.618534	-0.521316
C	-5.924581	-0.043673	1.685379
H	-5.298858	0.565111	2.350108
H	-6.949020	0.342477	1.744164
H	-5.928714	-1.070278	2.071363
C	-1.607918	1.863942	-0.386407
O	-2.116372	2.853613	-0.157954
H	0.004676	0.193405	-1.790958
H	-0.823176	-0.434480	-1.639784

TSC2-3

Coordinates (Angstroms)			
	X	Y	Z

C	4.704910	0.863088	-0.079066
C	3.865729	-0.232227	-0.243488
C	2.479236	-0.073401	-0.148542
C	1.933078	1.187131	0.118317
C	2.786475	2.285235	0.278110
C	4.163301	2.123112	0.178585
H	5.780530	0.736996	-0.153398
H	4.290229	-1.213392	-0.439350

H	2.376504	3.271583	0.476530
H	4.818231	2.979942	0.303349
P	0.105717	1.351952	0.241168
P	1.332847	-1.481440	-0.347364
C	-0.126727	2.194433	1.860858
H	0.463790	3.118077	1.837746
H	-1.177043	2.492475	1.926461
C	-0.273397	2.672486	-0.981556
H	-1.342783	2.894609	-0.887209
H	0.270462	3.580159	-0.695102
C	0.267269	1.339037	3.061757
H	-0.377627	0.460548	3.159378
H	1.305495	0.997162	2.989516
H	0.170344	1.921157	3.983718
C	0.076817	2.263810	-2.411139
H	1.153414	2.098790	-2.524255
H	-0.438466	1.342732	-2.707850
H	-0.217081	3.050019	-3.113569
C	1.785604	-2.231540	-1.959694
H	2.855993	-2.467810	-1.945477
H	1.241219	-3.180737	-2.024758
C	1.445709	-1.329221	-3.143427
H	0.373160	-1.108603	-3.178944
H	1.989879	-0.380048	-3.091448
H	1.716511	-1.820446	-4.083295
C	1.884821	-2.718397	0.897923
H	1.124485	-3.507628	0.906465
H	2.816874	-3.169742	0.538278
C	2.082462	-2.135232	2.297092
H	2.912272	-1.421995	2.315374

H	1.189336	-1.617379	2.659970
H	2.311801	-2.937719	3.005123
Co	-0.773787	-0.708463	-0.222394
C	-3.871327	0.308441	-0.121523
C	-3.495595	1.246851	1.030261
H	-2.815201	0.761150	1.737708
H	-3.007187	2.151145	0.649174
H	-4.391673	1.557770	1.580163
C	-4.895447	1.032211	-1.020766
H	-4.487238	1.974169	-1.407054
H	-5.179681	0.409002	-1.876691
H	-5.803838	1.266691	-0.453380
C	-4.522756	-0.962583	0.432585
H	-4.941659	-1.585801	-0.365232
H	-3.820787	-1.575028	1.006909
H	-5.346179	-0.692279	1.102919
C	-2.666718	0.025108	-1.015413
H	-2.319201	0.903322	-1.557054
C	-2.380383	-1.207292	-1.592230
H	-1.858642	-1.242097	-2.546369
H	-2.974779	-2.086479	-1.360535
H	-1.037231	-2.082083	-0.803240
C	-1.259929	-1.432383	1.459540
O	-1.526156	-2.014926	2.405489

TSC4-5

Coordinates (Angstroms)

X	Y	Z

C	-4.727037	-0.211137	-0.912473
C	-3.666978	0.682817	-1.000090
C	-2.393361	0.314170	-0.549898
C	-2.186096	-0.965755	-0.016273
C	-3.261503	-1.858887	0.063774
C	-4.524187	-1.483075	-0.377674
H	-5.712103	0.082082	-1.262235
H	-3.832489	1.667502	-1.428621
H	-3.118153	-2.850921	0.484172
H	-5.350648	-2.183574	-0.307158
P	-0.509418	-1.453686	0.558822
P	-0.960612	1.440910	-0.695910
C	-0.758047	-2.028264	2.303496
H	-1.011162	-3.094168	2.285067
H	0.222547	-1.945225	2.786957
C	-0.236018	-3.047770	-0.329032
H	0.660219	-3.508276	0.100530
H	-1.073771	-3.704927	-0.068614
C	-1.815686	-1.253907	3.093968
H	-1.729636	-0.170113	2.968987
H	-2.825953	-1.534399	2.783815
H	-1.715665	-1.473911	4.161452
C	-0.118949	-2.916634	-1.844208
H	-1.032235	-2.494499	-2.276173
H	0.722639	-2.280492	-2.135942
H	0.038245	-3.903219	-2.292234
C	-0.746603	1.705222	-2.509943
H	-1.529754	2.400844	-2.834318
H	0.213829	2.218975	-2.636439

C	-0.797503	0.435210	-3.355239
H	-0.028598	-0.285210	-3.065789
H	-1.771548	-0.057470	-3.273753
H	-0.634976	0.686866	-4.408169
C	-1.556552	3.089140	-0.141968
H	-0.759145	3.800521	-0.387309
H	-2.416424	3.353653	-0.767639
C	-1.923762	3.180077	1.336218
H	-2.608402	2.379071	1.636379
H	-1.036835	3.139768	1.973886
H	-2.421517	4.134812	1.533704
Co	0.802401	0.495641	0.398351
C	0.519241	1.003516	2.232359
C	1.956235	1.792654	0.123110
O	0.477688	1.288871	3.334167
O	2.463302	2.818902	-0.074929
C	3.546334	-0.595960	-0.771908
C	2.814597	-0.074182	-2.015515
H	1.729861	-0.203794	-1.900975
H	3.013933	0.988577	-2.194555
H	3.124265	-0.625100	-2.910933
C	5.058276	-0.380309	-0.964581
H	5.283515	0.676032	-1.154570
H	5.620412	-0.694323	-0.076924
H	5.425508	-0.962793	-1.818019
C	3.279987	-2.097443	-0.635661
H	3.908600	-2.553881	0.136056
H	2.237849	-2.288410	-0.374887
H	3.489540	-2.608884	-1.581815
C	3.115132	0.176540	0.507886

C	3.152466	-0.597173	1.826110
H	4.159202	-1.017936	1.963690
H	2.436009	-1.420814	1.878970
H	3.822183	0.998168	0.639627
H	2.978428	0.069497	2.675963

TSC6-1

	Coordinates (Angstroms)		
	X	Y	Z

C	4.766743	0.165981	-1.462169
C	3.722559	-0.735566	-1.291760
C	2.527565	-0.336499	-0.681454
C	2.394617	0.988515	-0.233486
C	3.454625	1.887249	-0.402307
C	4.632753	1.479961	-1.016448
H	5.686872	-0.156580	-1.939661
H	3.842536	-1.760227	-1.632975
H	3.361719	2.912454	-0.053214
H	5.446452	2.186924	-1.145904
P	0.847781	1.538517	0.578047
P	1.155118	-1.527567	-0.416279
C	1.388383	2.199798	2.206923
H	2.075987	3.030693	2.007749
H	0.496061	2.627461	2.679259
C	0.368875	3.081764	-0.307783
H	-0.496853	3.490651	0.227184
H	1.186773	3.800931	-0.182223

C	2.046586	1.173692	3.123619
H	1.352469	0.376608	3.403205
H	2.923638	0.718205	2.652382
H	2.377322	1.660422	4.046652
C	0.048040	2.895904	-1.787570
H	0.877447	2.418653	-2.321311
H	-0.851361	2.288319	-1.935443
H	-0.132498	3.870157	-2.253153
C	0.922086	-2.346934	-2.047463
H	1.892897	-2.733884	-2.378075
H	0.278111	-3.213587	-1.861865
C	0.307336	-1.447107	-3.116491
H	-0.727587	-1.189134	-2.871149
H	0.875552	-0.518405	-3.241406
H	0.297823	-1.965476	-4.080649
C	1.922949	-2.870453	0.587499
H	1.106156	-3.545479	0.869952
H	2.600780	-3.440343	-0.059433
C	2.666598	-2.377252	1.827499
H	3.544707	-1.783375	1.553946
H	2.031826	-1.760825	2.471239
H	3.010320	-3.230787	2.420567
Co	-0.613731	-0.183073	0.387865
C	-0.668473	-0.920506	2.040877
C	-2.359190	-1.270907	-0.264646
O	-0.655523	-1.451643	3.052978
O	-2.175360	-2.401457	-0.625539
C	-4.091671	0.625536	-0.579707
C	-3.804275	0.502590	-2.086481
H	-2.732314	0.478127	-2.315751

H	-4.257291	-0.405685	-2.502057
H	-4.223740	1.362196	-2.621001
C	-5.602422	0.852397	-0.410130
H	-6.176362	0.020553	-0.834811
H	-5.887822	0.964981	0.640863
H	-5.902943	1.768456	-0.931637
C	-3.347528	1.836268	0.003114
H	-3.675673	2.058324	1.024018
H	-2.260435	1.686267	0.027166
H	-3.539504	2.725594	-0.608167
C	-3.716385	-0.708458	0.137246
C	-3.787044	-0.650147	1.668201
H	-4.799068	-0.388915	1.988429
H	-3.102288	0.095493	2.084341
H	-4.428100	-1.471109	-0.203978
H	-3.546504	-1.625449	2.104054
H	-1.469188	-0.280772	-0.929596
H	-0.637990	0.377119	-1.058410

TSE2-3

	Coordinates (Angstroms)		
	X	Y	Z

C	4.581673	0.842308	-1.021522
C	3.731794	-0.193151	-0.657081
C	2.380376	0.032375	-0.357459
C	1.889443	1.353345	-0.412500
C	2.756536	2.385954	-0.800554

C	4.088094	2.139153	-1.105258
H	5.623589	0.632555	-1.242538
H	4.137001	-1.193865	-0.611738
H	2.396055	3.403363	-0.864990
H	4.735946	2.959253	-1.398949
P	0.162601	1.708781	0.129303
P	1.254370	-1.364516	0.101512
C	0.343790	2.910696	1.596811
C	-0.720825	2.546382	-1.324370
C	1.365613	2.305635	2.574293
H	1.014662	1.370125	3.013896
H	2.338887	2.126247	2.107524
H	1.516066	3.012192	3.399118
C	0.114621	3.525979	-2.159136
H	0.492104	4.371539	-1.578766
H	0.956994	3.031914	-2.651118
H	-0.531792	3.933004	-2.946839
C	1.216991	-2.475308	-1.446055
C	0.647305	-3.862635	-1.103371
H	1.367809	-4.482074	-0.563442
H	-0.269841	-3.822334	-0.513987
H	0.414460	-4.380720	-2.041817
C	2.122337	-2.278857	1.533872
C	2.621822	-1.219068	2.526654
H	3.423897	-0.606198	2.104698
H	1.820760	-0.552980	2.854392
H	3.015490	-1.723711	3.417171
Co	-0.792185	-0.318956	0.620575
C	-4.076673	-0.932922	-0.290603
C	-5.251212	-1.785242	0.242685

H	-4.975389	-2.843378	0.314507
H	-5.573835	-1.446028	1.234088
H	-6.105427	-1.700491	-0.438299
C	-4.507689	0.536513	-0.304300
H	-4.611662	0.934155	0.712517
H	-3.782302	1.150955	-0.842958
H	-5.474950	0.641923	-0.808807
C	-3.750767	-1.393278	-1.714204
H	-2.866731	-0.892520	-2.119169
H	-3.586991	-2.475051	-1.767590
H	-4.592156	-1.154667	-2.374238
C	-2.956688	-1.193567	0.710797
C	-1.947879	-2.122069	0.533790
C	1.089143	-3.173388	2.241781
H	1.583325	-3.686043	3.075983
H	0.259958	-2.599330	2.660246
H	0.675809	-3.941493	1.583194
C	3.316155	-3.167666	1.147160
H	3.711725	-3.615544	2.067277
H	3.037725	-3.988963	0.484012
H	4.137618	-2.612458	0.690407
C	2.565227	-2.675598	-2.156070
H	3.333468	-3.106938	-1.510892
H	2.405637	-3.374529	-2.986825
H	2.947495	-1.745144	-2.584148
C	0.283779	-1.772775	-2.440891
H	0.691236	-0.801694	-2.736066
H	0.193850	-2.382119	-3.348550
H	-0.720454	-1.621463	-2.036801
C	0.830012	4.320903	1.224585

H	0.819284	4.932334	2.135650
H	1.856235	4.326781	0.850188
H	0.183164	4.815877	0.496863
C	-1.008312	3.055347	2.321654
H	-1.520164	2.101420	2.469186
H	-0.829580	3.496929	3.309405
H	-1.690183	3.719173	1.786689
C	-1.969376	3.275968	-0.807640
H	-2.615707	3.514804	-1.660676
H	-2.551535	2.671140	-0.107934
H	-1.716734	4.219815	-0.317347
C	-1.147540	1.394941	-2.244398
H	-1.648826	0.601633	-1.681460
H	-1.842546	1.763712	-3.008613
H	-0.285551	0.961722	-2.757683
H	-3.241667	-0.942473	1.732163
H	-1.826574	-2.583190	-0.439425
H	-1.549214	-2.672320	1.379463
H	-2.052077	0.540748	0.681561
C	-0.801704	-0.322899	2.554744
O	-1.059196	-0.367986	3.666664

TSE4-5

Coordinates (Angstroms)		
X	Y	Z

C	1.913899	1.659291	-0.143327
C	2.627841	2.866848	-0.163120

H	2.099801	3.809867	-0.141406
C	4.015169	2.894249	-0.210987
H	4.535387	3.846837	-0.221263
C	4.724843	1.699949	-0.244372
H	5.809760	1.701906	-0.282871
C	4.037565	0.494132	-0.225385
H	4.611893	-0.421724	-0.249998
C	2.636599	0.445988	-0.170391
C	-0.942196	-0.860596	1.943777
C	-1.240914	-2.220431	-0.332149
Co	-0.501013	-0.665179	0.067125
O	-1.309534	-1.042857	3.006721
O	-1.637914	-3.292630	-0.509912
P	0.069424	1.652469	-0.026609
P	1.759375	-1.173705	-0.065389
H	-3.623515	-2.029279	0.756123
C	-0.570277	2.541456	-1.586538
C	-2.029180	2.989683	-1.395497
H	-2.420428	3.303614	-2.370721
H	-2.688862	2.202820	-1.022229
H	-2.109392	3.846302	-0.722367
C	-0.368119	2.650234	1.531003
C	-0.147775	4.168262	1.451000
H	-0.502423	4.609412	2.390986
H	0.906481	4.435831	1.351797
H	-0.710967	4.638720	0.642502
C	2.144457	-2.104497	-1.677332
C	3.598637	-1.996952	-2.158335
H	3.697762	-2.593442	-3.073537
H	3.870329	-0.967809	-2.408924

H	4.319605	-2.385540	-1.434957
C	2.486531	-2.084199	1.436265
C	1.538578	-3.234234	1.823598
H	1.904561	-3.687245	2.752619
H	0.515456	-2.896789	2.003079
H	1.503436	-4.020078	1.066498
C	-2.576958	-0.699119	-0.609489
C	-3.689537	-0.997392	0.385651
H	-2.454998	0.371389	-0.743516
H	-2.749385	-1.125921	-1.600514
H	-3.563185	-0.345155	1.259033
C	-5.122780	-0.784009	-0.162119
C	-5.279545	0.632943	-0.729511
H	-6.320751	0.819548	-1.018703
H	-4.999004	1.389535	0.014720
H	-4.657495	0.784786	-1.619212
C	-5.443127	-1.818151	-1.249546
H	-4.792537	-1.709900	-2.125044
H	-5.326707	-2.839482	-0.866198
H	-6.477301	-1.704346	-1.596251
C	-6.101365	-0.969645	1.005721
H	-5.928943	-0.221722	1.790000
H	-7.138714	-0.865630	0.665281
H	-5.993702	-1.963310	1.458367
C	3.886348	-2.682138	1.229329
H	4.646865	-1.927596	1.018150
H	4.180808	-3.178539	2.162261
H	3.909935	-3.437836	0.441257
C	2.557527	-1.083040	2.599728
H	1.582603	-0.650412	2.835151

H	2.904888	-1.610755	3.495774
H	3.256417	-0.265052	2.400327
C	1.774209	-3.588783	-1.538577
H	0.764007	-3.738542	-1.150812
H	1.814562	-4.046095	-2.534366
H	2.473923	-4.136204	-0.902347
C	1.248653	-1.478148	-2.753851
H	1.499654	-0.427318	-2.912802
H	1.404827	-2.003416	-3.703783
H	0.182965	-1.554111	-2.504940
C	0.502248	2.112194	2.677631
H	1.570940	2.249181	2.486876
H	0.252528	2.658860	3.594601
H	0.322829	1.054576	2.876838
C	-1.854063	2.399043	1.859322
H	-2.037807	2.665731	2.906807
H	-2.516119	3.012214	1.243717
H	-2.152019	1.355496	1.724233
C	0.246603	3.765793	-2.026238
H	1.271755	3.501273	-2.298838
H	-0.229881	4.187056	-2.920284
H	0.276532	4.555006	-1.271225
C	-0.501738	1.515472	-2.725850
H	0.536062	1.267722	-2.961738
H	-1.043129	0.591464	-2.498978
H	-0.947143	1.951132	-3.628497

TSE6-1

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.977322	2.270633	-1.587756
C	-2.754913	2.482312	-0.964405
C	-1.926570	1.416704	-0.581292
C	-2.377906	0.093982	-0.796060
C	-3.598522	-0.096019	-1.460825
C	-4.390658	0.972274	-1.860247
H	-4.593056	3.118930	-1.870420
H	-2.444507	3.502820	-0.786333
H	-3.948290	-1.098816	-1.668709
H	-5.330937	0.787085	-2.370371
P	-1.449237	-1.363749	-0.141024
P	-0.253654	1.760154	0.116064
Co	0.597302	-0.347236	0.707202
C	0.387973	-0.465409	2.503371
C	2.121243	-1.869756	1.031412
O	0.338905	-0.623922	3.634950
O	1.819493	-3.005972	1.246107
C	4.686668	-0.523501	-0.776617
C	4.972328	0.735445	-1.607152
H	4.042699	1.203693	-1.952864
H	5.526398	1.479076	-1.021118
H	5.571801	0.490671	-2.491960
C	6.019806	-1.159359	-0.360241
H	6.603462	-0.479213	0.272132
H	5.874897	-2.094890	0.191860
H	6.621906	-1.395149	-1.245720
C	3.897628	-1.520387	-1.635431

H	3.677702	-2.448730	-1.093205
H	2.951330	-1.090464	-1.986793
H	4.477876	-1.800163	-2.522743
C	3.890076	-0.089253	0.473367
H	3.008643	0.487265	0.155368
C	3.420606	-1.201785	1.415871
H	3.222896	-0.766724	2.406628
H	4.173558	-1.983406	1.562762
H	4.511537	0.605023	1.050441
H	1.537606	-1.221089	-0.209146
H	0.976384	-0.479335	-0.775861
C	0.690322	2.655078	-1.277231
C	1.003925	1.626591	-2.372405
C	-0.073903	3.803814	-1.955606
C	2.011492	3.201934	-0.713659
H	1.697874	0.853710	-2.030954
H	0.094852	1.146400	-2.747725
H	1.478662	2.142794	-3.215605
H	-0.438484	4.558389	-1.256807
H	0.616087	4.302662	-2.647086
H	-0.916549	3.435572	-2.546969
H	2.657230	3.492541	-1.551156
H	1.859968	4.092893	-0.099018
H	2.555820	2.461627	-0.120162
C	-0.477339	2.915179	1.611566
C	0.817769	2.880266	2.444923
C	-0.791246	4.388731	1.313095
C	-1.631894	2.339996	2.446068
H	1.138894	1.864523	2.691337
H	1.648327	3.380189	1.940685

H	0.642526	3.406149	3.391056
H	-1.721679	4.524798	0.757092
H	-0.916403	4.905511	2.272857
H	0.018479	4.891738	0.779699
H	-1.698197	2.891871	3.391132
H	-2.592753	2.435723	1.931013
H	-1.483402	1.286167	2.690795
C	-2.654648	-2.155731	1.097220
C	-1.959673	-3.406462	1.657948
C	-2.870898	-1.138261	2.227744
C	-4.058022	-2.532121	0.594086
H	-1.936219	-4.218112	0.924147
H	-0.930498	-3.201358	1.974084
H	-2.515416	-3.766191	2.532549
H	-3.262421	-0.186145	1.854107
H	-3.607208	-1.544406	2.932221
H	-1.962850	-0.947151	2.797712
H	-4.576037	-3.048307	1.412310
H	-4.651669	-1.646919	0.350165
H	-4.060109	-3.204139	-0.262820
C	-1.144317	-2.514973	-1.637601
C	-0.739350	-1.645691	-2.837476
C	0.034014	-3.444313	-1.300621
C	-2.321005	-3.405839	-2.060737
H	-1.553460	-1.000275	-3.181416
H	0.128439	-1.019710	-2.613553
H	-0.459534	-2.305783	-3.667791
H	-0.116609	-4.001591	-0.373442
H	0.151584	-4.170707	-2.114302
H	0.975627	-2.898258	-1.218063

H	-2.024797	-3.948253	-2.967354
H	-2.562318	-4.154922	-1.302490
H	-3.224625	-2.843606	-2.306562

TSF2-3

	Coordinates (Angstroms)		
	X	Y	Z

C	4.277639	2.019703	0.180884
C	3.697469	0.758406	0.187131
C	2.314143	0.588084	0.040879
C	1.487869	1.724554	-0.094146
C	2.097940	2.987835	-0.122830
C	3.472725	3.139395	0.008228
H	5.351201	2.123554	0.302924
H	4.340273	-0.104993	0.299461
H	1.499900	3.881356	-0.227330
H	3.908414	4.133445	-0.011493
P	-0.360033	1.548927	-0.027382
P	1.579291	-1.095561	-0.075379
C	-0.778209	2.444589	1.607424
C	-1.091535	2.498695	-1.506889
C	0.215358	1.934949	2.664135
H	0.251514	0.843330	2.699289
H	1.231099	2.302306	2.491635
H	-0.107056	2.287534	3.651161
C	-0.447162	3.851657	-1.845136
H	-0.457965	4.561242	-1.015297

H	0.580604	3.734159	-2.199252
H	-1.020708	4.302143	-2.665113
C	2.192509	-1.718286	-1.762518
C	1.500517	-0.838074	-2.810913
H	0.411925	-0.890157	-2.746682
H	1.803912	0.208469	-2.710353
H	1.791426	-1.174299	-3.813501
C	2.264777	-2.168439	1.338274
C	2.218913	-1.334405	2.627290
H	2.865800	-0.453411	2.576283
H	1.206370	-1.004313	2.870474
H	2.564262	-1.957744	3.460691
Co	-0.704380	-0.808654	-0.058899
C	-4.071736	-1.464059	-0.181268
C	-4.452429	-0.417884	0.871718
H	-3.801290	-0.470618	1.747331
H	-4.399004	0.597498	0.464016
H	-5.478613	-0.588272	1.217505
C	-5.182675	-1.487421	-1.254401
H	-5.317185	-0.498712	-1.709727
H	-4.946807	-2.201036	-2.052136
H	-6.136602	-1.782616	-0.801490
C	-3.992035	-2.851378	0.467395
H	-3.941005	-3.648780	-0.282094
H	-3.123858	-2.952069	1.126925
H	-4.889778	-3.028681	1.069791
C	-2.801274	-1.082857	-0.933268
H	-2.853874	-0.118755	-1.429515
C	-1.910328	-2.014000	-1.435783
H	-1.316043	-1.770308	-2.313991

H	-2.058889	-3.076621	-1.266220
H	-0.547680	-2.278324	-0.335772
C	-1.200477	-1.190400	1.708261
O	-1.481178	-1.476667	2.780297
C	-0.701263	3.977030	1.566993
H	-0.907078	4.352486	2.577296
H	0.285452	4.348945	1.284703
H	-1.449020	4.414839	0.900940
C	-2.194785	2.058354	2.056243
H	-2.400309	2.543524	3.018312
H	-2.966786	2.379265	1.354497
H	-2.296823	0.984382	2.206020
C	-2.591303	2.723077	-1.249998
H	-2.764720	3.509455	-0.510478
H	-3.063350	3.044440	-2.186290
H	-3.106103	1.819168	-0.911843
C	-0.920094	1.611636	-2.749750
H	-1.364464	0.619335	-2.633205
H	-1.413772	2.096090	-3.601188
H	0.134644	1.490628	-3.007380
C	1.359120	-3.402326	1.507655
H	1.743277	-3.999301	2.343482
H	0.324924	-3.142650	1.736447
H	1.355884	-4.041258	0.620282
C	3.697179	-2.690026	1.144157
H	3.974294	-3.251927	2.044472
H	3.772874	-3.377314	0.298288
H	4.437432	-1.896393	1.024838
C	1.768585	-3.180037	-1.964000
H	1.957704	-3.458158	-3.008064

H	2.345880	-3.863471	-1.334731
H	0.703444	-3.338519	-1.765665
C	3.704664	-1.590652	-2.007504
H	3.912674	-1.981613	-3.011264
H	4.033377	-0.548046	-1.992610
H	4.314426	-2.159054	-1.304647

TSF4-5

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.653136	1.133473	-0.039846
C	-3.391530	1.692191	0.117235
C	-2.228251	0.908758	0.088296
C	-2.354527	-0.490032	-0.078700
C	-3.635718	-1.029717	-0.262906
C	-4.774890	-0.235074	-0.249154
H	-5.532425	1.769861	-0.016700
H	-3.316030	2.764457	0.243590
H	-3.753718	-2.093844	-0.425958
H	-5.750386	-0.687719	-0.397609
P	-0.895278	-1.621462	0.021755
P	-0.580985	1.739511	0.094436
C	-1.203935	-2.552872	1.660215
C	-1.004731	-2.831312	-1.453411
C	-1.185146	-1.518146	2.792383
H	-0.248303	-0.968882	2.853824
H	-2.006776	-0.802507	2.690101

H	-1.320385	-2.040044	3.747667
C	-1.890368	-4.076279	-1.295232
H	-1.520434	-4.755986	-0.523323
H	-2.935716	-3.837988	-1.085809
H	-1.868860	-4.623971	-2.245918
C	-0.633456	2.897309	-1.433377
C	-1.371417	2.151578	-2.559441
H	-1.083386	1.101626	-2.651902
H	-2.454376	2.174161	-2.407355
H	-1.153186	2.641549	-3.515653
C	-0.445126	2.771400	1.685153
C	-1.597569	3.747266	1.976473
H	-1.327406	4.321554	2.871474
H	-1.795398	4.463714	1.181231
H	-2.523600	3.214215	2.209837
Co	1.009970	-0.024987	-0.209539
C	1.726464	-0.353569	1.373007
C	1.064467	-0.048734	-2.078064
O	2.041000	-0.585929	2.462098
O	1.248765	-0.111748	-3.202172
C	4.240352	0.070923	-0.077895
C	3.835622	1.298293	-0.901503
H	3.677210	1.044374	-1.956336
H	2.909054	1.739745	-0.510464
H	4.613160	2.069114	-0.857741
C	4.621007	0.536073	1.334459
H	3.855495	1.182658	1.776451
H	4.798133	-0.302166	2.015981
H	5.546533	1.120676	1.284203
C	5.488572	-0.561672	-0.728655

H	5.915378	-1.350916	-0.101301
H	5.258110	-0.989451	-1.711905
H	6.260219	0.204456	-0.867497
C	3.112098	-0.986919	-0.126761
H	2.912753	-1.199696	-1.177203
C	3.369847	-2.329050	0.537518
H	2.498297	-2.981473	0.441811
H	3.628766	-2.251342	1.596827
H	4.198940	-2.830904	0.024653
C	-2.549531	-3.286619	1.788232
H	-2.571085	-3.764154	2.775885
H	-3.394759	-2.594496	1.750472
H	-2.703181	-4.070515	1.049054
C	-0.058128	-3.553483	1.864882
H	-0.175583	-4.034925	2.843317
H	-0.058676	-4.343504	1.108173
H	0.920043	-3.064811	1.856616
C	0.425977	-3.339281	-1.713876
H	1.143512	-2.535089	-1.888278
H	0.798584	-3.937582	-0.876734
H	0.423258	-3.981015	-2.603394
C	-1.525188	-2.053512	-2.673775
H	-1.333441	-2.639684	-3.580440
H	-2.603130	-1.880959	-2.605878
H	-1.051282	-1.079961	-2.809315
C	-0.398012	1.815523	2.882140
H	-0.329226	2.412355	3.799959
H	-1.307418	1.213668	2.949704
H	0.467141	1.154973	2.861472
C	0.884620	3.539193	1.613510

H	1.086588	3.990445	2.592353
H	1.726528	2.876599	1.375138
H	0.857223	4.348784	0.878594
C	0.813101	3.198012	-1.866746
H	0.788471	3.864505	-2.737394
H	1.385011	3.703231	-1.084011
H	1.370468	2.308057	-2.159726
C	-1.326922	4.254925	-1.248257
H	-0.781006	4.907873	-0.562622
H	-1.347366	4.754640	-2.224781
H	-2.362960	4.169733	-0.913277

TSF6-1

Coordinates (Angstroms)

	X	Y	Z
C	4.846241	0.576422	-0.398839
C	3.863606	-0.403112	-0.449022
C	2.500714	-0.104596	-0.293207
C	2.136071	1.250422	-0.114090
C	3.143025	2.224436	-0.046314
C	4.485830	1.899891	-0.178281
H	5.889359	0.300291	-0.518648
H	4.177607	-1.426217	-0.596188
H	2.880749	3.262873	0.108039
H	5.240354	2.677842	-0.116390
P	0.376275	1.788329	-0.033475
P	1.255800	-1.471418	-0.124010

Co	-0.830280	-0.177154	0.292761
C	-0.878517	-0.365213	2.100277
C	-2.391892	-1.725917	0.049457
O	-0.929730	-0.515109	3.232779
O	-2.003252	-2.860079	0.039334
C	-4.450907	-0.303171	-0.654771
C	-4.105056	-0.680367	-2.105956
H	-3.045428	-0.523223	-2.340421
H	-4.345571	-1.730625	-2.310857
H	-4.680611	-0.061400	-2.803166
C	-5.980611	-0.330899	-0.510682
H	-6.382637	-1.324471	-0.741117
H	-6.304845	-0.056668	0.498514
H	-6.432643	0.384379	-1.207522
C	-3.950179	1.112759	-0.352852
H	-4.314946	1.481800	0.611557
H	-2.854500	1.154664	-0.338888
H	-4.294340	1.809800	-1.125461
C	-3.846248	-1.353281	0.320346
C	-3.984616	-1.001780	1.807839
H	-5.041056	-0.901875	2.069997
H	-3.490653	-0.058872	2.058318
H	-4.381149	-2.296987	0.152239
H	-3.562142	-1.793351	2.434994
H	-1.663483	-0.825416	-0.877351
H	-0.986049	-0.093150	-1.239727
C	0.120555	2.735174	-1.671947
C	1.192474	3.801139	-1.957598
C	0.187894	1.731779	-2.828793
C	-1.265471	3.394674	-1.676118

H	1.291250	4.547033	-1.169159
H	2.172004	3.351340	-2.139700
H	0.903143	4.330494	-2.873543
H	-0.618346	0.993450	-2.795954
H	0.090497	2.279293	-3.773948
H	1.149347	1.209064	-2.850340
H	-1.436534	3.840908	-2.663285
H	-2.064727	2.670630	-1.501985
H	-1.352206	4.195398	-0.937276
C	0.176250	2.968283	1.449655
C	-1.319540	2.962707	1.825139
C	1.006466	2.399618	2.611348
C	0.589614	4.436097	1.258500
H	-1.946290	3.372034	1.026791
H	-1.693387	1.963628	2.065041
H	-1.464060	3.588246	2.713954
H	2.077918	2.550057	2.451213
H	0.726602	2.918024	3.535951
H	0.844104	1.332448	2.772435
H	0.420403	4.954286	2.210597
H	1.648022	4.557960	1.017168
H	-0.007680	4.949400	0.501714
C	1.348565	-2.534287	-1.710427
C	0.516361	-1.830387	-2.791235
C	2.759931	-2.735827	-2.280911
C	0.709979	-3.909174	-1.456932
H	-0.548218	-1.809769	-2.541831
H	0.858955	-0.809829	-2.969175
H	0.621096	-2.382558	-3.733210
H	3.445221	-3.211866	-1.575600

H	2.682453	-3.396856	-3.153280
H	3.202306	-1.795662	-2.623160
H	0.579566	-4.408207	-2.425590
H	1.337331	-4.558553	-0.842100
H	-0.272297	-3.821145	-0.988612
C	1.916927	-2.478563	1.357249
C	2.339791	-1.476184	2.445372
C	0.763312	-3.351742	1.885222
C	3.115470	-3.402653	1.092746
H	3.273656	-0.967917	2.187926
H	1.589964	-0.705600	2.635973
H	2.499346	-2.016413	3.386097
H	0.508283	-4.156043	1.192051
H	1.074304	-3.814447	2.829900
H	-0.150839	-2.786105	2.076445
H	3.366207	-3.910698	2.032843
H	2.899129	-4.177954	0.355495
H	4.009504	-2.859958	0.777990

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	Coordinates (Angstroms)		
	X	Y	Z

C	-2.750106	0.693650	-0.075239
C	-3.958088	1.378778	-0.283441
H	-3.956249	2.454888	-0.384130
C	-5.175322	0.721271	-0.372866
H	-6.086774	1.286601	-0.540400

C	-5.207777	-0.661085	-0.243966
H	-6.147103	-1.202110	-0.304099
C	-4.022186	-1.356079	-0.054561
H	-4.079958	-2.430887	0.018582
C	-2.773932	-0.715731	0.024643
C	1.098687	0.041097	-1.685293
C	2.282963	-1.240171	0.664680
Co	0.660882	0.221939	0.093692
O	1.460436	-0.073259	-2.761903
O	2.062590	-2.370756	0.345424
P	-1.208903	1.694488	0.089841
P	-1.212709	-1.717345	0.061671
H	4.442937	-1.394570	-0.869535
C	3.654622	-0.719695	1.009977
C	4.465245	-0.472551	-0.275184
H	3.580002	0.175908	1.631460
H	4.130587	-1.506717	1.605039
H	3.972387	0.300773	-0.880309
C	5.938840	-0.063736	-0.055938
C	6.036442	1.266496	0.701797
H	7.086109	1.558260	0.824529
H	5.528899	2.072235	0.158107
H	5.597223	1.200252	1.704233
C	6.695646	-1.153950	0.714788
H	6.346103	-1.243961	1.749872
H	6.581549	-2.132113	0.231343
H	7.766356	-0.921434	0.752379
C	6.574966	0.101284	-1.443919
H	6.054493	0.869280	-2.029695
H	7.625865	0.400997	-1.355781

H	6.539177	-0.838170	-2.008933
C	2.066365	1.772225	0.392403
O	2.800337	2.629550	0.508445
H	0.465279	0.153949	1.647700
H	1.229530	-0.506121	1.415356
C	-1.478766	2.629544	1.735519
C	-0.328663	3.623025	1.946869
C	-2.817775	3.379094	1.856169
C	-1.460343	1.602812	2.876256
H	0.638135	3.116957	2.011201
H	-0.278966	4.385229	1.164239
H	-0.479441	4.140216	2.901861
H	-3.667537	2.692262	1.876111
H	-2.813815	3.913186	2.814104
H	-2.981320	4.119711	1.073701
H	-1.656539	2.123998	3.820991
H	-2.240597	0.844734	2.750322
H	-0.493813	1.101741	2.977348
C	-1.202404	2.906717	-1.397291
C	-1.668604	2.118313	-2.631650
C	-2.057287	4.178321	-1.275986
C	0.241739	3.380297	-1.637398
H	-1.133003	1.172110	-2.747614
H	-2.738941	1.896759	-2.599946
H	-1.474359	2.717965	-3.528790
H	-1.706240	4.839879	-0.479608
H	-1.965182	4.729276	-2.219930
H	-3.120747	3.983524	-1.127480
H	0.246608	4.072870	-2.487253
H	0.650235	3.920784	-0.778752

H	0.917215	2.560479	-1.893650
C	-1.354975	-2.743819	-1.547438
C	-1.731437	-1.777259	-2.683057
C	0.027914	-3.339390	-1.864780
C	-2.376246	-3.891373	-1.552375
H	-2.727195	-1.343279	-2.553311
H	-1.014598	-0.959149	-2.786414
H	-1.727798	-2.329147	-3.631027
H	0.334077	-4.094934	-1.138884
H	-0.016111	-3.821527	-2.849387
H	0.811669	-2.580074	-1.900164
H	-2.290430	-4.417642	-2.511653
H	-2.196172	-4.625800	-0.764801
H	-3.407272	-3.539860	-1.476484
C	-1.351691	-2.875061	1.587118
C	-0.416947	-4.085726	1.432629
C	-0.876117	-2.062435	2.802606
C	-2.757860	-3.399269	1.914581
H	-0.780008	-4.803493	0.692588
H	0.599936	-3.794919	1.166112
H	-0.375098	-4.609364	2.396323
H	-1.431392	-1.127514	2.914819
H	-1.037093	-2.652991	3.712904
H	0.191905	-1.831898	2.750584
H	-2.676476	-4.064765	2.783362
H	-3.448033	-2.595095	2.184616
H	-3.195984	-3.984648	1.102234

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	Coordinates (Angstroms)		
	X	Y	Z
C	-3.084342	3.427544	-1.822329
C	-1.767895	3.211989	-1.428377
C	-1.379652	1.963993	-0.934900
C	-2.321093	0.925037	-0.837870
C	-3.641294	1.154668	-1.233931
C	-4.021098	2.401029	-1.721522
H	-3.378167	4.397389	-2.211396
H	-1.042847	4.016114	-1.511010
H	-4.374333	0.355854	-1.166647
H	-5.048748	2.569042	-2.028266
P	-1.765099	-0.706158	-0.210697
P	0.326222	1.638687	-0.369691
Co	0.605872	-0.591323	-0.442140
C	0.927693	-0.876578	1.345818
C	1.297666	-2.519749	-0.905385
O	1.036502	-1.014635	2.471280
O	0.667814	-3.531104	-0.792841
C	4.949735	-2.807258	0.419685
C	5.525132	-3.823351	1.416019
H	4.946148	-3.836345	2.347848
H	5.512235	-4.836881	0.997205
H	6.563418	-3.577142	1.668432
C	5.779374	-2.836948	-0.870668
H	5.710568	-3.816009	-1.360821
H	5.445607	-2.076612	-1.586952
H	6.836632	-2.642705	-0.655008

C	5.013245	-1.406642	1.048114
H	4.647219	-0.628633	0.366771
H	4.418738	-1.359801	1.969502
H	6.047750	-1.149342	1.304445
C	3.486337	-3.206185	0.136963
H	2.920950	-3.116212	1.074523
C	2.795910	-2.376090	-0.950974
H	3.110231	-2.688152	-1.956816
H	3.038650	-1.306695	-0.868404
H	3.440847	-4.262447	-0.151503
H	0.694025	-1.477603	-1.741864
H	0.393243	-0.404468	-1.962212
C	0.433284	2.369708	1.297760
C	1.659960	2.279478	1.968668
C	-0.658378	2.963454	1.933810
C	1.792519	2.785617	3.255830
H	2.515413	1.813056	1.484111
C	-0.523432	3.461154	3.229080
H	-1.615130	3.043503	1.427682
C	0.698224	3.374885	3.889230
H	2.747502	2.714257	3.767213
H	-1.377775	3.918953	3.718351
H	0.800654	3.765748	4.897112
C	1.446337	2.644634	-1.394367
C	2.065584	2.061189	-2.504897
C	1.693789	3.989913	-1.093168
C	2.906416	2.818586	-3.315671
H	1.894555	1.013482	-2.735748
C	2.534985	4.742894	-1.906009
H	1.233426	4.449228	-0.223245

C	3.139711	4.159029	-3.018044
H	3.382347	2.358846	-4.176423
H	2.720163	5.786211	-1.669733
H	3.797459	4.749061	-3.649137
C	-2.404253	-0.814394	1.493547
C	-2.164359	-2.000990	2.200181
C	-3.043718	0.249550	2.134227
C	-2.571886	-2.121958	3.523778
H	-1.663452	-2.835865	1.714963
C	-3.437083	0.128924	3.465764
H	-3.240209	1.174958	1.601957
C	-3.204507	-1.054483	4.160316
H	-2.388992	-3.048052	4.060310
H	-3.928841	0.963300	3.956899
H	-3.513526	-1.147034	5.197246
C	-2.735393	-1.907595	-1.177546
C	-3.931752	-2.458856	-0.709188
C	-2.267518	-2.251276	-2.450990
C	-4.651948	-3.342614	-1.509093
H	-4.305783	-2.201179	0.276990
C	-2.993681	-3.128725	-3.249716
H	-1.337678	-1.826782	-2.821027
C	-4.185437	-3.676908	-2.778056
H	-5.579278	-3.768716	-1.138161
H	-2.626077	-3.389453	-4.237662
H	-4.749977	-4.365229	-3.399938

TSJ6-7

	Coordinates (Angstroms)		
	X	Y	Z
C	2.633728	1.519731	3.736366
C	2.907807	0.808242	2.572075
C	1.900396	0.591525	1.629762
C	0.606110	1.100254	1.851692
C	0.348067	1.819868	3.021159
C	1.356137	2.025931	3.958882
H	3.418680	1.676033	4.469741
H	3.905939	0.415639	2.403073
H	-0.644894	2.217177	3.207162
H	1.140123	2.581068	4.866566
P	-0.663992	0.786205	0.564128
P	2.201371	-0.329811	0.083025
Co	0.233045	-1.394719	-0.462092
C	1.238777	-2.998164	-1.445958
O	1.877652	-3.735630	-2.021183
C	-5.474400	-1.484010	-1.043941
C	-6.631666	-2.242227	-1.708552
H	-6.572878	-2.174488	-2.801944
H	-6.618228	-3.304763	-1.435985
H	-7.597992	-1.827277	-1.397819
C	-5.622803	-1.573052	0.480010
H	-5.598548	-2.616791	0.818306
H	-4.825529	-1.030529	0.999174
H	-6.575478	-1.136641	0.803201
C	-5.524746	-0.013991	-1.483132
H	-4.772692	0.592832	-0.966664
H	-5.359213	0.083378	-2.563667

H	-6.504782	0.421574	-1.254401
C	-4.157268	-2.148943	-1.498477
H	-4.114090	-2.137238	-2.595242
C	-2.888460	-1.496169	-0.952438
H	-2.805170	-0.440111	-1.234598
H	-4.170193	-3.203353	-1.196815
C	-0.095711	-2.332932	1.086385
O	-0.321271	-2.933640	2.028372
H	-2.859593	-1.505557	0.146580
C	-1.629477	-2.176894	-1.393020
O	-1.524483	-3.257116	-1.898665
C	3.706528	-1.313601	0.361605
C	4.972722	-0.832247	0.011821
C	3.586541	-2.572855	0.961323
C	6.104426	-1.600788	0.269566
H	5.078602	0.140593	-0.458884
C	4.720797	-3.335475	1.221285
H	2.608323	-2.964247	1.227437
C	5.979917	-2.849642	0.874723
H	7.084549	-1.221928	-0.003506
H	4.619312	-4.310108	1.688516
H	6.865412	-3.445715	1.073866
C	2.657442	0.933702	-1.153193
C	2.870962	2.270001	-0.812174
C	2.737916	0.541032	-2.494923
C	3.140013	3.208790	-1.806870
H	2.806456	2.590500	0.223071
C	3.024218	1.476083	-3.481904
H	2.563409	-0.497067	-2.768908
C	3.216174	2.814786	-3.139076

H	3.284060	4.250407	-1.536829
H	3.086309	1.163883	-4.520084
H	3.421029	3.549242	-3.912131
C	-2.251037	0.975403	1.451144
C	-3.236040	1.867218	1.018475
C	-2.505960	0.163502	2.565270
C	-4.449389	1.957294	1.699010
H	-3.060753	2.501851	0.155193
C	-3.712322	0.265844	3.249787
H	-1.750982	-0.534460	2.917589
C	-4.687046	1.165061	2.817697
H	-5.205789	2.654904	1.352440
H	-3.892478	-0.358446	4.119684
H	-5.630993	1.241577	3.348600
C	-0.566653	2.253993	-0.520609
C	-0.335707	3.535728	-0.007244
C	-0.721925	2.085034	-1.898527
C	-0.250164	4.627106	-0.864432
H	-0.213725	3.683820	1.061809
C	-0.634895	3.179216	-2.756169
H	-0.898419	1.095886	-2.310062
C	-0.395069	4.449334	-2.239771
H	-0.067035	5.617315	-0.458234
H	-0.749638	3.035706	-3.826104
H	-0.321076	5.301503	-2.908834
H	0.303211	-0.657226	-1.838810
H	-0.610978	-1.208466	-1.817276

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	Coordinates (Angstroms)		
	X	Y	Z
C	-4.903509	1.613156	-0.625624
C	-3.626830	1.997708	-0.233248
C	-2.601375	1.050519	-0.140443
C	-2.864513	-0.295269	-0.441504
C	-4.153765	-0.670038	-0.834820
C	-5.166746	0.277456	-0.927757
H	-5.693512	2.354572	-0.695198
H	-3.429117	3.040420	0.001079
H	-4.367324	-1.709693	-1.068991
H	-6.163729	-0.024667	-1.233825
P	-1.511050	-1.523576	-0.307024
P	-0.923722	1.561834	0.378601
Co	0.388053	-0.273834	0.323132
C	0.285027	-0.707633	2.089241
C	1.929092	-1.704952	-0.041056
O	0.135594	-0.993820	3.184083
O	1.664321	-2.825521	-0.380215
C	4.292974	0.778187	-0.619206
C	4.517124	2.277323	-0.375156
H	3.563034	2.803617	-0.243277
H	5.121659	2.446620	0.524107
H	5.038128	2.737912	-1.222643
C	5.657464	0.093702	-0.782635
H	6.248681	0.169406	0.138103
H	5.558746	-0.968219	-1.035216
H	6.227025	0.569448	-1.589611

C	3.477526	0.603760	-1.905491
H	3.276557	-0.452991	-2.125448
H	2.516957	1.129728	-1.840928
H	4.024106	1.012872	-2.763229
C	3.550604	0.215105	0.613544
H	2.629281	0.801953	0.767639
C	3.219078	-1.280791	0.619244
H	3.089452	-1.615369	1.659581
H	4.029129	-1.891591	0.205429
H	4.170335	0.418034	1.494979
H	1.281657	-0.696052	-0.901915
H	0.549417	0.104375	-1.164327
C	-1.171197	2.397155	1.983484
H	-0.205855	2.755384	2.355565
H	-1.850641	3.249044	1.880210
H	-1.588777	1.693310	2.709775
C	-0.466147	2.925778	-0.745148
H	0.510535	3.320646	-0.447130
H	-0.395006	2.549252	-1.769385
H	-1.203562	3.733952	-0.704623
C	-2.199077	-2.830416	0.771711
H	-2.417687	-2.416547	1.760803
H	-3.116098	-3.257898	0.353210
H	-1.455609	-3.626555	0.882809
C	-1.448740	-2.313370	-1.953355
H	-1.166511	-1.569133	-2.703917
H	-0.685709	-3.097212	-1.937100
H	-2.412670	-2.754518	-2.226389

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	Coordinates (Angstroms)		
	X	Y	Z
C	5.792252	-0.017617	0.211491
C	4.719880	0.865894	0.204853
C	3.406638	0.382934	0.156563
C	3.172006	-0.999946	0.114053
C	4.261297	-1.878771	0.119953
C	5.562275	-1.392459	0.168059
H	6.807398	0.365215	0.250363
H	4.907674	1.936034	0.236517
H	4.090555	-2.951604	0.086661
H	6.398063	-2.085552	0.172131
P	1.447510	-1.617828	0.064109
P	2.004355	1.556196	0.138039
Co	0.025479	0.403167	0.051689
C	-1.025549	2.227562	0.268649
O	-1.372821	3.308005	0.282460
C	-5.642821	-0.234172	0.144815
C	-6.757652	-1.283019	0.265412
H	-6.666309	-2.050458	-0.513248
H	-6.723102	-1.786051	1.239533
H	-7.744713	-0.816686	0.162000
C	-5.823070	0.814248	1.251786
H	-5.715869	0.362428	2.245939
H	-5.092153	1.627435	1.169376
H	-6.820328	1.266091	1.192879
C	-5.742401	0.444501	-1.228475

H	-5.007115	1.250210	-1.343321
H	-5.583089	-0.277990	-2.038720
H	-6.735022	0.889609	-1.366345
C	-4.294664	-0.971827	0.295387
H	-4.215965	-1.727816	-0.495115
C	-3.057462	-0.077223	0.244516
H	-3.003361	0.484163	-0.699927
H	-4.293168	-1.514457	1.249572
C	-0.154778	0.325498	-1.771531
O	-0.248009	0.229880	-2.903877
H	-3.054603	0.671936	1.045522
C	-1.765455	-0.841549	0.331579
O	-1.638147	-2.025481	0.196045
C	2.361413	2.662610	-1.272528
H	3.330245	3.157776	-1.152042
H	2.367294	2.086294	-2.202756
H	1.580283	3.427009	-1.339672
C	2.261489	2.625602	1.596087
H	3.241711	3.111566	1.561847
H	1.486614	3.398996	1.616244
H	2.183493	2.028984	2.509316
C	1.444470	-2.801363	-1.331910
H	0.438810	-3.219940	-1.438606
H	1.707571	-2.283657	-2.259491
H	2.152762	-3.620521	-1.170582
C	1.340339	-2.698426	1.536858
H	2.123079	-3.463990	1.530007
H	1.437698	-2.095299	2.444770
H	0.362648	-3.188326	1.544922
H	-0.790804	-0.241144	1.286047

H	0.086374	0.284623	1.617631

TSM6-1

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.857803	1.608643	-0.838821
C	-3.622603	1.986630	-0.324565
C	-2.609636	1.036616	-0.164070
C	-2.842985	-0.300753	-0.515984
C	-4.087851	-0.669970	-1.033871
C	-5.089512	0.280693	-1.195630
H	-5.640417	2.350604	-0.963682
H	-3.452798	3.025468	-0.050950
H	-4.279162	-1.703066	-1.313846
H	-6.052759	-0.013147	-1.601050
P	-1.496529	-1.504938	-0.259457
P	-0.986827	1.503978	0.520459
Co	0.392995	-0.250627	0.339169
C	0.344039	-0.762085	2.097099
C	1.916306	-1.648795	-0.183138
O	0.227023	-1.088415	3.182648
O	1.637483	-2.735914	-0.615924
C	4.282649	0.830073	-0.650346
C	4.505058	2.316560	-0.336325
H	3.550433	2.834541	-0.175889
H	5.114043	2.445121	0.566766
H	5.020145	2.817302	-1.164436

C	5.646150	0.160377	-0.873318
H	6.259470	0.197904	0.035346
H	5.545170	-0.889682	-1.170886
H	6.195426	0.672717	-1.672042
C	3.447124	0.715804	-1.930679
H	3.258235	-0.329383	-2.208330
H	2.479891	1.221456	-1.824396
H	3.973507	1.181061	-2.772267
C	3.566965	0.200518	0.566526
H	2.655919	0.784787	0.782193
C	3.219053	-1.289536	0.487791
H	3.093703	-1.681450	1.508858
H	4.017888	-1.883588	0.030322
H	4.211798	0.342100	1.441788
H	1.251396	-0.585645	-0.933685
H	0.494872	0.218232	-1.128400
N	-1.407870	1.882606	2.111002
H	-0.617842	2.072542	2.721030
H	-2.134487	2.584145	2.235201
N	-0.539673	2.841303	-0.404180
H	-1.100297	3.683437	-0.294560
H	0.450359	3.061034	-0.361753
N	-2.177791	-2.502032	0.926401
H	-3.066029	-2.943815	0.699397
H	-1.529066	-3.185689	1.306166
N	-1.342918	-2.241542	-1.770660
H	-0.472030	-2.759437	-1.853915
H	-2.127892	-2.792589	-2.109327

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	Coordinates (Angstroms)		
	X	Y	Z
C	3.235991	0.629557	0.059522
C	4.464425	1.276236	0.234029
H	4.520893	2.362238	0.221572
C	5.624459	0.535217	0.424102
H	6.574248	1.042841	0.560677
C	5.567320	-0.858332	0.441631
H	6.473410	-1.436633	0.593951
C	4.351019	-1.506425	0.264073
H	4.315793	-2.593173	0.280567
C	3.177815	-0.770391	0.069554
C	-0.406606	0.079702	1.503571
C	-1.644759	-1.308865	-0.858280
Co	-0.122573	0.223256	-0.315863
O	-0.532472	-0.018994	2.630519
O	-1.319509	-2.443752	-0.642234
P	1.708337	1.590546	-0.188343
P	1.564068	-1.581033	-0.183792
H	-3.732051	-1.581438	0.865009
C	-3.063328	-0.840025	-1.035634
C	-3.719885	-0.619414	0.337861
H	-3.075907	0.071998	-1.639071
H	-3.591219	-1.627990	-1.583554
H	-3.096708	0.060740	0.933970
C	-5.153295	-0.046452	0.295558
C	-5.144657	1.393969	-0.232720

H	-6.161095	1.804770	-0.241572
H	-4.529960	2.042433	0.403769
H	-4.759189	1.456005	-1.257041
C	-6.065620	-0.916530	-0.578666
H	-5.789810	-0.863175	-1.638470
H	-6.026063	-1.968439	-0.269323
H	-7.106175	-0.581226	-0.495045
C	-5.687214	-0.043387	1.735297
H	-5.040081	0.546895	2.396200
H	-6.692236	0.392911	1.775352
H	-5.745650	-1.061075	2.140121
C	-1.402525	1.843514	-0.601739
O	-1.885811	2.866498	-0.696951
H	0.094400	0.165994	-1.877549
H	-0.679205	-0.504930	-1.652177
N	1.697763	2.568865	1.188643
H	2.507837	3.163856	1.346820
H	0.836949	3.090289	1.327117
N	2.046860	2.408840	-1.624180
H	1.245291	2.856653	-2.057064
H	2.854124	3.028037	-1.624993
N	1.474330	-2.569008	1.188746
H	0.563817	-3.005210	1.301363
H	2.212857	-3.257320	1.317083
N	1.853874	-2.428399	-1.621992
H	2.624851	-3.092735	-1.616067
H	1.017999	-2.865295	-1.999484

TSO6-1

	Coordinates (Angstroms)		
	X	Y	Z
C	-5.174759	1.616945	-0.244901
C	-3.934499	1.871347	0.327432
C	-2.903175	0.934540	0.208709
C	-3.120414	-0.267651	-0.483653
C	-4.374584	-0.512927	-1.052219
C	-5.394130	0.424574	-0.933927
H	-5.970211	2.350162	-0.155845
H	-3.765524	2.801339	0.862946
H	-4.552016	-1.439541	-1.590515
H	-6.362083	0.227630	-1.384154
P	-1.743027	-1.466631	-0.633704
P	-1.267548	1.260307	0.951961
Co	0.182023	-0.356465	0.270918
C	0.243540	-1.343321	1.829417
C	1.754849	-1.531170	-0.625541
O	0.196944	-1.959941	2.785049
O	1.452265	-2.485870	-1.280213
C	3.996490	1.128812	-0.374674
C	4.263243	2.406282	0.435060
H	3.337195	2.800527	0.873108
H	4.967320	2.215053	1.254178
H	4.692631	3.189051	-0.200954
C	5.327467	0.612577	-0.940286
H	6.006124	0.299685	-0.137448
H	5.185423	-0.238099	-1.616763
H	5.827496	1.402032	-1.513479

C	3.048072	1.462921	-1.531367
H	2.831409	0.585741	-2.154906
H	2.096433	1.863471	-1.159685
H	3.495523	2.219658	-2.186419
C	3.380059	0.093501	0.591960
H	2.461952	0.520805	1.030809
C	3.086966	-1.306043	0.044648
H	3.069002	-2.022680	0.879597
H	3.864831	-1.662437	-0.639748
H	4.072421	-0.027946	1.433026
H	1.033757	-0.329408	-1.050424
H	0.223553	0.441175	-1.046164
H	-1.019763	2.601633	0.626463
H	-1.548067	1.400833	2.320774
H	-1.798022	-1.817871	-1.992128
H	-2.293810	-2.637234	-0.083553

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	Coordinates (Angstroms)		
	X	Y	Z

C	-5.955443	0.529724	0.279804
C	-4.790498	1.275102	0.150288
C	-3.557787	0.631540	-0.005880
C	-3.496986	-0.770999	-0.033467
C	-4.678248	-1.509503	0.100128
C	-5.898582	-0.863758	0.255717
H	-6.908510	1.034575	0.402246

H	-4.838561	2.360181	0.171594
H	-4.640837	-2.595027	0.082859
H	-6.808930	-1.445918	0.359590
P	-1.870202	-1.586478	-0.241612
P	-2.023910	1.611321	-0.170081
Co	-0.152914	0.250802	-0.299516
C	1.072423	1.897954	-0.596734
O	1.529229	2.922734	-0.761569
C	4.898289	-0.085580	0.270486
C	5.346506	0.146477	1.720627
H	4.741188	0.922763	2.205003
H	5.256501	-0.772161	2.312894
H	6.393922	0.468136	1.754903
C	5.781125	-1.171758	-0.357130
H	5.649756	-2.132537	0.155775
H	5.557691	-1.321749	-1.419739
H	6.839173	-0.894325	-0.282432
C	5.042602	1.223566	-0.516215
H	4.798400	1.093573	-1.576927
H	4.389017	2.004445	-0.108090
H	6.074150	1.590677	-0.462120
C	3.421769	-0.535409	0.316989
H	2.843562	0.245432	0.828570
C	2.785374	-0.818115	-1.054977
H	2.788696	0.073296	-1.689019
H	3.344633	-1.443252	0.928290
C	0.174929	0.045401	1.517100
O	0.324484	-0.084119	2.637503
H	3.327649	-1.619174	-1.568732
C	1.372846	-1.298123	-0.880742

O	1.021188	-2.419234	-0.665358
H	-2.132568	2.546066	0.872671
H	-2.292267	2.456275	-1.258234
H	-1.915913	-2.582827	0.749409
H	-2.089915	-2.401259	-1.365946
H	0.409684	-0.471378	-1.641809
H	-0.355296	0.205750	-1.868989

TSQ6-1

Coordinates (Angstroms)

	X	Y	Z

C	-5.228583	1.368081	-0.921091
C	-4.013832	1.791778	-0.390554
C	-3.044379	0.850912	-0.035286
C	-3.302303	-0.524573	-0.201073
C	-4.527687	-0.935751	-0.730874
C	-5.482551	0.009966	-1.093854
H	-5.976763	2.101645	-1.202486
H	-3.823967	2.852871	-0.257572
H	-4.738568	-1.992612	-0.865656
H	-6.429265	-0.317249	-1.511172
P	-2.046618	-1.723510	0.343543
P	-1.455232	1.364826	0.667838
Co	-0.089007	-0.436303	0.797336
C	-0.005761	-0.654259	2.631722
C	1.470676	-1.932911	0.446411
O	-0.010716	-0.752454	3.764457

O	1.143169	-3.071351	0.300294
C	3.682128	0.528163	-0.637582
C	3.744508	2.062104	-0.638210
H	2.740386	2.499040	-0.552637
H	4.345988	2.434667	0.199900
H	4.192837	2.435045	-1.566124
C	5.105652	-0.033613	-0.758095
H	5.722086	0.261269	0.099872
H	5.111874	-1.128144	-0.818856
H	5.588309	0.345639	-1.666191
C	2.848723	0.065745	-1.839114
H	2.742133	-1.026793	-1.875339
H	1.846006	0.509592	-1.825835
H	3.330516	0.371793	-2.774707
C	3.050992	0.093672	0.703621
H	2.099109	0.642947	0.833973
C	2.804429	-1.405910	0.908011
H	2.808606	-1.639804	1.983176
H	3.583521	-2.031160	0.457263
H	3.697313	0.442931	1.516091
H	0.728773	-1.028632	-0.426900
H	-0.022891	-0.282195	-0.742344
C	-1.822627	2.266184	2.262982
H	-2.858446	2.206410	2.646820
C	-0.809677	2.779409	-0.387089
H	-0.194881	3.517035	0.161524
C	-2.890546	-2.768298	1.631358
H	-3.747952	-2.303327	2.155198
C	-1.854231	-2.972981	-1.038512
H	-1.748174	-4.020886	-0.702873

O	-0.939718	2.860158	2.827367
O	-1.020578	2.839391	-1.567047
O	-2.489746	-3.877410	1.881210
O	-1.813038	-2.641150	-2.192898

TSR6-7

	Coordinates (Angstroms)		
	X	Y	Z

C	-5.557575	0.433277	-0.130073
C	-4.401748	1.206289	-0.099971
C	-3.149713	0.585569	-0.077106
C	-3.056305	-0.818255	-0.070578
C	-4.226628	-1.582932	-0.100712
C	-5.469048	-0.957045	-0.134775
H	-6.528311	0.917501	-0.149428
H	-4.474128	2.290565	-0.091362
H	-4.169339	-2.667936	-0.099811
H	-6.372567	-1.557751	-0.159574
P	-1.411821	-1.588875	0.043081
P	-1.636320	1.576838	-0.082389
Co	0.279253	0.282498	-0.185442
C	1.485792	1.920984	-0.577011
O	2.043005	2.888851	-0.762885
C	5.341000	-0.032337	0.130218
C	5.936880	-0.057697	1.545282
H	5.312749	0.508403	2.247934
H	6.024003	-1.084233	1.921432

H	6.937688	0.389408	1.550463
C	6.219868	-0.876254	-0.802076
H	6.199356	-1.935441	-0.516862
H	5.899460	-0.799160	-1.847883
H	7.260855	-0.536010	-0.753881
C	5.295316	1.418478	-0.365293
H	4.862957	1.498617	-1.369446
H	4.705220	2.047933	0.312237
H	6.306696	1.838599	-0.412932
C	3.915360	-0.618368	0.225626
H	3.308960	0.052184	0.849352
C	3.213803	-0.825907	-1.129252
H	3.181248	0.095136	-1.716177
H	3.955177	-1.586545	0.738866
C	0.704288	0.177207	1.635335
O	0.905982	0.129581	2.752974
H	3.727544	-1.597756	-1.712149
C	1.818842	-1.323324	-0.900024
O	1.466797	-2.439470	-0.681106
C	-1.802510	2.821009	-1.460328
H	-2.555461	2.602326	-2.240080
C	-1.737833	2.694109	1.415904
H	-1.248115	3.679281	1.298987
C	-1.494223	-2.617775	1.592257
H	-2.212520	-2.278005	2.363301
C	-1.388557	-2.929977	-1.256874
H	-0.977111	-3.898357	-0.918376
O	-2.255756	2.331310	2.438025
O	-1.083157	3.787947	-1.482909
O	-0.774810	-3.573856	1.740534

O	-1.758483	-2.725927	-2.383317
H	0.791529	-0.474290	-1.553182
H	0.015737	0.158828	-1.758678

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	Coordinates (Angstroms)		
	X	Y	Z

C	4.549925	-1.870976	-1.092885
C	3.342361	-2.182756	-0.477478
C	2.404172	-1.172339	-0.246698
C	2.683471	0.149484	-0.625475
C	3.896082	0.451785	-1.249190
C	4.825766	-0.557612	-1.476195
H	5.279328	-2.653387	-1.276947
H	3.128377	-3.206286	-0.183964
H	4.109707	1.470310	-1.558156
H	5.769054	-0.322759	-1.959377
P	1.407719	1.417465	-0.340773
P	0.833066	-1.527236	0.596215
Co	-0.505646	0.244386	0.387795
C	-0.446811	0.769842	2.143449
C	-2.065062	1.657613	-0.067865
O	-0.352248	1.069600	3.238758
O	-1.793470	2.736880	-0.509109
C	-4.470920	-0.772940	-0.543050
C	-4.622492	-2.287357	-0.344268
H	-3.643987	-2.782193	-0.293474

H	-5.159442	-2.513027	0.585051
H	-5.181770	-2.736267	-1.173370
C	-5.867462	-0.137715	-0.601686
H	-6.402820	-0.276430	0.345374
H	-5.825545	0.937158	-0.812528
H	-6.462583	-0.602360	-1.396529
C	-3.742582	-0.515773	-1.867802
H	-3.585916	0.555077	-2.052676
H	-2.767935	-1.017229	-1.894691
H	-4.332975	-0.901711	-2.706934
C	-3.681094	-0.220186	0.664610
H	-2.757934	-0.812168	0.784447
C	-3.340112	1.273781	0.640037
H	-3.180261	1.629814	1.668742
H	-4.151948	1.885211	0.231242
H	-4.266934	-0.416347	1.569640
H	-1.432330	0.545656	-0.851796
H	-0.726348	-0.267962	-1.062173
O	1.235220	-2.004707	2.086545
O	0.345988	-2.968638	0.062430
O	2.199134	2.412172	0.660187
O	1.416333	2.290337	-1.713981
C	2.222905	-1.254752	2.810631
H	2.172436	-0.182849	2.590463
H	2.020337	-1.415272	3.869659
H	3.222084	-1.621474	2.560807
C	-0.217207	-3.060916	-1.251442
H	-0.414616	-4.118999	-1.423225
H	-1.156032	-2.499583	-1.312149
H	0.486813	-2.695312	-2.006451

C	1.502650	3.578161	1.127873
H	1.533772	4.361941	0.367120
H	0.457589	3.352886	1.370341
H	2.020421	3.911885	2.027585
C	0.624713	1.819893	-2.809646
H	0.788029	2.519648	-3.629947
H	0.942723	0.819217	-3.124519
H	-0.438068	1.812366	-2.549819

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Coordinates (Angstroms)

	X	Y	Z

C	5.523585	-0.107275	-0.791301
C	4.457724	-0.964179	-0.541903
C	3.190886	-0.430779	-0.282022
C	2.997447	0.957104	-0.262616
C	4.074091	1.809564	-0.520878
C	5.331579	1.275335	-0.780261
H	6.507397	-0.516918	-0.997283
H	4.605960	-2.040225	-0.555416
H	3.925364	2.884938	-0.522883
H	6.167473	1.938644	-0.979667
P	1.323062	1.606542	0.053278
P	1.790565	-1.523565	0.085017
Co	-0.160399	-0.394810	0.059523
C	-1.175495	-2.329903	-0.166533
O	-1.440030	-3.430536	-0.205365

C	-5.840113	0.077881	-0.265665
C	-6.979915	1.098389	-0.396768
H	-6.922734	1.859582	0.390989
H	-6.940857	1.612105	-1.365108
H	-7.955790	0.605058	-0.316308
C	-5.969572	-0.961734	-1.387744
H	-5.853934	-0.495614	-2.374312
H	-5.220369	-1.757714	-1.299673
H	-6.955807	-1.439384	-1.355185
C	-5.947870	-0.618267	1.098178
H	-5.196596	-1.408349	1.217752
H	-5.819875	0.098842	1.918689
H	-6.932133	-1.087398	1.213751
C	-4.510262	0.854148	-0.381437
H	-4.472925	1.610837	0.411398
C	-3.252007	-0.007487	-0.296022
H	-3.210099	-0.566210	0.649375
H	-4.499177	1.397108	-1.335071
C	-0.494022	-0.361027	1.873213
O	-0.704947	-0.373315	2.992129
H	-3.206905	-0.758915	-1.094487
C	-1.981287	0.790896	-0.364576
O	-1.880123	1.981148	-0.309220
O	2.182275	-2.295118	1.450930
O	1.952613	-2.792326	-0.901527
O	1.617523	2.420650	1.423972
O	1.206378	2.836390	-1.013164
C	2.701687	-1.528925	2.548536
H	2.494561	-2.101964	3.452385
H	3.779896	-1.393115	2.429087

H	2.226349	-0.544351	2.628786
C	1.694226	-2.612145	-2.299470
H	1.866482	-3.581622	-2.766819
H	0.657273	-2.304382	-2.475828
H	2.377470	-1.872741	-2.730231
C	0.526239	3.121445	2.037456
H	-0.395927	2.530579	2.018956
H	0.815013	3.306362	3.072714
H	0.355149	4.072046	1.526001
C	0.795272	2.511684	-2.343234
H	0.791686	3.447202	-2.903927
H	1.499290	1.815352	-2.814240
H	-0.212183	2.084578	-2.349583
H	-0.944851	0.147593	-1.231160
H	-0.025498	-0.350222	-1.507991

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Coordinates (Angstroms)

	X	Y	Z
C	-4.883883	1.679386	-0.619502
C	-3.611646	2.038354	-0.185561
C	-2.618895	1.061015	-0.098217
C	-2.903724	-0.273471	-0.444063
C	-4.184081	-0.622589	-0.875197
C	-5.168154	0.357483	-0.961152
H	-5.658667	2.435598	-0.691294
H	-3.393773	3.068750	0.077717

H	-4.411048	-1.649561	-1.143607
H	-6.164113	0.088611	-1.297716
P	-1.563121	-1.476521	-0.308679
P	-0.957724	1.454460	0.468193
Co	0.403289	-0.296984	0.321641
C	0.440752	-0.901094	2.088905
C	2.004714	-1.730273	-0.242434
O	0.404612	-1.262272	3.164451
O	1.673271	-2.806134	-0.626044
C	4.299230	0.883434	-0.622147
C	4.397557	2.372873	-0.262978
H	3.402010	2.819237	-0.141839
H	4.948318	2.518727	0.674239
H	4.918994	2.929064	-1.050545
C	5.716385	0.320770	-0.799490
H	6.294544	0.417458	0.127279
H	5.709248	-0.737393	-1.085400
H	6.247805	0.867153	-1.587368
C	3.517824	0.739240	-1.933263
H	3.404091	-0.310100	-2.236424
H	2.518510	1.182873	-1.847959
H	4.040096	1.254772	-2.747448
C	3.585712	0.170935	0.548208
H	2.650530	0.713666	0.767900
C	3.308504	-1.326933	0.391628
H	3.258557	-1.798416	1.384063
H	4.105127	-1.850339	-0.149432
H	4.200591	0.297099	1.446308
H	1.313190	-0.645952	-0.941438
H	0.590390	0.152839	-1.153930

F	-1.212369	2.138443	1.879209
F	-0.593490	2.762880	-0.351190
F	-2.197199	-2.587071	0.639940
F	-1.671980	-2.255600	-1.689712

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Coordinates (Angstroms)

	X	Y	Z
C	-5.799051	-0.001407	-0.426247
C	-4.730111	0.884643	-0.349754
C	-3.433072	0.383724	-0.212423
C	-3.211091	-1.004537	-0.146003
C	-4.293489	-1.883092	-0.221200
C	-5.581647	-1.377249	-0.362386
H	-6.807341	0.383925	-0.536261
H	-4.905637	1.954957	-0.399026
H	-4.132251	-2.955374	-0.171770
H	-6.421494	-2.061813	-0.422094
P	-1.509980	-1.592876	0.043490
P	-2.020847	1.490801	-0.100422
Co	-0.013209	0.474059	-0.000393
C	1.018641	2.270116	-0.288224
O	1.479390	3.293273	-0.433382
C	5.669620	-0.300548	-0.215106
C	6.784446	-1.342593	-0.384945
H	6.700859	-2.137592	0.366150
H	6.742330	-1.808405	-1.376881

H	7.770733	-0.877180	-0.272348
C	5.832322	0.787210	-1.286036
H	5.708275	0.372792	-2.294328
H	5.105203	1.598465	-1.160112
H	6.831205	1.234766	-1.226296
C	5.781954	0.327921	1.180585
H	5.035813	1.116070	1.340165
H	5.651565	-0.427070	1.965815
H	6.768979	0.785448	1.316348
C	4.322485	-1.039080	-0.374521
H	4.237680	-1.794669	0.415406
C	3.091438	-0.133358	-0.329850
H	3.049483	0.458042	0.597468
H	4.320461	-1.576745	-1.330879
C	0.297560	0.451047	1.846915
O	0.498154	0.460659	2.963714
H	3.072534	0.585135	-1.157416
C	1.804172	-0.892339	-0.364368
O	1.596807	-2.048827	-0.190292
F	-2.427859	2.453025	1.099432
F	-2.263900	2.509493	-1.294573
F	-1.635665	-2.504832	1.347169
F	-1.459349	-2.747869	-1.053225
H	0.802467	-0.233180	-1.224278
H	-0.050702	0.302023	-1.573250

TSW6-1

Coordinates (Angstroms)

	X	Y	Z
C	-3.858752	2.907933	-0.496009
C	-2.482822	2.893792	-0.289505
C	-1.813109	1.674447	-0.170939
C	-2.529796	0.460748	-0.266362
C	-3.909410	0.492824	-0.479678
C	-4.566795	1.714643	-0.590598
H	-4.375025	3.857774	-0.585171
H	-1.946843	3.833101	-0.217977
H	-4.479193	-0.424945	-0.558122
H	-5.639168	1.729707	-0.754234
P	-1.585899	-1.088623	-0.113587
P	-0.021759	1.576870	0.089229
Co	0.643789	-0.540566	0.411025
C	0.493405	-0.711407	2.257217
C	1.825611	-2.454234	0.280171
O	0.372743	-0.792681	3.383677
O	1.260731	-3.482827	0.094546
C	4.686521	-0.664826	-0.528580
C	5.240821	0.766242	-0.496950
H	4.432981	1.507434	-0.492986
H	5.855183	0.931955	0.396251
H	5.866608	0.959450	-1.375765
C	5.862738	-1.651842	-0.512088
H	6.419462	-1.587711	0.430576
H	5.535019	-2.689144	-0.644669
H	6.556727	-1.424902	-1.329556
C	3.879375	-0.858624	-1.817333
H	3.431855	-1.859640	-1.882913

H	3.080623	-0.113434	-1.906716
H	4.531344	-0.744826	-2.691103
C	3.815828	-0.849466	0.733199
H	3.049653	-0.053146	0.764753
C	3.160657	-2.219895	0.934843
H	2.943083	-2.370321	2.003039
H	3.816268	-3.047749	0.642998
H	4.447510	-0.663863	1.609256
H	1.412124	-1.426023	-0.672891
H	0.948065	-0.542871	-1.109197
C	0.361077	2.797074	1.470867
C	0.727839	2.446026	-1.403314
C	-2.574595	-2.137021	1.094300
C	-1.904018	-1.989181	-1.734707
F	0.109752	4.071706	1.175441
F	-0.366611	2.454662	2.538085
F	1.656171	2.693174	1.790580
F	0.311371	3.702592	-1.555757
F	2.061285	2.457381	-1.284014
F	0.408609	1.760850	-2.503121
F	-2.626185	-1.478032	2.259129
F	-1.938674	-3.293678	1.292379
F	-3.823442	-2.409792	0.711877
F	-1.366016	-3.208624	-1.672466
F	-3.196395	-2.118221	-2.041632
F	-1.308636	-1.309639	-2.720598

TSX6-7

	Coordinates (Angstroms)		
	X	Y	Z
C	5.285724	0.330890	0.133472
C	4.274567	-0.621470	0.071890
C	2.938244	-0.214714	0.021614
C	2.616129	1.159549	0.027518
C	3.645534	2.101923	0.085988
C	4.971982	1.685820	0.139954
H	6.320890	0.009380	0.176998
H	4.536861	-1.672444	0.068918
H	3.426813	3.162547	0.096172
H	5.761314	2.428697	0.187300
P	0.854805	1.631515	-0.025000
P	1.576831	-1.404009	-0.061543
Co	-0.505200	-0.482675	0.048459
C	-1.451570	-2.380477	-0.165640
O	-1.911951	-3.408599	-0.267016
C	-6.267871	-0.188572	-0.115156
C	-7.443350	0.797113	-0.181532
H	-7.378794	1.545994	0.617364
H	-7.460407	1.328634	-1.140860
H	-8.398843	0.270787	-0.071981
C	-6.402203	-1.205487	-1.256971
H	-6.331792	-0.713740	-2.235092
H	-5.627819	-1.980573	-1.211180
H	-7.372738	-1.712426	-1.204125
C	-6.303518	-0.917274	1.235391
H	-5.525232	-1.686379	1.310732
H	-6.169032	-0.214359	2.066979

H	-7.268126	-1.419439	1.373695
C	-4.971081	0.636522	-0.258827
H	-4.926236	1.369781	0.555085
C	-3.681295	-0.185276	-0.250214
H	-3.580988	-0.775896	0.672007
H	-5.013745	1.204426	-1.196542
C	-0.807250	-0.413202	1.892579
O	-1.033886	-0.396798	3.004919
H	-3.629226	-0.894795	-1.084510
C	-2.458278	0.675444	-0.315385
O	-2.360433	1.849877	-0.167728
C	0.743408	2.955674	1.317458
C	0.760895	2.661563	-1.603631
C	1.920931	-2.670610	1.289024
C	1.896553	-2.405934	-1.623649
F	1.956425	-2.028030	2.460106
F	3.054776	-3.355393	1.147618
F	0.906801	-3.545935	1.319921
F	0.994409	-3.393144	-1.700103
F	3.111544	-2.947765	-1.691795
F	1.734406	-1.604180	-2.678650
F	1.311432	2.469135	2.428174
F	-0.533809	3.224288	1.586811
F	1.349392	4.107337	1.008910
F	-0.422870	3.266402	-1.699774
F	1.710253	3.593988	-1.710456
F	0.891727	1.821704	-2.639912
H	-1.419502	0.095239	-1.170692
H	-0.513051	-0.366168	-1.522838

TSY6-1

	Coordinates (Angstroms)		
	X	Y	Z
C	-4.072797	2.395863	-1.211601
C	-2.788225	2.545477	-0.703556
C	-1.993550	1.425633	-0.426325
C	-2.513245	0.135061	-0.640043
C	-3.819262	0.001341	-1.129312
C	-4.589479	1.120132	-1.425127
H	-4.673168	3.273872	-1.429113
H	-2.408624	3.543669	-0.509851
H	-4.249336	-0.985626	-1.265933
H	-5.596670	0.995692	-1.810934
P	-1.504128	-1.335071	-0.193686
P	-0.313769	1.637337	0.273493
Co	0.557063	-0.439044	0.536890
C	0.476291	-0.768546	2.315077
C	1.943784	-2.067753	0.276106
O	0.442460	-1.014113	3.431543
O	1.563880	-3.180051	0.039762
C	4.559626	-0.003306	-0.721370
C	4.903443	1.492799	-0.750221
H	3.994425	2.107880	-0.714769
H	5.531658	1.772665	0.104391
H	5.446522	1.752537	-1.666367
C	5.862777	-0.814555	-0.756150
H	6.472973	-0.617515	0.133674

H	5.676091	-1.893390	-0.807838
H	6.456656	-0.544955	-1.637573
C	3.714684	-0.341192	-1.955831
H	3.412096	-1.396792	-1.974438
H	2.810423	0.277948	-2.000481
H	4.286280	-0.154274	-2.872436
C	3.794985	-0.276382	0.592808
H	2.942162	0.421201	0.655789
C	3.300868	-1.707819	0.837389
H	3.180416	-1.863149	1.919674
H	4.019538	-2.462867	0.500744
H	4.453668	-0.004345	1.425674
H	1.381277	-1.044313	-0.657555
H	0.808557	-0.192438	-0.957653
C	-0.551155	2.688936	1.776888
C	0.794613	2.890684	2.480942
C	-1.596378	2.092010	2.720313
H	-0.920786	3.657935	1.420619
H	1.560093	3.304196	1.815125
H	0.673619	3.584195	3.320184
H	1.175255	1.944214	2.883135
H	-2.576546	1.999080	2.242670
H	-1.297591	1.102636	3.080962
H	-1.708529	2.741185	3.595807
C	0.672286	2.670026	-0.934126
C	0.454781	4.183561	-0.855479
C	0.467568	2.177516	-2.369559
H	1.710989	2.460400	-0.645346
H	0.663359	4.592858	0.136614
H	1.134759	4.673537	-1.561505

H	-0.565426	4.462285	-1.137985
H	0.632836	1.101360	-2.481470
H	-0.545522	2.400627	-2.721619
H	1.175900	2.687571	-3.031347
C	-2.606871	-2.290703	0.948822
C	-3.037106	-1.443430	2.148125
C	-1.893259	-3.572150	1.388387
H	-3.506953	-2.558396	0.382993
H	-3.579380	-0.543078	1.842440
H	-3.701195	-2.033976	2.789556
H	-2.181489	-1.136933	2.757995
H	-1.638811	-4.216464	0.540277
H	-0.966162	-3.345668	1.927769
H	-2.541377	-4.146687	2.059957
C	-1.346785	-2.389230	-1.728306
C	-0.784011	-1.581571	-2.902813
C	-2.603371	-3.147248	-2.165723
H	-0.589764	-3.123170	-1.426344
H	0.204851	-1.166311	-2.691769
H	-0.681689	-2.236435	-3.775503
H	-1.451967	-0.758203	-3.181674
H	-3.041379	-3.750201	-1.365218
H	-3.370576	-2.468307	-2.551484
H	-2.335735	-3.831431	-2.979298

TSZ6-7

Coordinates (Angstroms)

X	Y	Z

C	4.120712	2.975903	0.451031
C	3.859264	1.613580	0.384372
C	2.558706	1.144827	0.153877
C	1.507087	2.063287	-0.004615
C	1.787694	3.434801	0.069711
C	3.081640	3.889541	0.291665
H	5.133086	3.323377	0.632563
H	4.674578	0.912513	0.529501
H	0.988506	4.159539	-0.038768
H	3.276691	4.955965	0.348834
P	-0.200931	1.434824	-0.242418
P	2.225578	-0.651791	0.062355
Co	-0.023314	-0.963525	-0.062985
C	1.234536	-4.291923	-1.139462
O	1.110117	-5.357864	-0.770996
C	-5.066178	-0.294666	0.214592
C	-5.246560	0.873670	1.194835
H	-4.925944	0.596331	2.206842
H	-4.660270	1.747797	0.881957
H	-6.298059	1.179384	1.248653
C	-5.492831	0.158788	-1.187419
H	-4.863242	0.980475	-1.548864
H	-5.440154	-0.656842	-1.918109
H	-6.529466	0.515862	-1.172164
C	-5.942316	-1.470761	0.666801
H	-5.890951	-2.311420	-0.034665
H	-5.636840	-1.834452	1.655823
H	-6.992713	-1.163356	0.731953
C	-3.572544	-0.683487	0.247167

H	-3.329314	-1.003104	1.268450
C	-3.146338	-1.779263	-0.732208
H	-3.725417	-2.698125	-0.598571
H	-2.977180	0.211045	0.041499
C	-0.521240	-1.091552	1.686506
O	-0.903027	-1.166491	2.760296
H	-3.278654	-1.439374	-1.768024
C	-1.699094	-2.152398	-0.589931
O	-1.285315	-3.268703	-0.403638
C	3.114394	-1.376036	1.519383
C	2.865119	-2.885334	1.572516
C	2.722954	-0.694001	2.831648
H	4.183083	-1.199555	1.353526
H	3.235785	-3.395851	0.676874
H	3.382362	-3.316121	2.437062
H	1.794883	-3.104136	1.680383
H	2.892846	0.386617	2.804605
H	1.674951	-0.873015	3.087656
H	3.329038	-1.107939	3.645071
C	3.123095	-1.258178	-1.459983
C	4.634303	-1.445858	-1.308134
C	2.810867	-0.358192	-2.658865
H	2.669886	-2.239021	-1.640642
H	4.894968	-2.143265	-0.506810
H	5.032231	-1.859825	-2.241866
H	5.148804	-0.496244	-1.128922
H	1.735190	-0.220514	-2.812414
H	3.268617	0.630716	-2.543572
H	3.217120	-0.813103	-3.568721
C	-1.240458	2.330425	1.032223

C	-1.832966	3.694544	0.673503
C	-0.471474	2.406055	2.359334
H	-2.076476	1.638534	1.183975
H	-2.457052	3.658118	-0.223204
H	-2.467592	4.030849	1.502517
H	-1.059941	4.454918	0.525344
H	0.044631	1.473020	2.610438
H	0.282401	3.199204	2.336265
H	-1.171940	2.628617	3.171529
C	-0.643739	1.920028	-1.988253
C	-0.369464	3.359140	-2.429031
C	-2.081711	1.496280	-2.299704
H	0.026236	1.268175	-2.564948
H	0.684496	3.625986	-2.314272
H	-0.615858	3.454449	-3.493274
H	-0.975364	4.087528	-1.883355
H	-2.244224	0.433907	-2.096517
H	-2.808436	2.070779	-1.716191
H	-2.296265	1.670149	-3.360094
H	-0.785006	-1.330693	-1.402648
H	0.260780	-0.949059	-1.577826

U1

Coordinates (Angstroms)

	X	Y	Z
C	3.961591	0.165619	-0.000231
C	2.888437	1.050268	-0.000108

C	1.589624	0.540117	-0.000029
C	1.369186	-0.849968	-0.000093
C	2.452924	-1.728885	-0.000228
C	3.745160	-1.213027	-0.000302
H	4.974557	0.553982	-0.000270
H	3.058540	2.121750	-0.000040
H	2.289086	-2.801664	-0.000261
H	4.591422	-1.892071	-0.000396
P	-0.345099	-1.405311	0.000126
P	0.127641	1.580340	0.000098
Co	-1.730235	0.431394	-0.000221
H	-2.347484	1.807580	-0.000305
C	-3.509838	-0.149708	-0.000208
O	-4.608691	-0.425643	-0.000274
F	-0.392163	-2.431634	1.205989
F	-0.392228	-2.432412	-1.205078
F	0.353172	2.568262	1.208964
F	0.353344	2.568670	-1.208401

U5

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.721159	-1.319102	0.590613
C	-3.559009	-1.715692	-0.062800
C	-2.439071	-0.881435	-0.042260
C	-2.494823	0.351501	0.636103
C	-3.666478	0.741419	1.287658

C	-4.775332	-0.097454	1.262052
H	-5.591014	-1.967747	0.577894
H	-3.523250	-2.668243	-0.582171
H	-3.710180	1.691693	1.810279
H	-5.686718	0.201574	1.769304
P	-1.018028	1.385146	0.620149
P	-0.893192	-1.338193	-0.860321
Co	0.671434	0.405867	-0.595628
C	0.514776	1.223547	-2.299165
C	2.141775	1.740434	-0.105839
O	0.399595	1.744700	-3.301777
O	2.016992	2.847903	0.300643
C	3.293647	-1.264615	0.929347
C	2.966329	-2.737424	0.653195
H	1.964839	-2.839813	0.216153
H	3.687335	-3.180267	-0.044207
H	2.990032	-3.321543	1.580111
C	4.682254	-1.160623	1.577118
H	5.457257	-1.565898	0.916207
H	4.944869	-0.123215	1.814795
H	4.708524	-1.727093	2.515006
C	2.253200	-0.701404	1.910433
H	2.434612	0.351066	2.158518
H	1.221062	-0.796296	1.523796
H	2.273651	-1.263801	2.850332
C	3.312220	-0.530259	-0.435478
H	2.440027	-0.828232	-1.055729
C	3.433682	0.997848	-0.411999
H	3.692636	1.358388	-1.417488
H	4.206992	1.356219	0.275676

H	4.163880	-0.915235	-1.007451
F	-1.390004	-1.714998	-2.326288
F	-0.658606	-2.815185	-0.307997
F	-1.584860	2.787148	0.126546
F	-0.824278	1.737976	2.158707

U6

Coordinates (Angstroms)

	X	Y	Z
C	-5.219046	1.149131	-0.365377
C	-3.968731	1.729369	-0.180437
C	-2.827943	0.922422	-0.170775
C	-2.951831	-0.469154	-0.348075
C	-4.211930	-1.041451	-0.533503
C	-5.340645	-0.229190	-0.540590
H	-6.105328	1.775311	-0.371489
H	-3.882070	2.802582	-0.043251
H	-4.310214	-2.113888	-0.670270
H	-6.320344	-0.673420	-0.682991
P	-1.450536	-1.471350	-0.320414
P	-1.179767	1.626153	0.078372
Co	0.442255	-0.128340	0.201490
C	0.335364	-0.284460	2.095750
C	1.934008	-1.616660	0.191119
O	0.221567	-0.355154	3.224163
O	1.724642	-2.706152	-0.230438
C	4.632680	0.642120	-0.539284

C	4.743450	2.159919	-0.738481
H	3.795690	2.585073	-1.092880
H	5.010761	2.664231	0.198209
H	5.514286	2.399308	-1.480035
C	5.985744	0.107863	-0.048384
H	6.258645	0.554838	0.915118
H	5.984630	-0.981624	0.071484
H	6.774046	0.354313	-0.768981
C	4.272778	-0.017178	-1.876213
H	4.121975	-1.099178	-1.777900
H	3.362916	0.418201	-2.305245
H	5.078823	0.132887	-2.603853
C	3.541914	0.389713	0.527389
H	2.635524	0.936813	0.217180
C	3.216393	-1.089745	0.811688
H	3.054953	-1.244312	1.887037
H	4.023985	-1.766422	0.514651
H	3.864791	0.859170	1.462584
H	1.374227	0.057234	-1.632374
H	0.741750	0.404003	-1.862024
F	-1.414635	2.530622	1.369880
F	-1.144033	2.785622	-1.014031
F	-1.846327	-2.623440	0.707249
F	-1.582592	-2.309216	-1.667914

V6

Coordinates (Angstroms)

X Y Z

C	-5.063329	-1.756240	0.195966
C	-4.488204	-0.500488	0.365282
C	-3.113355	-0.350626	0.182239
C	-2.321150	-1.461303	-0.164485
C	-2.905274	-2.717899	-0.327890
C	-4.278070	-2.856417	-0.148478
H	-6.132519	-1.878723	0.332961
H	-5.103222	0.353298	0.630821
H	-2.299445	-3.576910	-0.597441
H	-4.739835	-3.829312	-0.279938
P	-0.553198	-1.182775	-0.350881
P	-2.259952	1.221574	0.390270
Co	-0.072160	1.043701	-0.312651
C	0.209035	2.879672	-0.735979
O	0.348834	3.982729	-0.955523
C	4.567424	-0.893935	0.418807
C	4.670805	-2.326909	0.959960
H	3.877917	-2.533812	1.689524
H	4.588816	-3.063835	0.151708
H	5.634515	-2.482399	1.458886
C	5.678409	-0.662933	-0.613651
H	5.553955	-1.320910	-1.482362
H	5.694973	0.373037	-0.971822
H	6.659539	-0.870709	-0.171009
C	4.727336	0.090938	1.584145
H	4.693100	1.134824	1.251367
H	3.941912	-0.053816	2.336293
H	5.693689	-0.059005	2.079721
C	3.174135	-0.748428	-0.231214

H	2.418312	-0.929684	0.543601
C	2.912541	0.611825	-0.901363
H	3.053940	1.433845	-0.191173
H	3.047028	-1.533995	-0.987171
C	0.707652	1.085568	1.477813
O	1.141943	1.113860	2.524390
H	3.575625	0.760406	-1.759380
C	1.500380	0.684609	-1.403890
O	1.117375	0.585787	-2.535138
F	-2.531629	1.596378	1.909518
F	-3.239234	2.261984	-0.294595
F	0.076987	-2.056421	0.816809
F	-0.167005	-2.091698	-1.586980

V7

Coordinates (Angstroms)

	X	Y	Z
C	-1.547271	-0.869899	0.039817
C	-2.650987	-1.716028	0.141359
H	-2.511541	-2.783150	0.282541
C	-3.932453	-1.177548	0.062820
H	-4.793546	-1.832891	0.141220
C	-4.116713	0.192867	-0.113903
H	-5.119831	0.601566	-0.173535
C	-3.022266	1.046486	-0.214538
H	-3.170419	2.112509	-0.352849
C	-1.735600	0.512551	-0.139851

C	2.199315	0.676389	1.461639
Co	1.572547	0.408307	-0.286199
O	2.577816	0.830541	2.517373
P	0.155157	-1.451047	0.157892
P	-0.283375	1.560972	-0.233094
C	3.001640	-0.499752	-1.058318
O	3.836966	-1.061272	-1.577206
H	1.048567	0.340758	-1.695641
F	0.157777	-2.258958	1.526568
F	0.185910	-2.676964	-0.850406
F	-0.591196	2.555851	-1.418731
F	-0.472600	2.573790	0.971258

W1

Coordinates (Angstroms)

	X	Y	Z

C	-1.163730	3.798569	-0.656270
C	-1.738977	2.546345	-0.458841
C	-0.918011	1.433053	-0.272980
C	0.485320	1.587309	-0.275653
C	1.049668	2.847821	-0.473562
C	0.219148	3.948226	-0.667359
H	-1.805255	4.661288	-0.800361
H	-2.817844	2.452970	-0.450962
H	2.124568	2.983670	-0.471653
H	0.659591	4.927477	-0.821269
P	1.465164	0.097727	0.037713

P	-1.559022	-0.242571	0.007786
Co	0.069429	-1.729269	0.202730
H	-0.860092	-2.621818	-0.647442
C	1.180687	-3.136916	-0.109318
O	1.827946	-4.032737	-0.369206
C	2.505296	0.472272	1.559639
C	2.739316	-0.022251	-1.341945
C	-2.614061	-0.128286	1.564090
C	-2.843590	-0.555839	-1.336612
F	1.676952	0.819424	2.547273
F	3.157692	-0.634673	1.924084
F	3.391531	1.449700	1.383485
F	3.585994	-1.016964	-1.062935
F	3.443410	1.090704	-1.534938
F	2.091606	-0.314916	-2.471921
F	-1.809814	0.217610	2.573851
F	-3.140778	-1.324620	1.831569
F	-3.599906	0.762355	1.483693
F	-3.788215	0.383302	-1.390912
F	-3.437697	-1.729494	-1.126661
F	-2.214954	-0.593604	-2.511919

W5

Coordinates (Angstroms)

	X	Y	Z

C	-4.970943	0.379398	-1.137249
C	-3.882483	1.180829	-0.808620

C	-2.657236	0.595372	-0.480433
C	-2.527030	-0.812466	-0.489785
C	-3.630986	-1.602859	-0.819035
C	-4.845878	-1.005482	-1.139914
H	-5.918870	0.843822	-1.387402
H	-4.002925	2.257467	-0.806029
H	-3.555763	-2.683270	-0.825480
H	-5.696796	-1.629105	-1.393122
P	-0.905645	-1.527312	-0.063515
P	-1.202636	1.576025	-0.008524
Co	0.618926	0.174396	0.521471
C	0.594332	0.121191	2.421816
C	2.367960	-0.870235	0.515249
O	0.606167	0.044422	3.555467
O	2.527670	-2.018019	0.764466
C	5.937690	0.458970	-0.446643
C	7.211001	-0.389640	-0.578896
H	7.444100	-0.902214	0.362267
H	7.101399	-1.152152	-1.360024
H	8.069981	0.239200	-0.841335
C	5.658461	1.154053	-1.785969
H	5.448370	0.421566	-2.575323
H	4.806842	1.842344	-1.724271
H	6.528260	1.743327	-2.099349
C	6.149773	1.509040	0.651945
H	5.293297	2.187587	0.743431
H	6.312487	1.033817	1.627256
H	7.029151	2.124049	0.427758
C	4.790939	-0.502964	-0.073078
H	5.051183	-1.022411	0.856870

C	3.419838	0.156678	0.116493
H	3.070808	0.660112	-0.794086
H	3.423983	0.911462	0.913555
H	4.701240	-1.270107	-0.851797
C	-1.815950	2.721504	1.354332
C	-0.906505	2.772254	-1.428623
C	-1.295886	-2.826429	1.241578
C	-0.461651	-2.593458	-1.550686
F	-0.773557	3.384491	1.866572
F	-2.350881	1.967686	2.320010
F	-2.723721	3.618401	0.965197
F	0.083727	3.605838	-1.085564
F	-0.502678	2.054889	-2.486221
F	-1.956423	3.502970	-1.796151
F	-2.086309	-3.814830	0.813604
F	-1.903913	-2.215184	2.264564
F	-0.160625	-3.365786	1.685643
F	-1.425876	-3.417279	-1.962231
F	0.618859	-3.324626	-1.268256
F	-0.160483	-1.766641	-2.562324

W6

Coordinates (Angstroms)			
	X	Y	Z

C	-4.586137	1.805285	-0.608624
C	-3.260024	2.189568	-0.439586
C	-2.267231	1.222066	-0.266641

C	-2.612657	-0.148920	-0.277338
C	-3.951633	-0.516497	-0.436123
C	-4.930531	0.458322	-0.598881
H	-5.349899	2.563925	-0.743104
H	-3.011697	3.244134	-0.445381
H	-4.244061	-1.558910	-0.437897
H	-5.965869	0.158782	-0.723245
P	-1.275492	-1.376832	-0.103478
P	-0.523784	1.664051	0.001144
Co	0.838713	-0.282279	0.226212
C	0.910198	-0.327111	2.126041
C	2.181522	-1.905799	0.223974
O	0.968705	-0.374142	3.260076
O	1.840547	-2.930703	-0.268268
C	5.118395	-0.053928	-0.480891
C	5.422359	1.439299	-0.663313
H	4.524339	1.992955	-0.966888
H	5.795446	1.885674	0.266550
H	6.184249	1.590804	-1.436772
C	6.410104	-0.783752	-0.085716
H	6.814587	-0.387897	0.853923
H	6.253206	-1.861207	0.041591
H	7.174170	-0.655828	-0.861377
C	4.593816	-0.624255	-1.804522
H	4.325808	-1.684639	-1.722590
H	3.715435	-0.072573	-2.158919
H	5.362069	-0.544778	-2.582370
C	4.073259	-0.183951	0.651052
H	3.251055	0.523597	0.454221
C	3.513581	-1.597893	0.887422

H	3.308671	-1.750962	1.955286
H	4.215985	-2.382633	0.589005
H	4.535792	0.161376	1.581990
H	1.731431	-0.293174	-1.563357
H	1.100639	0.036241	-1.822029
C	-0.559224	2.819590	1.485972
C	-0.105396	2.853843	-1.398432
C	-1.855175	-2.509147	1.285395
C	-1.467748	-2.475143	-1.624041
F	-1.358940	3.877923	1.365423
F	-0.966652	2.107849	2.544945
F	0.681766	3.259708	1.724784
F	-0.761714	4.014996	-1.366472
F	1.206374	3.121059	-1.362915
F	-0.379824	2.248740	-2.558741
F	-2.028786	-1.752029	2.377059
F	-0.903135	-3.409019	1.547336
F	-2.991352	-3.168331	1.048376
F	-0.753002	-3.589890	-1.471533
F	-2.722264	-2.825405	-1.914656
F	-0.979846	-1.794753	-2.671415

X6

Coordinates (Angstroms)

	X	Y	Z
C	-4.034562	2.833188	-0.872559
C	-3.777650	1.473393	-0.735539

C	-2.499487	1.042525	-0.373914
C	-1.464840	1.981176	-0.170073
C	-1.742810	3.343758	-0.305343
C	-3.024671	3.762397	-0.648490
H	-5.029592	3.163696	-1.151147
H	-4.575466	0.762456	-0.912093
H	-0.972786	4.088060	-0.148276
H	-3.228341	4.823321	-0.747680
P	0.204997	1.353040	0.216137
P	-2.098679	-0.701606	-0.116166
Co	0.112969	-1.021724	0.545689
C	-0.142569	-2.797461	1.278813
O	-0.274919	-3.854261	1.665779
C	5.034809	-0.837524	-0.610967
C	5.507659	0.403570	-1.381915
H	4.741007	0.749317	-2.086253
H	5.734972	1.230207	-0.697844
H	6.415825	0.181588	-1.954666
C	6.113860	-1.250986	0.397105
H	6.255175	-0.480720	1.165633
H	5.863598	-2.191862	0.901358
H	7.074717	-1.397508	-0.109927
C	4.786096	-1.977447	-1.606943
H	4.431645	-2.889271	-1.111636
H	4.044365	-1.686802	-2.360422
H	5.712857	-2.233081	-2.133844
C	3.726473	-0.449261	0.108444
H	2.981318	-0.212419	-0.657690
C	3.150933	-1.509276	1.057299
H	3.005834	-2.467414	0.545369

H	3.892075	0.469446	0.682037
C	0.773687	-1.645213	-1.183156
O	1.147536	-2.081509	-2.160877
H	3.799038	-1.665236	1.925175
C	1.808779	-1.065580	1.571540
O	1.528511	-0.722210	2.682169
C	1.264883	2.049966	-1.195794
C	0.775924	2.413713	1.668246
C	-2.626026	-1.584828	-1.690336
C	-3.356642	-1.332658	1.135224
F	-2.002430	-1.000536	-2.718885
F	-3.937837	-1.562851	-1.920367
F	-2.229584	-2.860523	-1.627585
F	-3.204515	-2.656281	1.264831
F	-4.628574	-1.088672	0.828467
F	-3.087345	-0.758439	2.311450
F	1.339704	1.122366	-2.160749
F	2.499665	2.311907	-0.763075
F	0.773625	3.158522	-1.743612
F	2.010351	2.061243	2.029247
F	0.783289	3.726231	1.420450
F	-0.054490	2.181964	2.687863

X7

Coordinates (Angstroms)

	X	Y	Z

C	-0.547959	1.706756	-0.155253

C	-1.144727	2.967758	-0.171136
H	-2.222295	3.072682	-0.123731
C	-0.349472	4.108082	-0.250115
H	-0.820167	5.085109	-0.266726
C	1.036064	4.000251	-0.304701
H	1.649637	4.892860	-0.363450
C	1.646956	2.749790	-0.281171
H	2.728343	2.681439	-0.327563
C	0.858826	1.599892	-0.215273
C	-0.003488	-2.453926	1.249782
Co	0.030459	-1.612591	-0.424500
O	-0.033851	-2.990851	2.246187
P	-1.482896	0.157497	-0.020688
P	1.572795	-0.061072	-0.149379
C	-1.029960	-2.774115	-1.393910
O	-1.660446	-3.470569	-2.027071
H	0.182322	-0.975779	-1.777748
C	2.487085	-0.130111	1.497201
C	2.988954	-0.150457	-1.392181
C	-2.327824	0.255760	1.657431
C	-2.932790	0.320719	-1.208436
F	1.573169	-0.065012	2.471560
F	3.122666	-1.302545	1.595309
F	3.366484	0.849350	1.675441
F	3.324774	-1.434220	-1.551874
F	4.073561	0.520817	-1.005800
F	2.580735	0.331966	-2.563361
F	-1.374446	0.316001	2.593178
F	-3.033840	-0.865448	1.846695
F	-3.141181	1.297048	1.816338

F	-3.643624	-0.811749	-1.167722
F	-3.755376	1.335733	-0.942095
F	-2.451181	0.475419	-2.442626

Y1

	Coordinates (Angstroms)		
	X	Y	Z

C	1.614398	3.644197	-0.658285
C	2.030646	2.337102	-0.430095
C	1.092475	1.326789	-0.191639
C	-0.279752	1.634871	-0.207682
C	-0.686723	2.950295	-0.459045
C	0.255734	3.950676	-0.671553
H	2.350992	4.420604	-0.839778
H	3.090082	2.104498	-0.456042
H	-1.742643	3.196609	-0.505981
H	-0.071342	4.968070	-0.862482
P	-1.478835	0.265477	0.010780
P	1.584648	-0.424912	0.043636
Co	-0.268337	-1.653391	0.183394
H	0.736739	-2.804217	0.301709
C	-1.539964	-2.942760	0.333290
O	-2.272560	-3.809759	0.445146
C	-2.627199	0.399436	-1.434348
C	-3.838433	-0.520202	-1.263836
C	-1.863071	0.086111	-2.722097
H	-2.976509	1.438171	-1.473596

H	-4.449650	-0.250592	-0.396895
H	-4.475358	-0.447403	-2.152250
H	-3.537731	-1.569461	-1.160528
H	-1.026899	0.774910	-2.878327
H	-1.472429	-0.939262	-2.709752
H	-2.535412	0.175941	-3.582375
C	-2.493685	0.601259	1.523589
C	-3.271317	1.917655	1.510135
C	-1.621360	0.476513	2.772703
H	-3.209442	-0.231201	1.524477
H	-3.861062	2.048910	0.597231
H	-3.964580	1.934417	2.358636
H	-2.598265	2.774771	1.616753
H	-1.159235	-0.514354	2.846302
H	-0.828903	1.232785	2.782531
H	-2.233787	0.623323	3.669195
C	2.626670	-0.813395	-1.436674
C	1.752885	-0.802275	-2.692610
C	3.363340	-2.144926	-1.280145
H	3.366051	-0.006586	-1.513631
H	1.245529	0.157396	-2.832687
H	2.374714	-0.982683	-3.576311
H	0.996603	-1.595941	-2.654605
H	4.080357	-2.131402	-0.453488
H	2.662436	-2.971377	-1.116075
H	3.922218	-2.354834	-2.198996
C	2.689415	-0.555661	1.522482
C	1.894100	-0.323316	2.807043
C	3.943177	0.319951	1.473876
H	2.991459	-1.609790	1.497780

H	1.085417	-1.053109	2.917208
H	2.557778	-0.432521	3.671952
H	1.466621	0.684779	2.839173
H	4.493217	0.219455	0.532519
H	3.697224	1.376182	1.623435
H	4.616194	0.021149	2.285203

Y5

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.326836	1.973451	-0.967627
C	-3.044066	2.278683	-0.529338
C	-2.089257	1.269637	-0.345613
C	-2.442946	-0.069883	-0.593018
C	-3.745054	-0.363384	-1.020228
C	-4.677041	0.648247	-1.216647
H	-5.055629	2.766643	-1.103569
H	-2.791532	3.312812	-0.315858
H	-4.044725	-1.393697	-1.179153
H	-5.681085	0.401263	-1.547869
P	-1.248647	-1.414807	-0.207923
P	-0.393065	1.662075	0.230076
Co	0.734401	-0.409679	0.555767
C	0.770904	-0.613173	2.406097
C	1.958340	-2.011724	0.424345
O	0.804824	-0.804017	3.532702
O	1.665580	-3.113135	0.059459

C	4.169379	0.231290	-0.839492
C	4.502578	1.729108	-0.831287
H	3.648390	2.322918	-0.480187
H	5.351084	1.942591	-0.169999
H	4.762066	2.078045	-1.837470
C	5.380749	-0.551688	-1.363045
H	6.254460	-0.404857	-0.716930
H	5.178650	-1.627183	-1.421917
H	5.647914	-0.214618	-2.371502
C	2.972939	-0.011815	-1.762405
H	2.762391	-1.080165	-1.887220
H	2.068588	0.487727	-1.382720
H	3.155702	0.399221	-2.762394
C	3.840672	-0.182044	0.610140
H	3.085418	0.514576	1.013962
C	3.385859	-1.628493	0.839810
H	3.395255	-1.833224	1.919714
H	4.066773	-2.350364	0.375676
H	4.736334	-0.024301	1.222860
C	-0.616996	2.767001	1.700293
C	0.758754	3.113876	2.278630
C	-1.524634	2.129261	2.753840
H	-1.095869	3.686330	1.345111
H	1.432558	3.544105	1.528687
H	0.651705	3.846732	3.086095
H	1.244389	2.224851	2.699089
H	-2.525618	1.924792	2.361608
H	-1.106820	1.191421	3.135009
H	-1.630389	2.811851	3.604720
C	0.354901	2.740137	-1.106653

C	-0.020508	4.223302	-1.074979
C	0.060303	2.139665	-2.485328
H	1.433914	2.660270	-0.922842
H	0.252758	4.710539	-0.134338
H	0.515331	4.740173	-1.879957
H	-1.090852	4.375794	-1.246413
H	0.274271	1.068295	-2.533008
H	-0.991684	2.281963	-2.755413
H	0.675744	2.636963	-3.243113
C	-2.201384	-2.444885	1.010812
C	-2.653224	-1.607815	2.210068
C	-1.378661	-3.657261	1.451099
H	-3.098562	-2.796713	0.487621
H	-3.262315	-0.749033	1.910910
H	-3.259566	-2.229776	2.878373
H	-1.801426	-1.238610	2.789484
H	-1.092970	-4.294573	0.608368
H	-0.462387	-3.348298	1.966076
H	-1.968108	-4.266163	2.146165
C	-1.044184	-2.474090	-1.719982
C	-0.413317	-1.650341	-2.845207
C	-2.276806	-3.232465	-2.215183
H	-0.301159	-3.204997	-1.378914
H	0.526138	-1.185271	-2.527906
H	-0.188311	-2.298011	-3.699998
H	-1.091525	-0.861412	-3.191065
H	-2.775242	-3.797984	-1.421566
H	-3.006722	-2.558526	-2.674702
H	-1.966521	-3.950130	-2.983416

Y6

	Coordinates (Angstroms)		
	X	Y	Z
C	-4.590797	1.831310	-0.752009
C	-3.287888	2.184437	-0.424459
C	-2.295706	1.204796	-0.284812
C	-2.624924	-0.150822	-0.462019
C	-3.947273	-0.491547	-0.778231
C	-4.919783	0.489094	-0.931603
H	-5.350279	2.600068	-0.856658
H	-3.046260	3.230804	-0.265053
H	-4.227887	-1.533814	-0.887805
H	-5.938861	0.205822	-1.176835
P	-1.343220	-1.436540	-0.162151
P	-0.577905	1.668802	0.146696
Co	0.707804	-0.298826	0.334291
C	0.782660	-0.485339	2.152481
C	1.997549	-1.846899	0.304115
O	0.856861	-0.660943	3.280074
O	1.705811	-2.952023	-0.061797
C	4.817327	0.193404	-0.675082
C	5.090485	1.698688	-0.801056
H	4.163468	2.255938	-0.988830
H	5.543140	2.097692	0.114986
H	5.777773	1.903384	-1.630282
C	6.142848	-0.527544	-0.389874
H	6.566468	-0.208704	0.570369

H	6.023993	-1.616584	-0.362454
H	6.875768	-0.299716	-1.172754
C	4.227810	-0.320168	-1.994980
H	3.934918	-1.375879	-1.932099
H	3.348661	0.263438	-2.292255
H	4.965809	-0.234263	-2.801289
C	3.834020	-0.007955	0.500398
H	2.954838	0.633721	0.321224
C	3.392111	-1.457913	0.777808
H	3.353861	-1.630929	1.862299
H	4.097825	-2.193103	0.377327
H	4.306008	0.394122	1.404077
H	1.480018	-0.437552	-1.308787
H	1.047136	0.201995	-1.381825
C	-0.723697	2.770016	1.630145
C	0.677933	3.151307	2.119304
C	-1.557241	2.128442	2.740898
H	-1.241934	3.675985	1.296048
H	1.292251	3.596370	1.328678
H	0.603171	3.882478	2.931733
H	1.213079	2.276484	2.507387
H	-2.577678	1.909691	2.412323
H	-1.109095	1.198517	3.104231
H	-1.618240	2.816925	3.591259
C	0.026773	2.775974	-1.242146
C	-0.347044	4.256719	-1.135823
C	-0.411419	2.215864	-2.599895
H	1.119144	2.693915	-1.170637
H	0.034680	4.726380	-0.224982
H	0.088851	4.791817	-1.987421

H	-1.430882	4.406377	-1.175811
H	-0.212832	1.145381	-2.711749
H	-1.484491	2.368609	-2.756417
H	0.123501	2.737327	-3.401202
C	-2.141239	-2.486652	1.146200
C	-2.551005	-1.658795	2.366391
C	-1.216477	-3.642839	1.535356
H	-3.054186	-2.897701	0.699199
H	-3.257850	-0.864876	2.106497
H	-3.036638	-2.311479	3.100895
H	-1.688066	-1.201030	2.858952
H	-0.941507	-4.262858	0.676184
H	-0.290781	-3.273240	1.989938
H	-1.718621	-4.285540	2.267456
C	-1.267850	-2.521348	-1.680490
C	-1.019408	-1.673955	-2.932273
C	-2.433522	-3.486322	-1.909772
H	-0.365389	-3.114168	-1.487691
H	-0.092122	-1.099604	-2.861871
H	-0.932062	-2.329312	-3.806308
H	-1.845790	-0.978246	-3.119015
H	-2.638114	-4.124351	-1.045303
H	-3.353278	-2.957436	-2.179145
H	-2.182175	-4.146485	-2.748272

Z6

Coordinates (Angstroms)

X Y Z

C	-4.286080	2.493780	-0.830263
C	-3.890970	1.161729	-0.848945
C	-2.597001	0.800376	-0.452608
C	-1.670697	1.794610	-0.096630
C	-2.094294	3.129582	-0.052028
C	-3.394113	3.474421	-0.403135
H	-5.293492	2.763053	-1.131983
H	-4.598754	0.402417	-1.166028
H	-1.407274	3.911689	0.247168
H	-3.704161	4.513832	-0.359187
P	0.085552	1.315464	0.175117
P	-2.123370	-0.948569	-0.239655
Co	0.088668	-1.045438	0.442626
C	-0.087849	-2.731700	1.208522
O	-0.178583	-3.766989	1.674813
C	4.961323	-0.125913	-0.449579
C	5.122896	1.018965	-1.460546
H	4.387580	0.936926	-2.271463
H	4.986680	1.995369	-0.978556
H	6.122109	1.005428	-1.911513
C	6.010423	0.029187	0.658881
H	5.879710	0.978319	1.193529
H	5.953519	-0.782865	1.392990
H	7.021728	0.019412	0.235241
C	5.162032	-1.463989	-1.172502
H	5.132237	-2.311194	-0.477853
H	4.389863	-1.622197	-1.936005
H	6.136499	-1.486057	-1.674339
C	3.534301	-0.024656	0.126875

H	2.833907	-0.017340	-0.714875
C	3.113290	-1.132007	1.096384
H	3.156878	-2.110040	0.600929
H	3.428902	0.945895	0.631458
C	0.894961	-1.804661	-1.145386
O	1.402096	-2.377361	-1.989833
H	3.761784	-1.160123	1.978464
C	1.689145	-0.936584	1.571902
O	1.406759	-0.737507	2.731825
C	-2.709082	-1.854692	-1.741376
C	-2.405347	-3.350052	-1.602909
C	-2.103004	-1.262383	-3.014540
H	-3.796369	-1.720904	-1.785765
H	-2.921257	-3.801252	-0.748933
H	-2.735795	-3.875147	-2.505596
H	-1.329680	-3.533465	-1.486890
H	-2.345020	-0.200755	-3.128085
H	-1.013659	-1.369705	-3.032845
H	-2.500627	-1.791202	-3.887674
C	-3.164938	-1.561239	1.178657
C	-4.678818	-1.508702	0.975723
C	-2.754543	-0.831785	2.461001
H	-2.871153	-2.614997	1.268421
H	-5.001123	-2.014170	0.060251
H	-5.166005	-2.013023	1.818129
H	-5.045261	-0.477567	0.955039
H	-1.681523	-0.928137	2.662878
H	-2.997174	0.235389	2.403714
H	-3.292115	-1.254687	3.316498
C	0.984369	2.048000	-1.299574

C	0.526098	3.448926	-1.724137
C	0.913784	1.125515	-2.517975
H	2.024259	2.111891	-0.957963
H	0.507703	4.173551	-0.909425
H	1.227901	3.821190	-2.479203
H	-0.467446	3.417553	-2.182042
H	1.454029	0.190740	-2.368792
H	-0.123864	0.893850	-2.783111
H	1.371086	1.626095	-3.378546
C	0.704613	2.207820	1.694053
C	-0.307383	2.053963	2.832626
C	1.166165	3.658625	1.544952
H	1.590878	1.621710	1.957227
H	-0.574760	1.007490	2.997444
H	0.132997	2.433301	3.761193
H	-1.222647	2.622963	2.636679
H	1.937464	3.772784	0.777624
H	0.342355	4.342730	1.321761
H	1.604462	3.976678	2.498086

Z7

Coordinates (Angstroms)

	X	Y	Z
C	0.406740	1.639256	-0.133403
C	0.936392	2.925462	-0.299313
H	2.008414	3.068210	-0.358926
C	0.102978	4.032738	-0.408025

H	0.534695	5.020979	-0.531843
C	-1.278745	3.868780	-0.372260
H	-1.935976	4.727421	-0.467749
C	-1.820607	2.598019	-0.221530
H	-2.898855	2.481570	-0.216428
C	-0.990164	1.479616	-0.083433
C	0.176313	-2.590916	-0.981049
Co	-0.018670	-1.579121	0.538681
O	0.365156	-3.264358	-1.881509
P	1.472844	0.152209	-0.014911
P	-1.716333	-0.192847	0.061895
C	1.047005	-2.494345	1.688633
O	1.723668	-3.001853	2.453273
H	-0.300593	-0.821028	1.790029
C	2.274434	-0.076036	-1.677955
C	3.364126	-1.150009	-1.558896
C	2.768622	1.170475	-2.413691
H	1.450134	-0.492020	-2.271763
H	3.026025	-2.030372	-0.998774
H	3.661122	-1.485537	-2.558307
H	4.257133	-0.759818	-1.059881
H	1.956405	1.878862	-2.600748
H	3.563057	1.692299	-1.872680
H	3.173948	0.868361	-3.386678
C	2.777256	0.481689	1.275803
C	2.104716	0.889634	2.592163
C	3.913059	1.451680	0.937155
H	3.223321	-0.513233	1.410103
H	1.352463	0.166478	2.920446
H	2.863247	0.963970	3.379049

H	1.619835	1.867927	2.498248
H	4.429149	1.194731	0.009659
H	3.563435	2.485803	0.868036
H	4.653567	1.415624	1.744900
C	-2.597442	-0.420308	-1.553802
C	-3.232204	-1.811061	-1.638294
C	-1.668092	-0.150798	-2.739911
H	-3.389459	0.338641	-1.560873
H	-3.891657	-2.029092	-0.791813
H	-3.827351	-1.888329	-2.554563
H	-2.467965	-2.595440	-1.676087
H	-1.270278	0.868426	-2.728600
H	-0.822318	-0.847206	-2.763296
H	-2.224052	-0.284720	-3.674324
C	-3.025203	-0.168700	1.392885
C	-4.409947	0.333648	0.970583
C	-2.538322	0.588586	2.632546
H	-3.114741	-1.231486	1.653060
H	-4.822014	-0.206909	0.114842
H	-5.100902	0.190625	1.808900
H	-4.404947	1.401981	0.735056
H	-1.561204	0.240230	2.983079
H	-2.467978	1.664078	2.438341
H	-3.255334	0.440043	3.447085

$A1_{M06\text{-}L}$

Coordinates (Angstroms)

X	Y	Z

C	-3.954554	0.607465	-0.000479
C	-3.066584	-0.462691	-0.000961
C	-1.686474	-0.231291	-0.000519
C	-1.200159	1.087595	0.000428
C	-2.103019	2.156582	0.000898
C	-3.472764	1.916462	0.000449
H	-5.024052	0.422505	-0.000830
H	-3.452313	-1.480265	-0.001698
H	-1.738815	3.182086	0.001627
H	-4.167641	2.750235	0.000827
P	0.609436	1.342939	0.001078
P	-0.466597	-1.590991	-0.001218
C	0.952384	2.418927	-1.445738
H	0.352121	3.331550	-1.344438
H	2.001285	2.726223	-1.363811
C	0.951716	2.415756	1.450409
H	2.000521	2.723629	1.369415
H	0.351109	3.328377	1.351176
C	0.685578	1.727962	-2.772283
H	1.297676	0.826061	-2.886013
H	-0.364627	1.435299	-2.867855
H	0.920566	2.387769	-3.609571
C	0.684935	1.721477	2.775234
H	-0.365169	1.428159	2.869895
H	1.297378	0.819530	2.886874
H	0.919524	2.379308	3.614186
C	-0.848106	-2.626326	1.458135
H	-1.908614	-2.902888	1.418710
H	-0.272015	-3.550066	1.337557

C	-0.501886	-1.931931	2.764952
H	0.563957	-1.677892	2.808506
H	-1.075592	-1.009273	2.896271
H	-0.716332	-2.577513	3.618603
C	-0.846155	-2.623055	-1.463406
H	-0.270948	-3.547459	-1.343701
H	-1.906941	-2.898899	-1.426625
C	-0.496819	-1.926099	-2.768035
H	-1.069555	-1.002721	-2.898546
H	0.569320	-1.672758	-2.808855
H	-0.709959	-2.569669	-3.623532
Co	1.569362	-0.711310	0.000031
H	1.936207	-2.182820	-0.000428
C	3.332612	-0.340159	0.000488
O	4.466665	-0.150801	0.000762

$A2_{M06\text{-}L}$

Coordinates (Angstroms)

	X	Y	Z
C	-4.429925	1.313951	-0.759618
C	-3.232882	1.767530	-0.216763
C	-2.126118	0.913631	-0.148584
C	-2.227625	-0.399162	-0.628435
C	-3.435597	-0.846462	-1.175954
C	-4.530686	0.007906	-1.240542
H	-5.287103	1.978012	-0.809882
H	-3.161262	2.789222	0.151635

H	-3.526060	-1.866124	-1.545998
H	-5.466476	-0.343402	-1.663748
P	-0.758295	-1.473361	-0.474912
P	-0.507068	1.446970	0.508470
C	-1.371462	-2.956656	0.429707
H	-1.986235	-3.539356	-0.267836
H	-0.492304	-3.573500	0.651894
C	-0.484898	-2.115628	-2.175308
H	0.274635	-2.902916	-2.098594
H	-1.408004	-2.612380	-2.498683
C	-2.152810	-2.638327	1.694146
H	-1.573938	-2.033920	2.397853
H	-3.072571	-2.091138	1.468686
H	-2.432555	-3.558178	2.211537
C	-0.071473	-1.040017	-3.164492
H	-0.853888	-0.283490	-3.280819
H	0.839852	-0.523506	-2.840128
H	0.124367	-1.467135	-4.150173
C	-0.051745	2.887270	-0.548861
H	-0.686564	3.729169	-0.245154
H	0.975404	3.161742	-0.280155
C	-0.184468	2.633896	-2.041678
H	0.404582	1.770947	-2.367164
H	-1.224774	2.446395	-2.323248
H	0.162767	3.499565	-2.609600
C	-0.891919	2.227185	2.126867
H	0.059884	2.576007	2.543099
H	-1.484183	3.126200	1.914035
C	-1.626486	1.324227	3.103409
H	-2.566505	0.955383	2.681086

H	-1.027185	0.458652	3.394404
H	-1.867740	1.870218	4.017696
Co	0.887524	-0.281435	0.498383
H	1.744295	0.828967	1.033814
C	0.784418	-0.959287	2.207360
O	0.907815	-1.387664	3.272084
C	3.894000	0.352440	-0.410114
C	4.232498	1.524817	0.508491
H	3.343026	2.119632	0.746454
H	4.667549	1.182477	1.453035
H	4.958119	2.189904	0.031627
C	5.195453	-0.382997	-0.776767
H	5.701622	-0.772017	0.111977
H	5.002432	-1.223028	-1.450578
H	5.885645	0.302768	-1.277112
C	3.224010	0.870697	-1.677699
H	3.030592	0.075155	-2.405457
H	2.271487	1.360132	-1.438688
H	3.860003	1.609764	-2.173237
C	3.037455	-0.671200	0.314934
H	3.360039	-0.869213	1.338564
C	2.271604	-1.649709	-0.309880
H	2.092927	-2.605051	0.176651
H	2.184847	-1.654647	-1.395514

$A3_{M06\text{-}L}$

Coordinates (Angstroms)		
X	Y	Z

C	4.471612	0.190130	-1.446824
C	3.388713	-0.680814	-1.405578
C	2.213354	-0.311120	-0.741341
C	2.128861	0.943401	-0.118260
C	3.225704	1.811411	-0.164019
C	4.390705	1.435669	-0.823454
H	5.381384	-0.101402	-1.962130
H	3.463400	-1.654774	-1.885918
H	3.169933	2.788414	0.312608
H	5.237712	2.113848	-0.854466
P	0.549215	1.406598	0.682095
P	0.777557	-1.430822	-0.601664
C	1.051566	2.058779	2.327693
H	1.676799	2.943714	2.153248
H	0.140574	2.420217	2.818257
C	0.055672	2.934293	-0.231335
H	-0.944729	3.209701	0.124513
H	0.726267	3.745134	0.079880
C	1.780612	1.049354	3.198099
H	1.151924	0.188727	3.441088
H	2.686094	0.676081	2.709031
H	2.081777	1.505258	4.143541
C	0.078076	2.771839	-1.742981
H	1.096604	2.617113	-2.110782
H	-0.521485	1.916637	-2.072757
H	-0.321844	3.661272	-2.234627
C	0.417911	-1.970288	-2.318700
H	1.319930	-2.450456	-2.718020
H	-0.343174	-2.756250	-2.245707

C	-0.040902	-0.836652	-3.218881
H	-0.936479	-0.346332	-2.819737
H	0.734265	-0.071177	-3.324429
H	-0.283400	-1.202957	-4.218504
C	1.447067	-2.948428	0.198576
H	0.582102	-3.569381	0.460394
H	2.007464	-3.503927	-0.563904
C	2.320837	-2.678516	1.413634
H	3.231023	-2.138186	1.138795
H	1.804002	-2.086642	2.173959
H	2.620745	-3.617749	1.882653
Co	-0.816631	-0.386755	0.504794
C	-4.044100	0.411344	-0.371672
C	-4.608909	1.528141	0.504217
H	-5.111506	1.127973	1.390657
H	-3.818858	2.208965	0.845167
H	-5.339726	2.126190	-0.047302
C	-3.340258	1.022154	-1.577882
H	-2.502357	1.658039	-1.263282
H	-2.955005	0.261419	-2.265700
H	-4.027806	1.651392	-2.150101
C	-5.169101	-0.518110	-0.826003
H	-4.789746	-1.326208	-1.459586
H	-5.681873	-0.972620	0.027612
H	-5.915239	0.036808	-1.402094
C	-3.048663	-0.416769	0.473434
H	-2.321494	0.419461	0.876653
C	-2.282707	-1.516308	-0.164790
H	-2.297748	-1.539705	-1.257839
H	-2.393478	-2.510636	0.263467

C	-0.688455	-1.183975	2.157534
O	-0.678856	-1.806561	3.129905
H	-3.513330	-0.742949	1.411406

$A4_{M06\text{-}L}$

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.602962	-1.882122	-0.377941
C	-4.075878	-0.597364	-0.312950
C	-2.694645	-0.411201	-0.183331
C	-1.844650	-1.523734	-0.115933
C	-2.383682	-2.813540	-0.186948
C	-3.756481	-2.989734	-0.319348
H	-5.674584	-2.022504	-0.477728
H	-4.743137	0.260694	-0.365643
H	-1.732586	-3.683876	-0.132895
H	-4.169879	-3.991869	-0.373979
P	-0.060114	-1.232088	0.136481
P	-1.933336	1.243842	-0.146945
C	0.272610	-2.047324	1.755983
H	0.263923	-3.130442	1.581218
H	1.296387	-1.788737	2.047817
C	0.766085	-2.292098	-1.111482
H	1.845236	-2.194338	-0.945472
H	0.513614	-3.335886	-0.887769
C	-0.715214	-1.669131	2.848294
H	-0.754097	-0.588207	3.011903

H	-1.728632	-2.004217	2.609728
H	-0.426839	-2.129147	3.795486
C	0.397450	-1.933013	-2.541932
H	-0.666014	-2.100370	-2.737934
H	0.614450	-0.882740	-2.766222
H	0.965006	-2.541630	-3.249084
C	-2.467020	2.011192	-1.731028
H	-3.562736	1.974765	-1.771058
H	-2.193909	3.072083	-1.681240
C	-1.853334	1.343249	-2.950312
H	-0.758561	1.398773	-2.933767
H	-2.131559	0.286219	-3.011748
H	-2.189264	1.826929	-3.869578
C	-2.864009	2.198309	1.115783
H	-2.471411	3.221495	1.085476
H	-3.905431	2.260775	0.774811
C	-2.784761	1.620546	2.517887
H	-3.167120	0.595703	2.554298
H	-1.758047	1.611100	2.895343
H	-3.377987	2.218348	3.212604
Co	0.340330	1.009544	-0.015212
C	0.715561	1.324642	1.766268
C	0.602368	2.670670	-0.674647
O	1.095308	1.450116	2.846573
O	0.755853	3.733200	-1.089983
C	4.601010	-0.473225	-0.101094
C	5.382077	-1.084694	1.061531
H	5.502656	-0.368941	1.881557
H	4.875825	-1.970687	1.461935
H	6.382401	-1.393530	0.742296

C	4.505630	-1.497345	-1.231901
H	4.058806	-2.436225	-0.880832
H	3.912095	-1.129666	-2.077770
H	5.498875	-1.742921	-1.620127
C	5.326302	0.777868	-0.594975
H	4.862023	1.196846	-1.493486
H	5.343149	1.559649	0.172696
H	6.364911	0.544340	-0.847936
C	3.185573	-0.117481	0.424763
H	3.309340	0.485068	1.335821
C	2.300823	0.623954	-0.552132
H	2.142800	0.073680	-1.489931
H	2.766742	1.576513	-0.816201
H	2.719984	-1.058114	0.755060

$A5_{M06\text{-}L}$

Coordinates (Angstroms)

	X	Y	Z
C	-4.530453	1.488049	-0.707211
C	-3.373283	1.817235	-0.011026
C	-2.262172	0.965600	-0.039658
C	-2.323863	-0.226528	-0.779424
C	-3.495765	-0.551292	-1.473868
C	-4.593137	0.300779	-1.437195
H	-5.386900	2.154399	-0.678851
H	-3.339278	2.740665	0.564543
H	-3.549793	-1.473000	-2.050293

H	-5.498168	0.042192	-1.977848
P	-0.841053	-1.286616	-0.846348
P	-0.751866	1.333663	0.926895
C	-1.408770	-2.981490	-0.437112
H	-2.103283	-3.291155	-1.228460
H	-0.522947	-3.619227	-0.530323
C	-0.435868	-1.393312	-2.638825
H	0.520539	-1.924587	-2.701022
H	-1.181945	-2.049490	-3.104518
C	-2.053191	-3.109931	0.932360
H	-1.351464	-2.871370	1.736161
H	-2.921487	-2.451399	1.037093
H	-2.395045	-4.133632	1.098267
C	-0.389296	-0.049551	-3.347863
H	-1.370509	0.434257	-3.354593
H	0.313359	0.643555	-2.874910
H	-0.074896	-0.174353	-4.386241
C	-0.372686	3.089152	0.501147
H	-1.218055	3.694943	0.851713
H	0.485676	3.389508	1.114205
C	-0.113553	3.340413	-0.974346
H	0.767104	2.801174	-1.335290
H	-0.966748	3.036005	-1.588755
H	0.061926	4.402885	-1.156942
C	-1.395483	1.484013	2.651920
H	-0.524641	1.590328	3.309312
H	-1.950975	2.427951	2.719704
C	-2.271800	0.320880	3.088953
H	-3.188049	0.266304	2.494092
H	-1.762503	-0.642320	2.996718

H	-2.561767	0.433979	4.135603
Co	0.737858	-0.422552	0.529335
C	0.690775	-1.187377	2.161116
C	2.042563	-1.797507	-0.015129
O	0.646698	-1.709075	3.191753
O	1.868310	-2.793635	-0.671787
C	3.736177	1.016803	-0.471385
C	3.626631	2.477676	-0.037865
H	2.637395	2.687142	0.390674
H	4.374937	2.726551	0.720910
H	3.772397	3.156681	-0.883698
C	5.112747	0.761132	-1.085543
H	5.910070	0.975818	-0.367609
H	5.231318	-0.274427	-1.419482
H	5.272759	1.402123	-1.957397
C	2.653236	0.717839	-1.502513
H	2.730803	-0.288300	-1.929110
H	1.643744	0.831561	-1.054312
H	2.679643	1.427437	-2.337295
C	3.529858	0.133719	0.770739
H	2.622065	0.495781	1.303784
C	3.404022	-1.365915	0.516407
H	3.502023	-1.913314	1.463701
H	4.190232	-1.753466	-0.142495
H	4.343901	0.321343	1.480917

$A6_{M06\text{-}L}$

Coordinates (Angstroms)

	X	Y	Z
C	-4.778767	1.189855	-1.224509
C	-3.676019	1.702896	-0.551807
C	-2.544661	0.906071	-0.337118
C	-2.524774	-0.419045	-0.805791
C	-3.644934	-0.924201	-1.476964
C	-4.764152	-0.126703	-1.684781
H	-5.651946	1.813811	-1.387198
H	-3.701481	2.727962	-0.186668
H	-3.645386	-1.950900	-1.838284
H	-5.627218	-0.529783	-2.205352
P	-1.026989	-1.431508	-0.521295
P	-1.111936	1.532555	0.607488
C	-1.626927	-2.957022	0.307214
H	-2.265869	-3.490508	-0.408494
H	-0.738880	-3.582852	0.453114
C	-0.598878	-2.066563	-2.195760
H	0.077050	-2.912103	-2.035561
H	-1.522688	-2.473737	-2.626037
C	-2.361025	-2.720761	1.615124
H	-1.717302	-2.252921	2.365175
H	-3.237697	-2.079745	1.477489
H	-2.708550	-3.666512	2.036138
C	0.026334	-1.043225	-3.128016
H	-0.559815	-0.118172	-3.179808
H	1.044109	-0.787055	-2.818041
H	0.095765	-1.439340	-4.143261
C	-0.751772	3.184773	-0.125457
H	-1.655778	3.794795	-0.004875

H	0.013922	3.652130	0.504823
C	-0.321364	3.156053	-1.581495
H	0.646617	2.661801	-1.720314
H	-1.055715	2.643620	-2.211151
H	-0.209862	4.171126	-1.968355
C	-1.821236	1.982085	2.248585
H	-0.981804	2.271760	2.891301
H	-2.425913	2.886419	2.103745
C	-2.651327	0.883608	2.891063
H	-3.523594	0.633197	2.280301
H	-2.077572	-0.034226	3.042791
H	-3.012906	1.204019	3.870246
Co	0.532757	-0.074804	0.509508
C	0.465437	-0.560924	2.218460
C	2.027148	-1.463245	0.340858
O	0.401001	-0.876427	3.329589
O	1.827072	-2.521588	-0.196171
C	4.647304	0.649200	-0.467156
C	4.874582	2.157460	-0.563309
H	3.924714	2.695977	-0.672671
H	5.375686	2.544067	0.330114
H	5.498138	2.409013	-1.426451
C	5.997392	-0.054496	-0.315779
H	6.508906	0.258972	0.600064
H	5.899435	-1.144651	-0.289022
H	6.651950	0.185780	-1.158910
C	3.967293	0.161510	-1.747636
H	3.692645	-0.899630	-1.701845
H	3.068078	0.746966	-1.978332
H	4.636506	0.276975	-2.605797

C	3.780017	0.382399	0.780113
H	2.891521	1.038396	0.753477
C	3.336853	-1.064998	0.989644
H	3.164695	-1.245869	2.059890
H	4.101287	-1.784671	0.674687
H	4.345130	0.711547	1.659820
H	1.411339	0.227651	-0.881409
H	0.808198	0.796443	-0.885212

$B2_{M06\text{-}L}$

	Coordinates (Angstroms)		
	X	Y	Z

C	-3.751710	1.592355	0.337636
C	-2.412733	1.931867	0.497169
C	-1.412059	0.992570	0.223121
C	-1.766910	-0.292395	-0.215470
C	-3.116993	-0.625621	-0.373185
C	-4.103820	0.314164	-0.096541
H	-4.523836	2.324288	0.552358
H	-2.149219	2.931108	0.838223
H	-3.401415	-1.620929	-0.708917
H	-5.149754	0.051367	-0.218778
P	-0.425717	-1.481545	-0.558500
P	0.361182	1.376690	0.425467
C	-0.789641	-2.957555	0.468015
H	-1.661219	-3.453530	0.022651
H	0.055784	-3.642650	0.338484

C	-0.692844	-2.032834	-2.285194
H	-0.041422	-2.900578	-2.437446
H	-1.726204	-2.392210	-2.366981
C	-1.034730	-2.648277	1.935832
H	-0.174876	-2.160250	2.402875
H	-1.901856	-1.994958	2.069543
H	-1.224798	-3.568705	2.491014
C	-0.404403	-0.943069	-3.303572
H	-1.050488	-0.072039	-3.154454
H	0.636875	-0.607517	-3.241403
H	-0.571226	-1.306980	-4.319085
C	0.641532	2.888409	-0.579097
H	-0.024992	3.673957	-0.201878
H	1.664023	3.221810	-0.364519
C	0.436985	2.666996	-2.068313
H	1.108195	1.894868	-2.460453
H	-0.589831	2.360096	-2.290205
H	0.634851	3.583799	-2.626801
C	0.526340	1.968799	2.156461
H	1.580052	2.232932	2.301609
H	-0.038920	2.906714	2.229657
C	0.057280	0.972346	3.202623
H	-0.993018	0.700789	3.058594
H	0.647786	0.052165	3.185301
H	0.153740	1.397245	4.203577
Co	1.527207	-0.439907	-0.261557
C	2.131157	-1.177965	1.317462
O	2.540458	-1.729603	2.240006
C	3.048006	0.382390	-0.817036
O	4.004029	0.894223	-1.196542

H	1.986564	-1.670500	-0.992616

$B3_{M06\text{-}L}$

	Coordinates (Angstroms)		
	X	Y	Z

C	-5.067356	0.106013	-0.225348
C	-4.047178	-0.824765	-0.066356
C	-2.710397	-0.409382	-0.037677
C	-2.405557	0.953300	-0.171175
C	-3.439709	1.884235	-0.329565
C	-4.763438	1.461569	-0.355588
H	-6.101591	-0.222902	-0.246905
H	-4.293009	-1.879743	0.040050
H	-3.212247	2.943012	-0.439582
H	-5.560704	2.187644	-0.479427
P	-0.653505	1.466989	-0.174552
P	-1.329356	-1.578334	0.206388
C	-0.449266	2.353539	-1.778460
H	-0.934414	3.332945	-1.682260
H	0.623521	2.552258	-1.895491
C	-0.580356	2.831223	1.057873
H	0.432947	3.247670	1.022827
H	-1.246240	3.622644	0.690666
C	-0.998739	1.600557	-2.979179
H	-0.560233	0.603853	-3.081091
H	-2.083129	1.476723	-2.910610
H	-0.783430	2.143701	-3.901532

C	-0.959356	2.425353	2.470891
H	-1.961180	1.985902	2.509146
H	-0.257100	1.701638	2.892395
H	-0.956913	3.295143	3.131015
C	-1.721290	-2.406442	1.807012
H	-2.525010	-3.130032	1.621869
H	-0.836896	-2.993432	2.081494
C	-2.114124	-1.452158	2.924012
H	-1.351684	-0.691058	3.111445
H	-3.048413	-0.931855	2.694517
H	-2.259387	-1.998751	3.858028
C	-1.623357	-2.907719	-1.031518
H	-0.803590	-3.626984	-0.921441
H	-2.536827	-3.437512	-0.732538
C	-1.736860	-2.417655	-2.465383
H	-2.557930	-1.703656	-2.582423
H	-0.820421	-1.933438	-2.811320
H	-1.930204	-3.254654	-3.139476
Co	0.630742	-0.377484	0.122146
H	1.401293	-1.652297	0.294054
C	1.170840	-0.665262	-1.577044
C	0.992353	-0.358417	1.889308
O	1.590088	-0.924943	-2.619303
O	1.277467	-0.474910	3.000964
C	4.763660	-0.069065	-0.072850
C	4.566513	-1.386884	-0.832294
H	3.628427	-1.875735	-0.546135
H	4.551500	-1.231106	-1.916184
H	5.383169	-2.079422	-0.607337
C	6.121645	0.532779	-0.471246

H	6.174617	0.727772	-1.546930
H	6.310368	1.473743	0.053348
H	6.927417	-0.163633	-0.219499
C	4.733195	-0.329544	1.428459
H	4.895220	0.585745	2.006623
H	3.777221	-0.765789	1.739139
H	5.520603	-1.035167	1.707119
C	3.705085	0.907516	-0.504429
H	3.641438	1.055641	-1.586810
C	2.891896	1.633094	0.278668
H	2.227921	2.380284	-0.148976
H	2.928084	1.580608	1.364783

$B6_{M06\text{-}L}$

Coordinates (Angstroms)

	X	Y	Z
C	-4.731427	-2.041423	0.440310
C	-4.184704	-0.782395	0.658461
C	-2.845249	-0.531864	0.337721
C	-2.052664	-1.553930	-0.202268
C	-2.614094	-2.817973	-0.419983
C	-3.945189	-3.059130	-0.100135
H	-5.770399	-2.231373	0.690336
H	-4.802609	0.005966	1.084044
H	-2.014931	-3.618713	-0.848874
H	-4.372714	-4.041564	-0.273817
P	-0.317564	-1.187120	-0.656828

P	-2.075577	1.091208	0.628263
C	0.623773	-2.556239	0.134072
H	0.137175	-3.486643	-0.184768
H	1.624122	-2.567956	-0.311935
C	-0.253221	-1.612919	-2.443890
H	0.780176	-1.465722	-2.774003
H	-0.464359	-2.687105	-2.524176
C	0.691591	-2.478233	1.648962
H	1.256704	-1.604172	1.988820
H	-0.307032	-2.427168	2.095309
H	1.188338	-3.361038	2.057431
C	-1.215654	-0.796154	-3.289440
H	-2.254089	-0.955040	-2.981360
H	-0.991112	0.271850	-3.221592
H	-1.135886	-1.080586	-4.340509
C	-3.176276	2.300091	-0.209009
H	-4.190540	2.165652	0.186853
H	-2.852346	3.297991	0.110522
C	-3.157369	2.174562	-1.723216
H	-2.149802	2.317464	-2.130006
H	-3.508518	1.190279	-2.048084
H	-3.803838	2.924612	-2.182922
C	-2.349195	1.421086	2.418373
H	-1.817757	2.351008	2.653193
H	-3.416751	1.634166	2.557112
C	-1.904023	0.287251	3.327671
H	-2.481174	-0.623245	3.141585
H	-0.846066	0.042162	3.195638
H	-2.044559	0.560105	4.375390
Co	0.089389	1.043653	-0.163022

C	0.079750	2.854993	-0.408053
O	0.013477	3.999919	-0.507632
C	4.819042	-0.614186	0.322943
C	4.973829	-2.097648	0.662164
H	4.181386	-2.434556	1.341997
H	4.934213	-2.720806	-0.238282
H	5.931578	-2.289941	1.154608
C	5.924787	-0.190881	-0.642477
H	5.851911	-0.724694	-1.596518
H	5.896482	0.883155	-0.853915
H	6.909540	-0.408132	-0.218464
C	4.903510	0.203801	1.610747
H	4.785349	1.278245	1.431703
H	4.136625	-0.104684	2.330411
H	5.877587	0.066983	2.089445
C	3.434418	-0.444778	-0.328913
H	2.673590	-0.741457	0.408032
C	3.101183	0.954477	-0.844378
H	3.202265	1.691477	-0.038291
H	3.348121	-1.151233	-1.168803
C	0.969740	1.004293	1.450471
O	1.558517	1.056185	2.440929
H	3.765106	1.241788	-1.666811
C	1.685293	0.987098	-1.357243
O	1.373100	0.994343	-2.522870

$B7_{M06\text{-}L}$

Coordinates (Angstroms)

	X	Y	Z
C	-0.155910	1.745402	-0.188986
C	-0.476926	3.104200	-0.284562
H	-1.516438	3.418225	-0.328724
C	0.526341	4.067579	-0.319227
H	0.263257	5.117480	-0.399554
C	1.862751	3.686152	-0.235278
H	2.645966	4.437385	-0.242010
C	2.198078	2.338959	-0.148002
H	3.243859	2.054206	-0.076195
C	1.198709	1.358769	-0.150622
C	-0.486333	-2.175811	1.298157
Co	-0.329378	-1.506009	-0.378171
O	-0.588883	-2.524762	2.390838
P	-1.429189	0.451429	0.003610
P	1.597928	-0.417110	-0.099796
C	-2.803506	0.904475	-1.124019
H	-2.973917	1.985528	-1.058295
H	-2.450413	0.709015	-2.142428
C	-4.088920	0.144482	-0.828871
H	-4.848660	0.378943	-1.576747
H	-3.944665	-0.939488	-0.844353
H	-4.502297	0.409080	0.148515
C	-2.105321	0.689718	1.700090
H	-2.822792	-0.127216	1.848089
H	-1.278887	0.485903	2.391917
C	-2.741466	2.037681	1.995247
H	-3.170009	2.041251	2.999983
H	-2.010116	2.848634	1.950554

H	-3.551454	2.273305	1.297760
C	2.810470	-0.814721	-1.423340
H	2.337119	-0.513037	-2.363440
H	2.834543	-1.911488	-1.449474
C	4.218069	-0.252858	-1.301252
H	4.861156	-0.705186	-2.059426
H	4.245057	0.826238	-1.465231
H	4.673293	-0.463172	-0.328943
C	2.499102	-0.667819	1.479991
H	3.306399	0.073343	1.530666
H	1.799237	-0.412853	2.284631
C	3.036998	-2.080941	1.643416
H	3.507291	-2.201747	2.621091
H	2.243721	-2.831701	1.569783
H	3.789707	-2.321505	0.887183
C	-1.585219	-2.409643	-1.313821
O	-2.378835	-2.925243	-1.966135
H	-0.018605	-0.937385	-1.733114

$C3_{M06\text{-}L}$

Coordinates (Angstroms)

	X	Y	Z
C	-4.451426	1.357677	-0.583074
C	-3.156854	1.823648	-0.382837
C	-2.100041	0.919708	-0.223281
C	-2.351370	-0.460816	-0.265438
C	-3.658983	-0.918772	-0.463313

C	-4.702842	-0.014081	-0.621043
H	-5.267194	2.062947	-0.707197
H	-2.971227	2.895463	-0.345752
H	-3.864587	-1.987086	-0.498370
H	-5.714408	-0.376324	-0.775291
P	-0.932426	-1.600486	-0.099150
P	-0.387526	1.469262	0.095313
C	-1.467926	-2.827239	1.161784
H	-2.361870	-3.335073	0.777710
H	-0.681828	-3.589563	1.213234
C	-0.983645	-2.574117	-1.665444
H	-0.168519	-3.306119	-1.613891
H	-1.916400	-3.151936	-1.676752
C	-1.733845	-2.222412	2.529709
H	-0.837877	-1.754464	2.947785
H	-2.520987	-1.462980	2.487453
H	-2.056444	-2.991298	3.234677
C	-0.868294	-1.711348	-2.911219
H	-1.708775	-1.015490	-2.994286
H	0.051673	-1.115380	-2.912087
H	-0.857620	-2.326711	-3.813217
C	-0.047323	2.732012	-1.193896
H	-0.772483	3.546865	-1.078508
H	0.935420	3.161786	-0.963890
C	-0.082472	2.163858	-2.603586
H	0.642429	1.350623	-2.729803
H	-1.071344	1.765549	-2.850623
H	0.158724	2.932741	-3.340280
C	-0.507222	2.428006	1.663364
H	0.518575	2.653599	1.977249

H	-0.980780	3.389941	1.429448
C	-1.265872	1.705295	2.765473
H	-2.312463	1.542768	2.492336
H	-0.827206	0.729975	2.994457
H	-1.250024	2.292380	3.685884
Co	0.955633	-0.316892	0.154467
C	3.574136	-0.338180	-0.604112
C	2.719293	-1.493386	-1.145499
H	2.055488	-1.933387	-0.365362
H	2.119299	-1.189096	-2.014745
H	3.322816	-2.351105	-1.462443
C	4.514776	0.147648	-1.710292
H	3.958289	0.465275	-2.598881
H	5.121041	0.993800	-1.373472
H	5.202632	-0.649562	-2.013210
C	4.397895	-0.826216	0.584426
H	5.041054	-0.033896	0.977144
H	3.771825	-1.183910	1.408578
H	5.048413	-1.653774	0.285613
C	2.590540	0.786341	-0.230874
H	2.237445	1.242602	-1.172363
C	3.101106	1.852525	0.700668
H	4.040361	2.289225	0.333078
H	3.303796	1.470059	1.706265
C	1.362426	-0.515258	1.900215
O	1.615296	-0.453365	3.027886
H	2.395239	2.683548	0.802972

$C4_{M06\text{-}L}$

	Coordinates (Angstroms)		
	X	Y	Z
C	-4.818889	0.472443	-0.301106
C	-3.680560	1.242898	-0.095048
C	-2.415633	0.643519	-0.053531
C	-2.301176	-0.747199	-0.222416
C	-3.457186	-1.513699	-0.416670
C	-4.707818	-0.908992	-0.456211
H	-5.794492	0.947079	-0.334063
H	-3.781778	2.317088	0.045632
H	-3.378869	-2.591654	-0.546407
H	-5.596724	-1.512598	-0.610139
P	-0.639966	-1.512164	-0.204086
P	-0.920604	1.608610	0.362760
C	-0.805817	-2.897299	1.002624
H	-1.581986	-3.560513	0.598745
H	0.128021	-3.469727	0.959960
C	-0.505912	-2.437823	-1.806661
H	0.563723	-2.468272	-2.048396
H	-0.801440	-3.476778	-1.618004
C	-1.137357	-2.494116	2.426570
H	-0.334422	-1.914742	2.887975
H	-2.056625	-1.901996	2.473616
H	-1.288453	-3.381054	3.045709
C	-1.303571	-1.865426	-2.970219
H	-2.376972	-2.011982	-2.832128
H	-1.139618	-0.794015	-3.109858
H	-1.017972	-2.361203	-3.900449

C	-1.047043	3.177078	-0.590847
H	-2.029242	3.605622	-0.354201
H	-0.311554	3.862014	-0.152393
C	-0.853781	3.058217	-2.091093
H	0.186190	2.849308	-2.350675
H	-1.478379	2.270376	-2.525706
H	-1.123330	3.994717	-2.583741
C	-1.269558	2.214143	2.073150
H	-0.340282	2.659269	2.448090
H	-1.987075	3.038956	1.977132
C	-1.799484	1.162503	3.032418
H	-2.765573	0.769847	2.701682
H	-1.116672	0.316540	3.141079
H	-1.939731	1.592938	4.026155
Co	0.887284	0.232027	0.031757
C	1.240403	0.051474	1.788782
C	0.982026	0.409761	-1.757817
O	1.422831	-0.080723	2.920568
O	1.067498	0.407441	-2.908473
C	3.944923	0.258659	-0.138933
C	3.727359	1.486441	-1.025140
H	3.599931	1.211093	-2.077800
H	2.843428	2.061813	-0.712212
H	4.584773	2.163743	-0.964682
C	4.153997	0.726791	1.299987
H	3.356788	1.402094	1.630333
H	4.215123	-0.104250	2.009774
H	5.090112	1.287447	1.379409
C	5.229485	-0.446102	-0.614097
H	5.516798	-1.263983	0.052308

H	5.116117	-0.853500	-1.624284
H	6.061319	0.264568	-0.634537
C	2.783811	-0.744173	-0.306759
H	2.756720	-1.020591	-1.369109
C	2.878549	-2.030269	0.487025
H	2.037902	-2.696756	0.270766
H	2.909237	-1.882481	1.570783
H	3.783650	-2.586529	0.211292

$C5_{M06\text{-}L}$

Coordinates (Angstroms)

	X	Y	Z
C	-4.666337	-0.625728	1.292501
C	-3.438170	-1.271004	1.206391
C	-2.334434	-0.618285	0.643933
C	-2.475445	0.693178	0.163212
C	-3.716891	1.334281	0.254260
C	-4.805604	0.678604	0.817226
H	-5.517512	-1.138260	1.729680
H	-3.338885	-2.288834	1.578970
H	-3.836036	2.349952	-0.119045
H	-5.765107	1.181748	0.884490
P	-1.025829	1.507882	-0.594366
P	-0.696554	-1.416127	0.525197
C	-1.633792	2.007207	-2.262160
H	-2.357896	2.820292	-2.124696
H	-0.781031	2.441516	-2.796894

C	-0.912727	3.119451	0.298646
H	-0.052686	3.657784	-0.117423
H	-1.797649	3.710970	0.031755
C	-2.254450	0.868158	-3.055207
H	-1.560959	0.034647	-3.194808
H	-3.147404	0.476971	-2.559014
H	-2.551164	1.211864	-4.048229
C	-0.801720	2.982091	1.808154
H	-1.686315	2.495354	2.229367
H	0.070424	2.392080	2.108812
H	-0.708081	3.962670	2.279787
C	-0.293350	-1.889992	2.253902
H	-1.058216	-2.596965	2.598673
H	0.648534	-2.447571	2.204097
C	-0.193622	-0.699255	3.192228
H	0.560289	0.021912	2.852859
H	-1.146399	-0.166241	3.271443
H	0.094057	-1.015544	4.197180
C	-0.991759	-3.020855	-0.310694
H	-0.014401	-3.511985	-0.362304
H	-1.614425	-3.626311	0.360426
C	-1.632269	-2.894517	-1.682565
H	-2.597818	-2.380736	-1.635910
H	-0.993519	-2.346250	-2.380297
H	-1.805724	-3.882361	-2.114299
Co	0.753684	0.019860	-0.451057
C	0.891886	-0.405113	-2.191992
C	2.261210	-1.241169	-0.088387
O	0.958778	-0.716985	-3.303907
O	2.162047	-2.421801	0.139535

C	3.673962	0.680793	0.798166
C	3.650929	0.189006	2.246126
H	2.808001	-0.491675	2.423507
H	4.566519	-0.356837	2.490664
H	3.561987	1.022570	2.950403
C	4.928139	1.519778	0.557126
H	5.832032	0.907796	0.632684
H	4.925918	1.995387	-0.427861
H	5.005475	2.312922	1.306812
C	2.429289	1.535581	0.546841
H	2.213999	1.659308	-0.532186
H	1.552785	1.111562	1.081827
H	2.509366	2.552577	0.944704
C	3.640652	-0.544615	-0.142876
C	3.988875	-0.243322	-1.597821
H	5.047503	0.009486	-1.688135
H	3.415254	0.596938	-2.005340
H	4.347673	-1.294775	0.235793
H	3.804856	-1.109850	-2.238492

$C6_{M06\text{-}L}$

Coordinates (Angstroms)			
	X	Y	Z

C	-4.541256	1.931216	-0.726903
C	-3.245530	2.172188	-0.285289
C	-2.320141	1.125477	-0.193259
C	-2.712478	-0.175320	-0.550325

C	-4.020744	-0.409180	-0.991834
C	-4.929179	0.638998	-1.081297
H	-5.251298	2.749472	-0.795229
H	-2.951650	3.183567	-0.010549
H	-4.336054	-1.415198	-1.262666
H	-5.941262	0.449825	-1.425086
P	-1.510853	-1.543145	-0.380163
P	-0.602107	1.392064	0.368655
C	-2.333291	-2.709974	0.787238
H	-3.161147	-3.183385	0.244154
H	-1.612532	-3.506654	1.005077
C	-1.630327	-2.447816	-1.982240
H	-1.013728	-3.349232	-1.888073
H	-2.665581	-2.798212	-2.079307
C	-2.838089	-2.061326	2.065536
H	-2.039192	-1.567870	2.624919
H	-3.607796	-1.312853	1.856310
H	-3.277071	-2.812844	2.724944
C	-1.230921	-1.632356	-3.199356
H	-1.820395	-0.713790	-3.281783
H	-0.172406	-1.351048	-3.183712
H	-1.387169	-2.206902	-4.114775
C	0.023370	2.736838	-0.723306
H	-0.562073	3.638816	-0.503657
H	1.046134	2.945340	-0.388029
C	-0.025795	2.421701	-2.209138
H	0.599869	1.563095	-2.473706
H	-1.046028	2.205051	-2.541805
H	0.336472	3.270064	-2.793880
C	-0.755310	2.244327	1.987729

H	0.270352	2.450110	2.312534
H	-1.227761	3.217626	1.802554
C	-1.525778	1.462901	3.037727
H	-2.543931	1.233585	2.707048
H	-1.032678	0.519829	3.288480
H	-1.602980	2.038872	3.962289
Co	0.518441	-0.616657	0.227683
C	0.547886	-1.228451	1.906362
C	2.306795	0.244264	0.724617
O	0.551396	-1.618149	2.994979
O	2.333714	1.339017	1.225376
C	4.518456	0.201632	-0.540218
C	5.141563	1.389874	0.191499
H	4.397950	2.118554	0.518237
H	5.698471	1.059645	1.074557
H	5.847575	1.902738	-0.468982
C	5.646274	-0.733438	-0.985070
H	6.163920	-1.176930	-0.127905
H	5.292181	-1.544632	-1.627497
H	6.386915	-0.166606	-1.556819
C	3.766765	0.702236	-1.776881
H	3.291863	-0.114980	-2.335325
H	2.999053	1.442017	-1.515548
H	4.458216	1.193535	-2.467602
C	3.554715	-0.586923	0.416084
C	3.214506	-1.989943	-0.067057
H	4.090516	-2.639748	-0.040776
H	2.843076	-1.996848	-1.099106
H	4.064637	-0.664904	1.389449
H	2.457427	-2.464519	0.566955

H	1.310013	-0.202865	-1.207325
H	0.644760	-0.624260	-1.453762

TSA2-3$_{M06-L}$

	Coordinates (Angstroms)		
	X	Y	Z

C	4.764139	-0.092434	-0.729583
C	3.671645	-0.950530	-0.668930
C	2.398087	-0.448105	-0.378848
C	2.229819	0.925095	-0.148370
C	3.333989	1.782434	-0.213197
C	4.595237	1.273937	-0.503320
H	5.750177	-0.487240	-0.953414
H	3.814074	-2.015290	-0.844678
H	3.212553	2.848734	-0.031874
H	5.449734	1.941573	-0.551518
P	0.548635	1.511632	0.259510
P	0.915153	-1.515079	-0.299738
C	0.731356	2.386722	1.864529
H	1.307488	3.300870	1.672333
H	-0.274226	2.709955	2.157811
C	0.213207	2.874454	-0.923982
H	-0.675292	3.395530	-0.547704
H	1.044107	3.588454	-0.865282
C	1.385444	1.557141	2.956563
H	0.811352	0.655286	3.185175
H	2.396496	1.247515	2.675029

H	1.461973	2.134445	3.880092
C	0.001242	2.396128	-2.349482
H	0.885247	1.878831	-2.735608
H	-0.846300	1.704384	-2.414546
H	-0.207177	3.234929	-3.016633
C	0.895471	-2.340568	-1.943737
H	1.871828	-2.818278	-2.091248
H	0.163350	-3.154950	-1.888563
C	0.580757	-1.384063	-3.081589
H	-0.386131	-0.886361	-2.938802
H	1.342513	-0.602421	-3.164551
H	0.541954	-1.909277	-4.038074
C	1.372522	-2.877686	0.847596
H	0.475946	-3.497972	0.966095
H	2.115516	-3.504793	0.338674
C	1.896760	-2.406279	2.194109
H	2.812267	-1.817532	2.083996
H	1.167113	-1.790674	2.726542
H	2.127802	-3.260202	2.834028
Co	-0.855034	-0.194528	0.147325
C	-4.061899	0.223440	-0.279367
C	-4.144486	1.738502	-0.456979
H	-3.402464	2.254898	0.164307
H	-3.976515	2.031599	-1.499735
H	-5.130214	2.110353	-0.164011
C	-5.164781	-0.441106	-1.121823
H	-5.045830	-0.223513	-2.188146
H	-5.159692	-1.527841	-0.996112
H	-6.146545	-0.068737	-0.815404
C	-4.254589	-0.134230	1.189628

H	-4.135265	-1.205911	1.380981
H	-3.548990	0.409811	1.825420
H	-5.262844	0.138677	1.513288
C	-2.752994	-0.301817	-0.852037
H	-2.502319	0.158599	-1.814682
C	-2.213332	-1.575523	-0.638154
H	-1.726528	-2.092085	-1.460169
H	-2.625058	-2.222069	0.134376
C	-1.130197	-0.638060	1.908476
O	-1.360955	-0.969725	2.989979
H	-1.767750	0.997754	0.159389

TSA4-5$_{M06-L}$

	Coordinates (Angstroms)		
	X	Y	Z

C	1.856521	1.377669	-0.661820
C	2.493567	2.465966	-1.270866
H	2.072610	3.464223	-1.184619
C	3.674154	2.285029	-1.983957
H	4.157612	3.136724	-2.451894
C	4.242845	1.017359	-2.082007
H	5.176340	0.878656	-2.618138
C	3.609086	-0.076392	-1.501610
H	4.058054	-1.062132	-1.589700
C	2.402270	0.087117	-0.810275
C	0.287302	-0.603942	2.627020
C	-1.277495	-2.008643	0.793782

Co	-0.361519	-0.524664	0.959153
O	0.767942	-0.710573	3.670779
O	-1.710030	-3.093609	0.882653
P	0.399863	1.584246	0.423238
P	1.464691	-1.326779	-0.139813
H	-3.733874	-1.109921	0.746365
C	-0.712205	2.761665	-0.448454
H	-0.106822	3.562789	-0.888350
H	-1.159038	2.221698	-1.292764
C	-1.789853	3.338278	0.458789
H	-2.480197	3.962501	-0.113217
H	-2.382827	2.554284	0.942697
H	-1.365440	3.963878	1.249170
C	1.009823	2.529240	1.883851
H	0.149600	2.596436	2.561910
H	1.731014	1.876830	2.389697
C	1.610251	3.900493	1.626290
H	1.835603	4.396405	2.573156
H	2.545565	3.834027	1.065438
H	0.929652	4.555842	1.073183
C	0.994775	-2.375459	-1.581480
H	0.325379	-1.762518	-2.196753
H	0.366344	-3.171026	-1.160791
C	2.113738	-2.963893	-2.424286
H	1.699661	-3.638023	-3.177657
H	2.672756	-2.190380	-2.955863
H	2.820105	-3.547056	-1.825670
C	2.667989	-2.328963	0.814432
H	3.537845	-2.540567	0.180644
H	3.030103	-1.691342	1.629039

C	2.055454	-3.612582	1.355841
H	2.784633	-4.161932	1.954287
H	1.190378	-3.411487	1.995087
H	1.724438	-4.278911	0.553633
C	-1.992379	-0.827050	-0.481253
C	-3.307177	-0.336172	0.094596
H	-1.451330	-0.051762	-1.033950
H	-2.098863	-1.665434	-1.172478
H	-3.117327	0.529911	0.746680
C	-4.376935	0.055008	-0.951054
C	-3.857553	1.153553	-1.877570
H	-4.634095	1.462366	-2.583734
H	-3.560206	2.044833	-1.311961
H	-2.999225	0.821160	-2.473963
C	-4.778605	-1.168803	-1.773979
H	-3.952729	-1.545663	-2.387303
H	-5.123196	-1.987075	-1.132932
H	-5.594728	-0.920282	-2.458834
C	-5.591511	0.576053	-0.183567
H	-5.337090	1.459727	0.413058
H	-6.394334	0.860581	-0.870386
H	-5.991321	-0.183173	0.496409

TSA6-$1_{M06\text{-}L}$

Coordinates (Angstroms)			
	X	Y	Z

C	4.683492	2.042255	-0.608314

C	4.284841	0.745097	-0.305322
C	2.926906	0.445703	-0.147650
C	1.968728	1.460757	-0.291229
C	2.379740	2.762858	-0.597398
C	3.730583	3.049888	-0.758700
H	5.737779	2.269214	-0.731202
H	5.034212	-0.037242	-0.200980
H	1.645318	3.558634	-0.705794
H	4.043354	4.061265	-0.998314
P	0.220097	1.049082	0.035324
P	2.335139	-1.250880	0.170432
C	-0.200932	2.124797	1.467820
H	-0.056884	3.162257	1.139472
H	-1.271421	1.998570	1.662863
C	-0.749294	1.811607	-1.325939
H	-1.806951	1.697673	-1.052613
H	-0.548509	2.890308	-1.298680
C	0.615643	1.823591	2.712165
H	0.455241	0.797163	3.053564
H	1.686071	1.967660	2.532289
H	0.326760	2.487947	3.529039
C	-0.474202	1.243836	-2.706821
H	0.583083	1.332192	-2.976512
H	-0.751028	0.188607	-2.778351
H	-1.052379	1.779861	-3.462567
C	3.029103	-2.239345	-1.217396
H	4.101854	-2.366244	-1.024001
H	2.582096	-3.237380	-1.144363
C	2.800141	-1.629960	-2.591470
H	1.739454	-1.464965	-2.800585

H	3.310424	-0.668001	-2.693183
H	3.183510	-2.292678	-3.369766
C	3.249958	-1.848679	1.642245
H	3.102347	-2.934560	1.670256
H	4.320505	-1.682048	1.469118
C	2.791089	-1.200716	2.936728
H	2.961233	-0.119885	2.927318
H	1.722083	-1.370523	3.110463
H	3.332443	-1.612543	3.790680
Co	0.111361	-1.203573	0.392383
C	-0.378657	-1.901328	-1.251878
O	-0.692035	-2.446346	-2.218381
C	-5.202226	0.282054	-0.194268
C	-6.284797	1.129781	0.473907
H	-6.696429	0.626902	1.354903
H	-5.890300	2.099216	0.797249
H	-7.112660	1.322077	-0.215305
C	-4.688034	1.020697	-1.432038
H	-4.265481	1.997181	-1.164365
H	-3.922163	0.452471	-1.975247
H	-5.501895	1.203505	-2.140164
C	-5.795026	-1.065654	-0.606283
H	-5.078728	-1.680385	-1.163048
H	-6.126939	-1.639724	0.265774
H	-6.664342	-0.923660	-1.255131
C	-4.066738	0.085829	0.826636
H	-4.477775	-0.304972	1.765222
C	-2.944359	-0.828889	0.360670
H	-3.276683	-1.874728	0.270609
H	-3.644219	1.069410	1.079607

H	-2.591928	-0.570978	-0.647368
C	-1.755341	-0.841646	1.279795
O	-1.730445	-0.413165	2.407574
H	-0.903093	-2.042914	1.171439
H	0.292887	-2.574342	1.021875

TSB3-4$_{M06-L}$

Coordinates (Angstroms)			
	X	Y	Z

C	-1.951790	-1.184900	-0.650877
C	-2.772635	-2.133348	-1.272853
H	-2.587063	-3.194035	-1.125367
C	-3.827882	-1.734967	-2.087031
H	-4.453241	-2.482120	-2.565531
C	-4.078023	-0.380360	-2.287503
H	-4.898721	-0.064525	-2.923731
C	-3.270202	0.573852	-1.677628
H	-3.472976	1.626241	-1.851138
C	-2.200927	0.187303	-0.861741
C	0.655179	0.358385	2.338303
C	1.770837	2.138433	0.619258
Co	0.848851	0.399073	0.553686
O	0.543664	0.225639	3.479755
O	2.020907	3.190279	1.018309
P	-0.555268	-1.634766	0.433271
P	-1.099366	1.413076	-0.066170
H	2.078211	-0.428853	0.864797

C	0.062498	-3.245594	-0.209959
H	-0.765052	-3.961275	-0.276618
H	0.400534	-3.077953	-1.239570
C	1.180079	-3.804200	0.660475
H	1.618173	-4.696620	0.208577
H	1.985599	-3.075670	0.810331
H	0.814072	-4.088842	1.651244
C	-1.344642	-2.087904	2.040251
H	-0.524303	-2.304228	2.735743
H	-1.811148	-1.170650	2.420017
C	-2.347357	-3.227671	2.004817
H	-2.770659	-3.393279	2.998270
H	-3.178895	-3.015639	1.326531
H	-1.887638	-4.169685	1.691555
C	-0.924180	2.802879	-1.276902
H	-0.832751	2.329119	-2.261420
H	0.052620	3.258313	-1.076871
C	-1.993520	3.887151	-1.288179
H	-1.751960	4.633019	-2.048896
H	-2.992228	3.508886	-1.517487
H	-2.056964	4.412085	-0.332168
C	-2.089001	2.111857	1.318258
H	-3.015217	2.519405	0.894622
H	-2.387578	1.268361	1.952126
C	-1.342684	3.160107	2.130308
H	-1.989746	3.573451	2.906711
H	-0.464422	2.741037	2.628788
H	-0.996199	3.995258	1.514206
C	1.267080	0.200118	-1.618326
C	2.261570	-0.601242	-1.092722

H	0.351600	-0.248015	-1.999238
H	1.509336	1.186497	-2.008982
H	2.014844	-1.654864	-0.954467
C	3.757932	-0.362249	-1.142260
C	4.165812	-0.863131	-2.543008
H	5.254101	-0.820758	-2.645907
H	3.857961	-1.900396	-2.710160
H	3.724046	-0.246522	-3.331258
C	4.174811	1.095975	-0.990507
H	3.599195	1.771754	-1.632291
H	4.081170	1.433952	0.044806
H	5.226324	1.209073	-1.269391
C	4.463789	-1.214876	-0.089100
H	4.213669	-2.275980	-0.200482
H	5.549376	-1.122192	-0.181873
H	4.189438	-0.905016	0.925521

TSB6-7$_{M06\text{-}L}$

Coordinates (Angstroms)		
X	Y	Z

C	3.029087	0.588997	0.075243
C	4.286996	1.198502	0.178103
H	4.382466	2.274847	0.065651
C	5.424971	0.438202	0.421314
H	6.392432	0.923803	0.500992
C	5.318092	-0.941947	0.571058
H	6.200929	-1.538478	0.778509

C	4.079808	-1.561007	0.442985
H	4.014600	-2.639968	0.552073
C	2.925662	-0.812327	0.173951
C	-0.624120	-0.020864	1.442105
C	-1.937392	-1.275828	-1.032100
Co	-0.287214	0.211143	-0.308127
O	-0.756045	-0.220703	2.572643
O	-1.678862	-2.439958	-0.921141
P	1.521252	1.586498	-0.163849
P	1.304380	-1.618031	-0.087863
H	-3.919704	-1.480150	0.758083
C	1.934907	2.641005	-1.612318
H	2.860647	3.180208	-1.376573
H	2.182964	1.955116	-2.429842
C	0.837927	3.607595	-2.025860
H	1.179875	4.242792	-2.845598
H	-0.053769	3.079814	-2.375814
H	0.534185	4.267262	-1.207132
C	1.394339	2.747121	1.262923
H	0.426333	3.246799	1.131441
H	1.278090	2.115611	2.151431
C	2.496490	3.772779	1.469423
H	2.219385	4.457251	2.274607
H	3.441450	3.306499	1.756477
H	2.671053	4.382967	0.578014
C	1.484524	-2.661292	-1.598667
H	1.611165	-1.960546	-2.432545
H	0.497491	-3.116760	-1.734227
C	2.576259	-3.717708	-1.611514
H	2.501932	-4.318218	-2.521468

H	3.575319	-3.275754	-1.596312
H	2.493946	-4.408287	-0.766435
C	1.218616	-2.792092	1.328741
H	2.115112	-3.423249	1.297723
H	1.315251	-2.180506	2.233248
C	-0.036693	-3.646732	1.386232
H	0.011424	-4.324323	2.241524
H	-0.938421	-3.038578	1.496236
H	-0.163946	-4.254387	0.486614
C	-3.302267	-0.669357	-1.133396
C	-3.913382	-0.499739	0.262284
H	-3.249390	0.291140	-1.656761
H	-3.907063	-1.363687	-1.727918
H	-3.265428	0.149480	0.869741
C	-5.338584	0.088966	0.271734
C	-5.332593	1.518039	-0.269773
H	-6.338744	1.945795	-0.231919
H	-4.678239	2.168123	0.321172
H	-5.007316	1.567602	-1.315217
C	-6.285470	-0.779082	-0.556043
H	-6.047070	-0.750542	-1.624736
H	-6.260848	-1.824894	-0.230594
H	-7.315955	-0.427138	-0.451836
C	-5.806966	0.104462	1.727563
H	-5.140058	0.704200	2.356481
H	-6.810137	0.533842	1.806502
H	-5.845332	-0.906482	2.146438
C	-1.470989	1.759404	-0.463944
O	-1.873578	2.791764	-0.137472
H	-0.040870	0.113362	-1.867431

H	-0.840921	-0.473831	-1.687985

TSC2-3$_{M06\text{-}L}$

	Coordinates (Angstroms)		
	X	Y	Z

C	4.672001	0.901287	-0.079422
C	3.848569	-0.209085	-0.224819
C	2.458534	-0.069134	-0.137026
C	1.895151	1.192068	0.100958
C	2.733854	2.303834	0.244116
C	4.113523	2.158413	0.153288
H	5.749537	0.789436	-0.147235
H	4.290685	-1.187614	-0.402999
H	2.311358	3.290304	0.425765
H	4.756758	3.025708	0.264477
P	0.069827	1.329492	0.214992
P	1.321717	-1.483543	-0.316665
C	-0.159414	2.198683	1.821519
H	0.420931	3.127875	1.755683
H	-1.209663	2.496859	1.891544
C	-0.318107	2.639787	-1.019608
H	-1.386705	2.869144	-0.922072
H	0.217581	3.551337	-0.727260
C	0.265189	1.384677	3.031073
H	-0.350826	0.490118	3.156696
H	1.310466	1.067236	2.957354
H	0.166337	1.975650	3.943972

C	0.035280	2.236007	-2.441851
H	1.111558	2.071051	-2.551708
H	-0.468835	1.309224	-2.741527
H	-0.254689	3.011357	-3.153899
C	1.802739	-2.252653	-1.913708
H	2.869291	-2.504342	-1.860185
H	1.260627	-3.202833	-1.981444
C	1.512913	-1.365874	-3.112537
H	0.448429	-1.115542	-3.177999
H	2.071383	-0.425923	-3.060217
H	1.790623	-1.863557	-4.043764
C	1.874605	-2.705601	0.941226
H	1.128946	-3.508956	0.945468
H	2.809547	-3.152282	0.580188
C	2.060291	-2.119243	2.331728
H	2.854461	-1.367139	2.345102
H	1.148081	-1.645860	2.705007
H	2.333267	-2.902314	3.041860
Co	-0.774385	-0.735683	-0.221391
C	-3.832048	0.275683	-0.124668
C	-3.492496	1.229336	1.019589
H	-2.795796	0.772963	1.731947
H	-3.039490	2.153430	0.638429
H	-4.394400	1.513821	1.569932
C	-4.869724	0.958708	-1.032830
H	-4.494903	1.910061	-1.425860
H	-5.135825	0.323760	-1.883191
H	-5.785071	1.169160	-0.471219
C	-4.436825	-1.010914	0.430803
H	-4.829263	-1.652649	-0.363852

H	-3.720886	-1.595735	1.015616
H	-5.274623	-0.773436	1.092009
C	-2.614712	0.026729	-1.004957
H	-2.290470	0.915816	-1.548799
C	-2.306372	-1.205498	-1.595019
H	-1.809602	-1.233960	-2.563633
H	-2.909609	-2.082194	-1.375447
H	-0.963012	-2.099649	-0.813473
C	-1.236400	-1.354448	1.439321
O	-1.492538	-1.827838	2.461791

TSC4-5$_{M06\text{-}L}$

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.616872	-0.180679	-1.335404
C	-3.540021	0.697828	-1.323488
C	-2.331397	0.326186	-0.721680
C	-2.208476	-0.940885	-0.129168
C	-3.299421	-1.818727	-0.150857
C	-4.495753	-1.441002	-0.749370
H	-5.551628	0.114838	-1.801283
H	-3.641922	1.678677	-1.784153
H	-3.214775	-2.802953	0.307065
H	-5.336700	-2.127293	-0.758352
P	-0.628098	-1.396468	0.673659
P	-0.883037	1.435311	-0.710471
C	-1.113055	-1.784784	2.419399

H	-1.471825	-2.820300	2.452515
H	-0.190047	-1.761816	3.011599
C	-0.255227	-3.071193	-0.020070
H	0.764330	-3.322530	0.295017
H	-0.912512	-3.785139	0.491652
C	-2.159354	-0.846630	3.003832
H	-1.897368	0.207723	2.879994
H	-3.133623	-0.993709	2.531100
H	-2.276710	-1.027281	4.074407
C	-0.412663	-3.200951	-1.526836
H	-1.456158	-3.079322	-1.829973
H	0.175496	-2.462189	-2.077570
H	-0.084806	-4.189054	-1.857518
C	-0.478234	1.681106	-2.487787
H	-1.332948	2.182256	-2.959413
H	0.358341	2.389907	-2.524122
C	-0.140685	0.389975	-3.214076
H	0.721259	-0.115455	-2.762918
H	-0.982416	-0.309938	-3.199338
H	0.109427	0.585768	-4.258807
C	-1.512001	3.079456	-0.190756
H	-0.646635	3.752999	-0.191567
H	-2.182144	3.440799	-0.981198
C	-2.214052	3.083958	1.156730
H	-3.069439	2.401219	1.168534
H	-1.542493	2.794828	1.969210
H	-2.587008	4.083461	1.388911
Co	0.746670	0.482149	0.495775
C	0.466802	1.076120	2.207961
C	2.032649	1.643488	0.165428

O	0.382261	1.419679	3.305764
O	2.578080	2.652570	-0.071150
C	3.657405	-0.580381	-0.710752
C	3.746147	0.446737	-1.840299
H	2.755860	0.805353	-2.146823
H	4.340178	1.319878	-1.555355
H	4.213067	-0.003967	-2.720628
C	5.076155	-1.109645	-0.438457
H	5.745261	-0.310356	-0.104954
H	5.086341	-1.901267	0.315639
H	5.497450	-1.530264	-1.356358
C	2.768593	-1.733658	-1.156898
H	2.785984	-2.569766	-0.450243
H	1.728801	-1.397380	-1.256773
H	3.085327	-2.121421	-2.129989
C	3.139772	0.054268	0.592416
C	2.947248	-0.889080	1.771711
H	3.917863	-1.323131	2.046558
H	2.268631	-1.721164	1.560826
H	3.850813	0.824964	0.909202
H	2.585582	-0.374670	2.664962

$TSC6\text{-}1_{M06\text{-}L}$

Coordinates (Angstroms)		
X	Y	Z

C	4.801339	-0.200660	-1.370690
C	3.680989	-1.002103	-1.184292

C	2.506084	-0.471690	-0.638010
C	2.470872	0.885786	-0.271594
C	3.605313	1.684317	-0.461139
C	4.762968	1.145707	-1.010446
H	5.706003	-0.624582	-1.795192
H	3.724277	-2.053479	-1.462697
H	3.588318	2.734789	-0.176381
H	5.636387	1.773749	-1.155062
P	0.960202	1.576718	0.491444
P	1.021185	-1.508700	-0.373389
C	1.538759	2.231072	2.111829
H	2.225477	3.059745	1.894899
H	0.667610	2.675620	2.606692
C	0.619147	3.122844	-0.448422
H	-0.192474	3.639539	0.077817
H	1.503967	3.763304	-0.342875
C	2.209219	1.198505	3.000924
H	1.528082	0.389169	3.276038
H	3.080674	0.753021	2.511367
H	2.552533	1.659808	3.929192
C	0.279209	2.918067	-1.913465
H	1.062094	2.357944	-2.435011
H	-0.664399	2.377200	-2.043579
H	0.170722	3.879778	-2.419545
C	0.743354	-2.316820	-2.003895
H	1.697513	-2.770461	-2.301220
H	0.045239	-3.140397	-1.822852
C	0.223594	-1.395380	-3.093332
H	-0.807769	-1.084933	-2.900166
H	0.836874	-0.493073	-3.196085

H	0.226104	-1.903565	-4.059985
C	1.610529	-2.919798	0.649423
H	0.719595	-3.516556	0.880662
H	2.245671	-3.550843	0.014441
C	2.347770	-2.516031	1.914719
H	3.256515	-1.950989	1.685770
H	1.729114	-1.900129	2.572809
H	2.643626	-3.399609	2.484071
Co	-0.587320	-0.035421	0.368339
C	-0.684225	-0.608422	2.061368
C	-2.354093	-1.235125	-0.180189
O	-0.699884	-1.021867	3.141442
O	-2.108348	-2.368227	-0.492589
C	-4.132671	0.590075	-0.586927
C	-3.859360	0.394921	-2.082667
H	-2.790428	0.361024	-2.326706
H	-4.312593	-0.530673	-2.453562
H	-4.281982	1.222654	-2.659647
C	-5.639197	0.794561	-0.405360
H	-6.206304	-0.070145	-0.764215
H	-5.912541	0.969895	0.638850
H	-5.971589	1.666591	-0.976396
C	-3.408321	1.837703	-0.074866
H	-3.692641	2.081795	0.952980
H	-2.313649	1.741182	-0.102164
H	-3.663253	2.701557	-0.697322
C	-3.724628	-0.697803	0.188009
C	-3.822958	-0.578854	1.707336
H	-4.848934	-0.344525	1.998363
H	-3.178658	0.212613	2.101779

H	-4.402961	-1.499974	-0.135926
H	-3.548305	-1.515492	2.199247
H	-1.491257	-0.234772	-0.873314
H	-0.606102	0.454854	-1.081779

$A1^{IV}$

	Coordinates (Angstroms)		
	X	Y	Z

C	3.653390	-0.782094	-1.208427
C	2.500005	-1.444432	-0.808159
C	1.368714	-0.731362	-0.391166
C	1.402354	0.676575	-0.388961
C	2.569797	1.330810	-0.803984
C	3.688227	0.610771	-1.205661
H	4.524068	-1.350924	-1.519877
H	2.480660	-2.531121	-0.816883
H	2.610379	2.416803	-0.809987
H	4.586719	1.135625	-1.515086
P	-0.037444	1.683004	0.156198
P	-0.114973	-1.663553	0.152581
C	0.642146	2.795812	1.451004
H	1.468368	3.381031	1.031976
H	-0.159630	3.498733	1.705484
C	-0.411602	2.775760	-1.271621
H	-1.157784	3.499045	-0.922855
H	0.493516	3.339411	-1.526041
C	1.087999	2.020316	2.690690
H	0.256388	1.454460	3.126699

H	1.895828	1.319942	2.453473
H	1.458331	2.712764	3.453324
C	-0.932972	2.002507	-2.481601
H	-0.191025	1.283947	-2.846179
H	-1.853221	1.456504	-2.240385
H	-1.159703	2.692898	-3.300052
C	-0.553088	-2.732628	-1.275890
H	0.309800	-3.364065	-1.518888
H	-1.354557	-3.396871	-0.932334
C	-1.002471	-1.929127	-2.494795
H	-1.875487	-1.307228	-2.263344
H	-0.202159	-1.276864	-2.859954
H	-1.280932	-2.604995	-3.309369
C	0.496974	-2.812862	1.448155
H	-0.348847	-3.461397	1.705605
H	1.282234	-3.452256	1.028950
C	0.993505	-2.063917	2.685001
H	1.857129	-1.433256	2.448401
H	0.206820	-1.427822	3.107169
H	1.299577	-2.775747	3.457921
Co	-1.672243	0.035705	1.027537
H	-2.271892	-0.080010	2.551671
C	-3.605737	0.051865	-0.249094
O	-4.602653	0.050954	-0.779696

$A1^{VI}$

Coordinates (Angstroms)		
X	Y	Z

C	-2.923714	0.552827	0.921514
C	-1.547286	0.202867	0.494546
C	-0.566692	1.325642	0.435197
C	-1.067934	2.541006	0.086049
C	-2.490226	2.751686	0.013796
C	-3.390507	1.772454	0.544794
H	-3.539044	-0.162917	1.458283
H	-0.410638	3.387745	-0.096715
H	-2.865447	3.727342	-0.275209
H	-4.424133	2.052039	0.730728
P	-1.256710	-1.199208	-0.625283
P	1.187497	0.899084	0.618406
Co	1.248337	-1.417253	-0.306718
H	1.799069	-2.731718	0.534536
C	-2.060354	-0.798537	-2.242923
H	-2.015918	-1.718585	-2.837925
H	-3.117240	-0.583070	-2.048031
C	-2.300626	-2.547311	0.060894
H	-3.346894	-2.220531	0.065824
H	-2.227605	-3.382214	-0.645856
C	-1.394450	0.360264	-2.980669
H	-0.327381	0.172648	-3.148253
H	-1.865559	0.500314	-3.959057
H	-1.497308	1.297249	-2.425055
C	-1.847738	-2.981868	1.454315
H	-2.479185	-3.798772	1.818151
H	-0.810970	-3.336592	1.440749
H	-1.913921	-2.159769	2.176024
C	2.157694	2.242476	-0.165293

H	1.857270	3.207459	0.258821
H	3.199709	2.074687	0.132310
C	1.528043	1.005191	2.422586
H	2.598088	0.802754	2.550495
H	1.339627	2.031424	2.757223
C	0.694723	0.002135	3.221261
H	0.853156	-1.022332	2.863732
H	0.977471	0.035770	4.278198
H	-0.375296	0.228156	3.155319
C	2.033650	2.236618	-1.689221
H	2.630089	3.047228	-2.119357
H	2.400858	1.293163	-2.111405
H	0.996847	2.376101	-2.012528
C	3.572582	-1.084732	-0.773269
O	4.689308	-0.979272	-0.622241

$A2^{IV}$

	Coordinates (Angstroms)		
	X	Y	Z

C	-2.440661	-2.468341	0.981012
C	-1.805647	-1.328307	0.470039
C	-2.576021	-0.339031	-0.161886
C	-3.960828	-0.512841	-0.280028
C	-4.578209	-1.649271	0.226268
C	-3.815430	-2.628153	0.861635
H	-1.859585	-3.243995	1.472701
H	-4.561263	0.251164	-0.766524

H	-5.652106	-1.773012	0.126736
H	-4.292091	-3.517052	1.263041
P	-1.781677	1.179041	-0.800956
P	0.020140	-1.175776	0.597396
Co	0.736686	0.992835	-0.454220
H	1.307698	2.104905	-1.575449
C	0.531340	2.809206	0.759531
O	0.471527	3.883820	1.115691
C	3.309081	1.123220	1.469998
H	3.026806	2.116364	1.810275
H	3.210702	0.318980	2.195711
C	3.818736	0.936360	0.247952
H	3.909539	1.800304	-0.412556
C	4.308040	-0.365224	-0.350372
C	5.767764	-0.169157	-0.796303
H	6.413895	0.058145	0.059244
H	6.145060	-1.079741	-1.276468
H	5.854325	0.653059	-1.516270
C	3.445900	-0.682763	-1.586707
H	2.385951	-0.770510	-1.311703
H	3.525879	0.107630	-2.341938
H	3.755722	-1.629128	-2.045326
C	4.230878	-1.522385	0.647143
H	4.560710	-2.453985	0.174098
H	4.870120	-1.341646	1.518646
H	3.207270	-1.672600	1.007597
C	-2.792501	2.550781	-0.101403
H	-2.309785	3.483149	-0.417154
H	-3.781375	2.530465	-0.574499
C	-2.926074	2.490551	1.420543

H	-3.421676	3.393664	1.789836
H	-3.523350	1.627402	1.731087
H	-1.953143	2.416822	1.919565
C	-2.179682	1.196486	-2.596221
H	-3.266099	1.124377	-2.725451
H	-1.867966	2.178203	-2.971528
C	-1.462326	0.080807	-3.354122
H	-1.703562	0.129654	-4.420761
H	-0.373970	0.173304	-3.256077
H	-1.761069	-0.907189	-2.987273
C	0.362134	-1.349983	2.395949
H	-0.115293	-2.267788	2.757856
H	1.444136	-1.486991	2.505751
C	-0.115321	-0.137908	3.195309
H	-1.193008	0.019362	3.075253
H	0.083488	-0.286897	4.261224
H	0.400412	0.778726	2.885149
C	0.617012	-2.751149	-0.148825
H	1.703955	-2.776531	-0.022166
H	0.208241	-3.587496	0.429465
C	0.247316	-2.885118	-1.625163
H	0.645959	-2.056072	-2.220426
H	0.661223	-3.813555	-2.031205
H	-0.838437	-2.914235	-1.764714

$A2^{VI}$

Coordinates (Angstroms)		
X	Y	Z

C	3.433360	-2.044128	0.024753
C	2.347800	-1.043152	0.173742
C	2.734627	0.389382	0.004254
C	3.742917	0.638371	-0.873169
C	4.527299	-0.441751	-1.417749
C	4.418296	-1.759714	-0.865907
H	3.394261	-2.986370	0.563134
H	4.015390	1.655482	-1.143974
H	5.320040	-0.214393	-2.121920
H	5.183855	-2.494139	-1.100998
P	0.626251	-1.486911	-0.198445
P	1.668967	1.636091	0.789695
Co	-0.604855	0.562073	0.546585
H	-1.557185	0.685771	1.869817
C	0.347310	-3.049126	0.731712
H	-0.614954	-3.447748	0.389963
H	1.112772	-3.775904	0.437799
C	0.545402	-2.021048	-1.968719
H	1.090508	-2.966433	-2.068082
H	-0.513141	-2.228364	-2.166555
C	0.334645	-2.838901	2.244431
H	-0.441129	-2.122643	2.538634
H	0.131450	-3.785833	2.754921
H	1.298221	-2.463671	2.605490
C	1.090228	-0.983819	-2.947304
H	0.898449	-1.302543	-3.976751
H	0.622378	-0.002140	-2.810916
H	2.170784	-0.858612	-2.829127
C	2.248441	1.741633	2.533238

H	3.289326	2.084633	2.535718
H	1.639676	2.519740	3.008693
C	2.107773	3.253411	0.043986
H	1.707716	4.015051	0.723502
H	3.197616	3.368317	0.049596
C	1.532876	3.438997	-1.359902
H	0.438188	3.469070	-1.334367
H	1.880230	4.384312	-1.788614
H	1.838892	2.633514	-2.036452
C	2.103654	0.419109	3.285069
H	2.368058	0.556638	4.338424
H	1.073077	0.047626	3.244331
H	2.766098	-0.349780	2.872595
C	-1.434470	1.251632	-1.378208
O	-1.843109	1.596051	-2.373918
C	-3.117477	-1.485151	-0.744232
H	-3.353266	-1.301711	-1.789851
H	-2.326230	-2.202623	-0.544712
C	-3.787078	-0.913850	0.260322
H	-3.496106	-1.162039	1.282692
C	-4.958042	0.040713	0.163720
C	-4.587436	1.355506	0.872406
H	-3.750689	1.855475	0.369184
H	-5.442363	2.042636	0.871032
H	-4.295512	1.178063	1.913721
C	-5.360123	0.333751	-1.283976
H	-4.545561	0.809663	-1.841618
H	-5.647981	-0.581027	-1.814761
H	-6.216957	1.016657	-1.304006
C	-6.144326	-0.607460	0.901859

H	-5.892694	-0.821952	1.947463
H	-7.010538	0.064953	0.895960
H	-6.439039	-1.548202	0.422873

$A3^{IV}$

	Coordinates (Angstroms)		
	X	Y	Z

C	4.646635	1.379975	-0.825696
C	3.835655	0.293487	-1.129658
C	2.551222	0.179178	-0.581868
C	2.083468	1.182929	0.286638
C	2.913095	2.270530	0.588498
C	4.184089	2.371873	0.037149
H	5.637800	1.454357	-1.262401
H	4.206481	-0.473310	-1.804749
H	2.563331	3.047613	1.263090
H	4.813285	3.222674	0.280155
P	0.413238	1.087391	1.045552
P	1.508475	-1.270221	-1.026086
C	0.736796	1.227147	2.850984
H	1.221616	2.190532	3.047292
H	-0.242763	1.251525	3.342821
C	-0.391542	2.679877	0.602222
H	-1.333637	2.716134	1.162688
H	0.227934	3.511897	0.957085
C	1.584867	0.078276	3.393377
H	1.104818	-0.893078	3.230043

H	2.572113	0.054061	2.920241
H	1.733860	0.197761	4.471175
C	-0.653064	2.792739	-0.898938
H	0.284137	2.779170	-1.466072
H	-1.283602	1.971637	-1.257507
H	-1.167290	3.732270	-1.124902
C	1.466687	-1.238122	-2.864224
H	2.489066	-1.324786	-3.250422
H	0.922352	-2.136839	-3.177480
C	0.784345	0.019049	-3.401746
H	-0.232674	0.121543	-3.006131
H	1.346387	0.921042	-3.136722
H	0.715860	-0.024454	-4.493383
C	2.551735	-2.725728	-0.609012
H	2.026505	-3.607007	-0.995539
H	3.501933	-2.650449	-1.149943
C	2.790435	-2.857906	0.893864
H	3.319692	-1.985689	1.292354
H	1.845315	-2.963304	1.438885
H	3.396977	-3.744279	1.105108
Co	-0.609087	-0.894619	0.087535
C	-4.642972	0.380736	-0.353796
C	-5.502294	0.789030	0.850143
H	-5.754464	-0.079738	1.471239
H	-4.975369	1.514375	1.483537
H	-6.441896	1.251380	0.523853
C	-4.360233	1.623382	-1.206886
H	-3.836476	2.391772	-0.623534
H	-3.746871	1.386331	-2.084009
H	-5.296346	2.063738	-1.571492

C	-5.394153	-0.661896	-1.188596
H	-4.827734	-0.940067	-2.084877
H	-5.578227	-1.575902	-0.609574
H	-6.365312	-0.270956	-1.516150
C	-3.313315	-0.216693	0.184210
H	-2.809696	0.592825	0.742320
C	-2.358437	-0.814799	-0.839690
H	-2.213140	-0.182820	-1.725261
H	-2.637385	-1.827318	-1.157804
C	-0.891946	-2.201933	1.696153
O	-1.216180	-2.889497	2.535336
H	-3.563934	-0.986303	0.929182

$A3^{VI}$

Coordinates (Angstroms)

	X	Y	Z
C	-3.511808	-1.412280	-1.239512
C	-2.303165	-0.753755	-0.685732
C	-2.125655	0.694180	-1.005326
C	-3.267996	1.419851	-1.142360
C	-4.551667	0.768889	-1.193320
C	-4.633250	-0.652929	-1.346350
H	-3.504051	-2.471383	-1.479767
H	-3.237128	2.499303	-1.267623
H	-5.446474	1.373355	-1.293993
H	-5.579848	-1.098384	-1.640694
P	-1.552763	-1.352798	0.857562

P	-0.437051	1.363278	-0.915198
Co	0.560808	-0.077683	0.824452
C	-1.525738	-3.180656	0.673157
H	-1.165085	-3.581250	1.627751
H	-2.550481	-3.545128	0.538256
C	-2.764932	-1.049916	2.222146
H	-3.722449	-1.507387	1.948902
H	-2.377153	-1.588437	3.095363
C	-0.620512	-3.634442	-0.471434
H	0.415201	-3.318395	-0.304717
H	-0.630313	-4.726228	-0.551237
H	-0.949242	-3.224714	-1.433132
C	-2.935594	0.435516	2.534993
H	-3.585047	0.566510	3.406517
H	-1.972592	0.910559	2.760547
H	-3.392284	0.966628	1.694208
C	0.284106	1.062153	-2.583132
H	-0.321287	1.584732	-3.332364
H	1.279282	1.522601	-2.580000
C	-0.594667	3.185618	-0.772882
H	0.410539	3.585924	-0.950339
H	-1.231830	3.562078	-1.581240
C	-1.108042	3.634009	0.596197
H	-0.428884	3.319960	1.397033
H	-1.182709	4.725479	0.632035
H	-2.099533	3.223335	0.812831
C	0.387153	-0.429479	-2.903194
H	0.901190	-0.575849	-3.858597
H	0.951568	-0.966438	-2.131915
H	-0.604077	-0.889170	-2.984535

C	0.944601	1.055777	2.582850
O	1.349181	1.586616	3.496625
C	2.328787	-0.940488	0.486466
H	2.683093	-1.384474	1.426783
C	3.246585	0.151746	-0.048963
H	2.796031	0.579579	-0.958433
C	4.703850	-0.250359	-0.405077
C	5.393652	0.972545	-1.024276
H	5.385440	1.823857	-0.331653
H	6.439947	0.753128	-1.270226
H	4.890492	1.284512	-1.948404
C	5.464621	-0.672461	0.857427
H	5.465733	0.131496	1.604776
H	5.019245	-1.561394	1.318931
H	6.509427	-0.909785	0.621646
C	4.710809	-1.398837	-1.420972
H	4.129858	-1.140003	-2.316154
H	5.735146	-1.625753	-1.741047
H	4.285503	-2.315399	-0.996884
H	2.162811	-1.741819	-0.244995
H	3.305081	0.977564	0.679446

$A4^{IV}$

Coordinates (Angstroms)		
X	Y	Z

C	3.322172	2.617359	-0.276191
C	2.505356	1.484313	-0.188727

C	3.090646	0.202979	-0.206955
C	4.479773	0.090716	-0.343040
C	5.279173	1.224513	-0.446672
C	4.700784	2.490373	-0.405438
H	2.879826	3.609035	-0.252695
H	4.949572	-0.887090	-0.367713
H	6.353827	1.117221	-0.557101
H	5.320926	3.378523	-0.478692
P	2.008264	-1.264827	0.015528
P	0.681991	1.665162	-0.059028
Co	-0.211438	-0.497021	-0.468636
C	2.267187	-1.746437	1.780869
C	3.685615	-2.129885	2.191458
H	1.576773	-2.577173	1.970039
H	1.908695	-0.902632	2.382628
H	3.701587	-2.401408	3.252561
H	4.053711	-2.990687	1.623525
H	4.384611	-1.299646	2.050640
C	2.775987	-2.620111	-0.964950
C	2.117482	-3.969987	-0.674229
H	3.851069	-2.681115	-0.767694
H	2.653536	-2.351814	-2.020495
H	2.510396	-4.730867	-1.355930
H	2.318528	-4.302632	0.349498
H	1.030782	-3.932230	-0.809100
C	0.445265	2.257485	1.670573
C	-1.003755	2.624394	1.985013
H	1.108808	3.113620	1.839306
H	0.785653	1.446535	2.325103
H	-1.109070	2.864392	3.047862

H	-1.330770	3.498334	1.412118
H	-1.687381	1.797458	1.762253
C	0.284670	3.126392	-1.119457
C	-1.152431	3.117647	-1.641893
H	0.984442	3.110361	-1.961826
H	0.485513	4.039729	-0.547539
H	-1.341954	4.024138	-2.226239
H	-1.328597	2.255684	-2.294303
H	-1.888650	3.085159	-0.832067
C	-0.994995	-1.006475	1.214882
O	-1.359689	-1.340303	2.241639
C	-0.902089	-1.912703	-1.608823
O	-1.285731	-2.760500	-2.263194
C	-3.259808	0.070513	-1.404320
C	-4.163601	-0.826432	-0.637800
H	-3.448856	0.319121	-2.444546
H	-2.474836	0.628084	-0.893313
H	-4.702744	-1.486648	-1.329012
H	-3.568007	-1.474993	0.023822
C	-5.216108	-0.099123	0.254749
C	-4.510920	0.798200	1.279310
H	-3.957820	1.608384	0.789447
H	-5.239508	1.259823	1.956679
H	-3.807964	0.221288	1.893080
C	-6.036312	-1.165492	0.989186
H	-6.796145	-0.701575	1.629727
H	-6.552623	-1.825144	0.280960
H	-5.396254	-1.789512	1.625792
C	-6.141664	0.750475	-0.623556
H	-5.582321	1.533715	-1.149859

H	-6.647957	0.133665	-1.376395
H	-6.913000	1.239566	-0.016346

$A4^{VI}$

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.031764	-0.210588	-0.171245
C	-2.725110	-0.376776	-0.508546
C	-2.045498	0.811409	-1.107982
C	-2.888958	1.714280	-1.928415
C	-4.185489	1.860528	-1.546730
C	-4.752121	0.968184	-0.581186
H	-4.575266	-0.979966	0.371844
H	-2.459018	2.276765	-2.751944
H	-4.829929	2.587961	-2.033290
H	-5.791298	1.078454	-0.290980
P	-1.667399	-1.789134	-0.064619
P	-0.604689	1.462989	-0.211109
Co	0.384236	-0.633684	0.599530
C	-1.494504	-2.754483	-1.626080
H	-0.789669	-3.566329	-1.410888
H	-2.464634	-3.209669	-1.856786
C	-2.650869	-2.874550	1.039584
H	-3.628418	-3.059987	0.579782
H	-2.123693	-3.835691	1.057465
C	-0.998591	-1.916584	-2.804775
H	-0.047359	-1.421969	-2.579071

H	-0.841171	-2.557733	-3.678071
H	-1.728426	-1.148615	-3.082847
C	-2.792258	-2.317517	2.455483
H	-3.412227	-2.982904	3.064739
H	-1.815630	-2.231009	2.944125
H	-3.261282	-1.327917	2.457621
C	0.309354	2.464815	-1.450126
H	-0.332876	3.278383	-1.806070
H	1.144054	2.928258	-0.909805
C	-1.250931	2.719499	0.984250
H	-0.378054	3.254336	1.377924
H	-1.853443	3.444217	0.424909
C	-2.062003	2.098255	2.118930
H	-1.484321	1.337980	2.658213
H	-2.354691	2.868755	2.839319
H	-2.975242	1.627391	1.742137
C	0.827504	1.618871	-2.612294
H	1.436356	2.232231	-3.284291
H	1.451501	0.791660	-2.255840
H	0.003928	1.194174	-3.196528
C	0.603634	-0.565640	2.665364
O	0.855109	-0.620290	3.768032
C	2.082697	-1.323682	-0.168940
H	2.268816	-2.294290	0.310879
C	3.193294	-0.312498	0.071792
H	2.834525	0.698327	-0.184805
C	4.525017	-0.520644	-0.700465
C	5.534975	0.515431	-0.189227
H	5.736937	0.375014	0.880169
H	6.489242	0.434252	-0.723949

H	5.158600	1.537073	-0.328222
C	5.073576	-1.930289	-0.453758
H	5.204696	-2.122323	0.618978
H	4.400736	-2.697028	-0.854641
H	6.049927	-2.057291	-0.937513
C	4.307722	-0.307452	-2.203851
H	3.935929	0.704498	-2.409390
H	5.249167	-0.434546	-2.752180
H	3.587326	-1.023630	-2.616420
H	1.866229	-1.486756	-1.233605
H	3.427086	-0.290960	1.146810
C	2.144485	2.174352	2.147836
O	2.927838	2.979165	1.991108

$A5^{IV}$

Coordinates (Angstroms)			
	X	Y	Z

C	2.194689	2.345343	-1.941930
C	1.802459	1.324140	-1.069149
C	2.237955	0.003976	-1.302459
C	3.043925	-0.260794	-2.416640
C	3.416733	0.761230	-3.283491
C	2.994838	2.066774	-3.044724
H	1.867985	3.366607	-1.765901
H	3.387897	-1.270959	-2.614465
H	4.037914	0.536697	-4.145246
H	3.286811	2.866909	-3.717985

P	1.753196	-1.318048	-0.121478
P	0.725679	1.692179	0.371378
Co	-0.066894	-0.419632	1.102710
C	3.256968	-1.604365	0.911091
C	4.530317	-2.037118	0.190623
H	2.966585	-2.349083	1.661723
H	3.422513	-0.666470	1.455426
H	5.337231	-2.168082	0.919738
H	4.398523	-2.990685	-0.331024
H	4.857464	-1.287357	-0.536456
C	1.542238	-2.839274	-1.132272
C	1.118625	-4.023914	-0.262718
H	2.465439	-3.074960	-1.671425
H	0.775623	-2.618757	-1.883666
H	0.963199	-4.911547	-0.883981
H	1.883655	-4.269187	0.481923
H	0.182440	-3.816990	0.268564
C	1.853127	2.596526	1.515247
C	1.135561	3.170308	2.736280
H	2.358877	3.391555	0.954318
H	2.619102	1.875597	1.824120
H	1.864913	3.592710	3.435008
H	0.442941	3.969807	2.454646
H	0.566865	2.400943	3.271329
C	-0.478367	2.953791	-0.236274
C	-1.772213	2.946116	0.579835
H	-0.694388	2.717608	-1.284377
H	-0.008965	3.943965	-0.218429
H	-2.478841	3.682546	0.182987
H	-2.254026	1.963035	0.539003

H	-1.594405	3.185630	1.633110
C	0.586341	-0.575604	2.912057
O	1.053285	-0.653487	3.947584
C	-1.890162	-1.226130	0.518138
O	-2.387474	-1.991410	1.289196
C	-2.320412	-0.934193	-0.906520
H	-2.047203	0.098293	-1.145312
H	-1.644058	-1.567380	-1.499678
C	-3.782437	-1.262314	-1.238100
H	-3.836481	-1.422466	-2.322001
H	-4.040503	-2.218208	-0.766684
C	-4.836075	-0.200535	-0.855721
C	-4.589083	1.107204	-1.621040
H	-3.635327	1.573169	-1.347796
H	-4.582855	0.935932	-2.704625
H	-5.379255	1.834419	-1.400297
C	-4.832909	0.078376	0.652815
H	-4.997476	-0.839503	1.228546
H	-3.887019	0.522605	0.987823
H	-5.628396	0.787597	0.910423
C	-6.210420	-0.756754	-1.256469
H	-6.428462	-1.692483	-0.727280
H	-7.005307	-0.041006	-1.015954
H	-6.256690	-0.959966	-2.333484

$A5^{VI}$

Coordinates (Angstroms)		
X	Y	Z

C	-3.776279	0.116254	-1.501003
C	-2.436020	0.085426	-0.867932
C	-1.964218	1.356158	-0.239924
C	-2.922965	2.154639	0.300349
C	-4.316794	1.891071	0.052775
C	-4.706488	0.929981	-0.939463
H	-4.007363	-0.533806	-2.339990
H	-2.661738	3.038583	0.877318
H	-5.062694	2.548186	0.486672
H	-5.734224	0.926183	-1.292948
P	-1.742412	-1.449147	-0.180835
P	-0.162450	1.563373	-0.090635
Co	0.435821	-0.716908	0.506801
C	-1.847435	-2.659703	-1.564047
H	-1.539113	-3.623704	-1.142099
H	-2.892031	-2.764795	-1.879080
C	-2.993532	-2.102456	1.018786
H	-3.898695	-2.365627	0.459204
H	-2.572899	-3.032641	1.419160
C	-0.952459	-2.283814	-2.742841
H	0.089147	-2.156704	-2.423816
H	-0.974517	-3.070599	-3.503943
H	-1.283144	-1.352049	-3.213443
C	-3.330235	-1.128829	2.144857
H	-4.009948	-1.603409	2.860095
H	-2.437306	-0.812204	2.694041
H	-3.824876	-0.232332	1.758092
C	0.310477	2.288170	-1.722672
H	-0.179801	3.265350	-1.803925

H	1.390939	2.466310	-1.692679
C	0.100842	2.975850	1.054873
H	1.134566	3.306026	0.895571
H	-0.541757	3.805161	0.736581
C	-0.125893	2.630099	2.525719
H	0.660548	1.966780	2.899227
H	-0.106494	3.539314	3.135239
H	-1.092383	2.139307	2.686342
C	-0.048767	1.410232	-2.918949
H	0.319885	1.868491	-3.842492
H	0.398750	0.413798	-2.840985
H	-1.133162	1.289572	-3.016306
C	0.326684	-0.753899	2.446557
O	0.373775	-0.886704	3.577197
C	3.421085	-1.544224	0.904469
C	3.625013	-0.029542	0.844315
H	2.656946	0.449054	1.066138
C	4.144397	0.535667	-0.493454
C	4.066419	2.065301	-0.402069
H	4.434402	2.536251	-1.320992
H	3.032559	2.397179	-0.241925
H	4.669085	2.440548	0.434123
C	5.601696	0.118850	-0.729084
H	5.710693	-0.970370	-0.790547
H	5.974077	0.538259	-1.671295
H	6.251430	0.477899	0.078298
C	3.274553	0.045356	-1.658750
H	3.512660	0.586675	-2.581859
H	3.427808	-1.022160	-1.860418
H	2.209320	0.196255	-1.444530

H	4.312992	0.263683	1.645165
H	4.239012	-2.118266	0.454927
C	2.106133	-2.005003	0.304982
H	3.334643	-1.863508	1.952943
O	1.833872	-3.096678	-0.096247

$A6^{IV}$

	Coordinates (Angstroms)		
	X	Y	Z

C	3.103034	2.585031	-0.703658
C	2.323424	1.468563	-0.379112
C	2.879744	0.178811	-0.487273
C	4.199860	0.043172	-0.935347
C	4.960537	1.159784	-1.265328
C	4.412695	2.434356	-1.145110
H	2.682406	3.583253	-0.617692
H	4.644678	-0.942301	-1.030661
H	5.980451	1.033275	-1.615560
H	5.002264	3.310048	-1.399363
P	1.870302	-1.286192	-0.022267
P	0.580845	1.694402	0.158658
Co	-0.364895	-0.487216	0.180546
C	2.584903	-1.871042	1.577462
C	4.048055	-2.304142	1.579519
H	1.939305	-2.695927	1.904038
H	2.425061	-1.053219	2.291283
H	4.323850	-2.669878	2.574465

H	4.232880	-3.113948	0.865517
H	4.714270	-1.471160	1.334891
C	2.302344	-2.577585	-1.260486
C	1.654111	-3.922269	-0.929008
H	3.388647	-2.689386	-1.338277
H	1.945831	-2.207157	-2.228592
H	1.863341	-4.643710	-1.725384
H	2.044932	-4.338262	0.005991
H	0.567544	-3.830341	-0.832038
C	0.755643	2.483815	1.815426
C	-0.584926	2.909345	2.412249
H	1.433494	3.341324	1.728975
H	1.245409	1.744427	2.460414
H	-0.440849	3.286267	3.429950
H	-1.049020	3.708900	1.825523
H	-1.290004	2.070816	2.461345
C	-0.066928	3.028032	-0.943678
C	-1.583776	2.951206	-1.112078
H	0.421276	2.908606	-1.916793
H	0.236817	4.002457	-0.544378
H	-1.937436	3.760163	-1.760010
H	-1.868782	2.001622	-1.576741
H	-2.111580	3.031354	-0.156162
C	-0.637226	-0.825456	2.075098
O	-0.744977	-1.040775	3.187326
C	-1.806353	-1.502856	-0.890624
O	-1.704471	-2.637485	-0.509763
C	-2.879289	-0.988857	-1.829242
H	-2.664219	0.046736	-2.099717
H	-2.789943	-1.601571	-2.735314

C	-4.293125	-1.148085	-1.231436
H	-5.000988	-1.159203	-2.068725
H	-4.359881	-2.134200	-0.756203
C	-4.744199	-0.061286	-0.229384
C	-4.997650	1.267721	-0.954676
H	-4.104838	1.633922	-1.473242
H	-5.795860	1.162132	-1.699429
H	-5.304192	2.041988	-0.241318
C	-3.701822	0.146435	0.876639
H	-3.486839	-0.792170	1.402674
H	-2.758149	0.542917	0.475444
H	-4.063406	0.870062	1.617226
C	-6.056793	-0.536142	0.409921
H	-5.907834	-1.465427	0.972959
H	-6.449613	0.218712	1.101490
H	-6.822525	-0.723443	-0.352737
H	0.320251	0.237029	-3.002297
H	0.240220	-0.058241	-2.321900

$A6^{VI}$

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.062954	0.413803	0.035083
C	-2.797904	0.220371	-0.423220
C	-1.936301	1.436893	-0.524500
C	-2.624238	2.718656	-0.817862
C	-3.885331	2.871636	-0.340769

C	-4.594264	1.743779	0.192177
H	-4.719203	-0.425965	0.248763
H	-2.104747	3.516206	-1.341403
H	-4.403551	3.821936	-0.438174
H	-5.607020	1.867801	0.559759
P	-1.978488	-1.386259	-0.654084
P	-0.364758	1.402571	0.387211
Co	0.209792	-0.958253	0.257130
C	-1.959431	-1.646755	-2.479133
H	-1.572649	-2.660089	-2.639949
H	-2.988790	-1.620218	-2.854069
C	-3.143893	-2.660426	-0.033543
H	-4.135094	-2.481031	-0.465818
H	-2.789458	-3.612681	-0.445454
C	-1.084274	-0.625726	-3.204272
H	-0.057396	-0.643088	-2.818356
H	-1.040316	-0.851731	-4.274619
H	-1.476212	0.391248	-3.092784
C	-3.200153	-2.735269	1.491580
H	-3.954797	-3.462939	1.806701
H	-2.236994	-3.056121	1.901863
H	-3.457339	-1.769764	1.940218
C	0.664792	2.681183	-0.446410
H	0.205968	3.664283	-0.291231
H	1.625865	2.690699	0.081073
C	-0.683801	2.151360	2.052213
H	0.269676	2.105404	2.592489
H	-0.931967	3.209585	1.912695
C	-1.787821	1.440545	2.831468
H	-1.606601	0.362939	2.910660

H	-1.850789	1.844883	3.846932
H	-2.761750	1.583497	2.353146
C	0.869668	2.410762	-1.935872
H	1.581530	3.128731	-2.356293
H	1.265378	1.405313	-2.115772
H	-0.069367	2.503603	-2.491566
C	0.237740	-1.554999	2.103632
O	0.359045	-1.905644	3.179842
C	3.237882	-1.497594	-0.360321
C	3.309450	-0.006699	-0.040252
H	2.816850	0.547248	-0.849514
C	4.720936	0.578013	0.160906
C	4.559364	2.072483	0.472043
H	3.972554	2.225504	1.386742
H	5.535756	2.549272	0.618644
H	4.053333	2.593649	-0.350761
C	5.430039	-0.108987	1.334670
H	4.834707	-0.039419	2.254179
H	5.619513	-1.169791	1.133198
H	6.399458	0.365183	1.527839
C	5.559453	0.421435	-1.115150
H	5.059642	0.882110	-1.976681
H	6.533627	0.909981	-0.993995
H	5.749841	-0.631279	-1.353680
H	2.722771	0.179989	0.872108
C	1.811036	-1.971117	-0.556812
H	3.622067	-2.107776	0.468768
H	3.801395	-1.773062	-1.258793
O	1.460342	-3.016662	-1.022278
H	2.918619	-0.412715	-3.231260

H	2.264745	-0.744850	-3.349460

$B2^{IV}$

	Coordinates (Angstroms)		
	X	Y	Z

C	1.459251	-1.046225	-0.354161
C	2.414572	-1.982360	-0.768121
H	2.095366	-2.949139	-1.147556
C	3.770459	-1.688023	-0.700526
H	4.500383	-2.422191	-1.026873
C	4.188769	-0.449955	-0.214942
H	5.247449	-0.216364	-0.157662
C	3.249274	0.488406	0.195031
H	3.586656	1.452372	0.567359
C	1.878996	0.205987	0.128055
Co	-1.638165	0.448532	0.437815
P	-0.318379	-1.467303	-0.445957
P	0.652932	1.474149	0.634722
C	1.144741	2.986046	-0.292625
H	0.405818	3.753693	-0.034851
H	2.114919	3.330585	0.085234
C	1.198903	2.774873	-1.805319
H	0.249727	2.395516	-2.199890
H	1.411241	3.723703	-2.307906
H	1.985712	2.064773	-2.079476
C	-0.618063	-1.902029	-2.204889
H	0.062786	-2.712752	-2.488267

H	-1.638719	-2.299675	-2.257466
C	-0.459063	-0.698178	-3.131623
H	-0.641428	-0.990198	-4.170481
H	-1.173159	0.094144	-2.877480
H	0.550993	-0.278397	-3.072900
C	-0.496881	-3.049509	0.469077
H	-1.512347	-3.410313	0.265945
H	0.197897	-3.789511	0.055501
C	-0.281227	-2.869242	1.970870
H	-0.998778	-2.153986	2.390806
H	-0.416350	-3.823254	2.490035
H	0.730158	-2.508967	2.187466
C	1.070799	1.848615	2.384858
H	2.135989	2.097971	2.452921
H	0.504303	2.747601	2.654791
C	0.719191	0.690705	3.317216
H	-0.354858	0.470661	3.287016
H	1.267255	-0.219589	3.050209
H	0.975836	0.943123	4.351063
H	-2.636538	1.392500	1.404248
C	-2.285283	1.938933	-0.966372
C	-3.658896	-0.852597	0.373070
O	-2.727190	2.860053	-1.456919
O	-4.674236	-1.269811	0.647938

$B2^{VI}$

Coordinates (Angstroms)		
X	Y	Z

C	2.461711	-1.830176	0.934807
C	1.354600	-0.937573	0.569712
C	1.745610	0.474156	0.301095
C	3.044940	0.736963	-0.109502
C	4.026441	-0.270419	-0.156158
C	3.609066	-1.683612	0.015281
H	2.646204	-2.034847	1.991473
H	3.338123	1.756463	-0.348058
H	5.074849	-0.006211	-0.261907
H	3.663825	-2.341869	-0.854931
P	-0.210226	-1.466436	-0.152947
P	0.358828	1.639770	0.324419
Co	-1.410143	0.458829	-0.459130
H	-1.911478	1.856793	-0.808160
C	-0.781969	-2.887351	0.852905
H	-1.687551	-3.268008	0.366506
H	-0.014635	-3.666497	0.769733
C	0.207292	-2.213156	-1.786488
H	0.939937	-3.012917	-1.628283
H	-0.712408	-2.676987	-2.163657
C	-1.051292	-2.549438	2.316820
H	-1.851418	-1.810130	2.419462
H	-1.363396	-3.450997	2.853257
H	-0.155330	-2.158177	2.810094
C	0.732100	-1.169254	-2.770408
H	0.925843	-1.629632	-3.744258
H	0.002416	-0.362960	-2.924456
H	1.666834	-0.720896	-2.417582
C	0.201914	2.238904	2.054817

H	1.009789	2.961204	2.218816
H	-0.745909	2.786405	2.112592
C	0.833328	3.104706	-0.660707
H	0.070700	3.861523	-0.443772
H	1.787585	3.491813	-0.285193
C	0.892302	2.813189	-2.158105
H	-0.074804	2.445909	-2.521558
H	1.134493	3.726646	-2.709937
H	1.655896	2.064760	-2.394186
C	0.260353	1.128589	3.102663
H	0.113881	1.557460	4.098833
H	-0.515957	0.371858	2.948923
H	1.232113	0.624055	3.092827
C	-2.653521	-0.175462	-1.652833
O	-3.426672	-0.538203	-2.405917
C	-2.590335	0.496031	1.075793
O	-3.340828	0.661986	1.914630

$B3^{IV}$

Coordinates (Angstroms)

	X	Y	Z
C	5.107544	0.034943	-0.479920
C	4.122455	0.709936	0.229472
C	2.774666	0.351991	0.095316
C	2.420245	-0.698081	-0.766648
C	3.422848	-1.372226	-1.476295
C	4.756095	-1.009594	-1.334825

H	6.148880	0.320459	-0.367275
H	4.402349	1.528034	0.888273
H	3.161639	-2.192689	-2.139353
H	5.523131	-1.541258	-1.889559
P	0.670772	-1.220263	-0.930349
P	1.480156	1.263545	1.015118
C	0.377769	-1.261694	-2.749564
H	1.113933	-1.937032	-3.200983
H	-0.605010	-1.724691	-2.899050
C	0.692298	-3.009048	-0.474305
H	-0.358218	-3.314763	-0.398101
H	1.132253	-3.575158	-1.303463
C	0.432768	0.111964	-3.413519
H	-0.361490	0.770971	-3.047764
H	1.396120	0.604202	-3.240196
H	0.300740	0.008875	-4.495350
C	1.439953	-3.311686	0.824337
H	2.515271	-3.144363	0.709743
H	1.096107	-2.689583	1.658014
H	1.288641	-4.358639	1.105236
C	2.031586	1.193347	2.770342
H	3.016215	1.670903	2.836302
H	1.332278	1.814946	3.341449
C	2.087876	-0.220886	3.342096
H	1.094689	-0.678927	3.378157
H	2.746301	-0.868265	2.752782
H	2.473877	-0.194032	4.366079
C	1.743587	3.032125	0.551946
H	0.856945	3.572269	0.905246
H	2.598460	3.419743	1.118349

C	1.963077	3.256701	-0.945759
H	2.947106	2.895305	-1.259093
H	1.217864	2.743921	-1.563781
H	1.906562	4.325482	-1.174751
Co	-0.781406	0.273845	0.471220
H	-1.714170	1.223177	1.505276
C	-1.201565	2.016467	-0.779429
C	-1.105094	-1.352609	2.080238
O	-1.571522	3.026442	-1.140501
O	-1.542577	-1.912119	2.962893
C	-4.770601	0.127099	-0.161841
C	-4.615972	1.653212	-0.079896
H	-3.760395	1.929334	0.545724
H	-4.480312	2.095036	-1.074652
H	-5.513453	2.100537	0.363039
C	-6.034629	-0.201145	-0.982882
H	-5.962620	0.201471	-2.000495
H	-6.186240	-1.284034	-1.055316
H	-6.919450	0.239689	-0.508432
C	-4.909724	-0.445847	1.251524
H	-5.101740	-1.524580	1.240281
H	-4.001724	-0.259913	1.837728
H	-5.749337	0.032419	1.768482
C	-3.596888	-0.470955	-0.911964
H	-3.306832	0.072355	-1.814996
C	-2.978469	-1.628127	-0.646398
H	-2.223315	-2.023968	-1.320516
H	-3.237161	-2.250173	0.207212

B3[VI]

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.513697	1.792738	-0.367382
C	-2.429647	0.932098	-0.193944
C	-2.640866	-0.426138	0.027840
C	-4.070482	-0.950147	0.057220
C	-5.142832	-0.062680	-0.081031
C	-4.928842	1.278446	-0.275588
H	-3.362055	2.846626	-0.577346
H	-4.231517	-2.013393	0.196562
H	-6.156978	-0.449263	-0.029084
H	-5.744159	1.986266	-0.367004
P	-0.708300	1.571594	-0.286257
P	-1.256106	-1.554811	0.253672
Co	0.909365	-0.338036	0.138052
C	-0.718836	3.002556	0.878574
H	0.243435	3.514564	0.759392
H	-1.491782	3.704292	0.544017
C	-0.664699	2.423318	-1.923257
H	-1.361638	3.268691	-1.877312
H	0.341756	2.844274	-2.034835
C	-0.944246	2.620178	2.339310
H	-0.110559	2.031341	2.733169
H	-1.025091	3.523145	2.952886
H	-1.868074	2.045879	2.468756
C	-1.004993	1.525597	-3.110623
H	-0.995766	2.112115	-4.035161

H	-0.280258	0.714640	-3.230482
H	-2.000563	1.081563	-3.006334
C	-1.615162	-2.429589	1.844576
H	-2.328465	-3.237055	1.645735
H	-0.676726	-2.899748	2.160426
C	-1.497199	-2.848961	-1.046006
H	-0.547164	-3.389421	-1.128941
H	-2.246644	-3.567480	-0.695924
C	-1.918764	-2.263157	-2.394782
H	-1.250808	-1.463125	-2.730530
H	-1.914590	-3.044360	-3.161512
H	-2.930423	-1.845575	-2.343534
C	-2.163101	-1.506108	2.934163
H	-2.231205	-2.047987	3.882903
H	-1.532565	-0.626798	3.099395
H	-3.166723	-1.147758	2.680015
H	1.482149	-1.912573	0.437254
C	1.041869	-0.234363	2.286796
C	1.284346	-0.935715	-1.862751
O	1.281305	-0.494118	3.365509
O	1.590438	-1.543503	-2.771578
C	2.768655	1.653285	0.290268
H	2.078562	2.371755	-0.144070
H	2.872136	1.670130	1.372727
C	3.552516	0.904799	-0.502137
H	3.429878	1.008293	-1.582614
C	4.686778	-0.002749	-0.081783
C	4.663268	-0.322213	1.414411
H	5.504942	-0.975557	1.669385
H	4.748575	0.580870	2.029176

H	3.741347	-0.848044	1.687766
C	4.622091	-1.309224	-0.888364
H	4.618555	-1.111994	-1.967190
H	5.494851	-1.933085	-0.664234
H	3.723643	-1.884488	-0.636187
C	5.991116	0.741189	-0.434228
H	6.856648	0.114466	-0.189307
H	6.038688	0.977893	-1.503681
H	6.074244	1.678119	0.127933

$B6^{IV}$

Coordinates (Angstroms)

	X	Y	Z
C	-4.596040	0.751172	-1.915895
C	-3.973964	-0.253157	-1.181720
C	-2.723323	-0.039933	-0.592119
C	-2.097619	1.217312	-0.734693
C	-2.733136	2.216361	-1.478265
C	-3.971499	1.985267	-2.069145
H	-5.563593	0.567171	-2.372738
H	-4.466777	-1.213521	-1.075222
H	-2.262488	3.184155	-1.610351
H	-4.447732	2.771631	-2.646718
P	-0.473540	1.484954	0.078771
P	-1.832771	-1.368616	0.304236
Co	0.451157	-0.688685	0.199497
C	1.205258	-2.282611	0.961903

O	1.500770	-3.298509	1.384532
C	4.764242	-0.351478	-0.818274
C	4.725599	0.144263	-2.270799
H	3.716364	0.056963	-2.693473
H	5.030614	1.195465	-2.339447
H	5.402316	-0.444777	-2.900710
C	6.183193	-0.180208	-0.261544
H	6.466055	0.879038	-0.222544
H	6.278222	-0.594291	0.749154
H	6.909491	-0.698992	-0.898063
C	4.367247	-1.833998	-0.788068
H	4.399378	-2.252899	0.224073
H	3.355572	-1.982170	-1.187977
H	5.053698	-2.425424	-1.405182
C	3.760078	0.502857	-0.016690
H	2.757784	0.327759	-0.434699
C	3.733174	0.243470	1.500871
H	3.646228	-0.822672	1.721849
H	3.979470	1.565527	-0.177890
C	0.624744	-1.081459	-1.683235
O	0.630661	-1.235756	-2.812253
H	4.632858	0.638433	1.986489
C	2.530669	0.964136	2.068787
O	2.445992	2.103386	2.394732
C	-2.204071	-2.959305	-0.565685
C	-3.462242	-3.749121	-0.206803
H	-1.322953	-3.583415	-0.370703
H	-2.180739	-2.728646	-1.637684
H	-3.458656	-4.696899	-0.756176
H	-3.498318	-3.986556	0.861104

H	-4.381812	-3.219781	-0.470312
C	-2.580799	-1.486247	1.989535
C	-4.081623	-1.228460	2.110153
H	-2.030733	-0.782027	2.622379
H	-2.323056	-2.488616	2.354193
H	-4.394299	-1.367272	3.150751
H	-4.330713	-0.202957	1.819666
H	-4.672690	-1.907481	1.489446
C	0.362794	2.890102	-0.777608
C	0.004676	4.318532	-0.365486
H	0.201024	2.734312	-1.850970
H	1.432966	2.725814	-0.605468
H	0.617021	5.022755	-0.938688
H	-1.044920	4.561889	-0.551750
H	0.209244	4.490461	0.695585
C	-0.887317	2.054784	1.793160
C	-2.187041	2.836401	1.966121
H	-0.026085	2.638417	2.134976
H	-0.903503	1.154891	2.418239
H	-2.302561	3.129746	3.015153
H	-2.203492	3.746586	1.358866
H	-3.057152	2.231731	1.690229

$B6^{VI}$

	Coordinates (Angstroms)		
	X	Y	Z

C	-3.534898	1.743114	-0.571618

C	-2.763761	0.664627	-0.277756
C	-2.335457	0.521266	1.144141
C	-3.262286	1.045541	2.176945
C	-4.000459	2.137487	1.844516
C	-4.067317	2.572937	0.481840
H	-3.800924	1.979880	-1.599105
H	-3.296834	0.602451	3.167848
H	-4.620454	2.634189	2.586374
H	-4.668189	3.437287	0.220494
P	-0.548480	0.438026	1.424783
P	-1.987914	-0.479842	-1.459085
Co	0.213338	-0.803950	-0.486873
C	2.755666	-1.927774	1.230046
O	2.939377	-2.918142	1.855661
C	3.759208	-1.039851	0.526387
H	3.768195	-1.395466	-0.513432
H	4.749726	-1.229603	0.955931
C	3.358727	0.435631	0.606306
C	1.210137	-1.005462	-2.108001
C	0.016350	-2.694668	-0.105389
O	-0.112513	-3.814048	0.059388
O	1.679466	-1.207361	-3.126238
C	-3.135206	-1.926210	-1.505261
H	-4.016630	-1.648445	-2.095017
H	-2.614756	-2.727115	-2.044148
C	-3.560756	-2.399722	-0.114643
H	-4.191361	-1.653067	0.379617
H	-4.136409	-3.327267	-0.195985
H	-2.702653	-2.597286	0.537157
C	-2.155203	0.287946	-3.119459

H	-1.869195	-0.492018	-3.835575
H	-3.209216	0.521398	-3.310622
C	-1.274168	1.524272	-3.302595
H	-1.549758	2.323818	-2.607834
H	-0.214845	1.291281	-3.144931
H	-1.378795	1.915264	-4.319799
C	-0.349589	-0.181811	3.141571
H	-0.838545	0.516557	3.830404
H	0.725650	-0.144145	3.354960
C	-0.878196	-1.602165	3.328269
H	-0.741498	-1.921172	4.366504
H	-1.946264	-1.671972	3.093678
H	-0.340097	-2.311413	2.690922
C	0.085079	2.174824	1.523582
H	-0.447081	2.694791	2.328161
H	1.138274	2.096995	1.820369
C	-0.050971	2.930077	0.203745
H	-1.102267	3.098724	-0.047782
H	0.435922	3.907880	0.275088
H	0.413975	2.383496	-0.626413
H	2.319763	0.534630	0.255863
H	3.363534	0.737434	1.662151
C	4.238086	1.411785	-0.202066
C	5.721906	1.234590	0.147432
H	6.109146	0.266160	-0.189379
H	6.322108	2.013822	-0.336854
H	5.886164	1.308756	1.229604
C	4.028899	1.194806	-1.706489
H	2.982296	1.373924	-1.986429
H	4.649190	1.887446	-2.287393

H	4.297918	0.178760	-2.017812
C	3.805766	2.839373	0.159015
H	4.372801	3.576408	-0.421824
H	2.741101	2.997485	-0.050903
H	3.975810	3.046754	1.222613

$B7^{IV}$

	Coordinates (Angstroms)		
	X	Y	Z

C	0.452626	1.730310	0.120331
C	0.513993	3.119632	0.281533
H	-0.391501	3.713818	0.219409
C	1.728882	3.753312	0.516076
H	1.759761	4.830723	0.645283
C	2.900171	3.004203	0.589677
H	3.850099	3.493119	0.782210
C	2.857594	1.627041	0.400646
H	3.782054	1.059933	0.444763
C	1.642476	0.977774	0.148632
Co	-0.792303	-1.527189	-0.411140
P	-1.155627	0.891705	-0.123718
P	1.586401	-0.818719	-0.203130
C	-1.901617	1.743690	-1.569501
H	-2.005715	2.810426	-1.339642
H	-1.171748	1.656142	-2.381906
C	-3.240418	1.139579	-1.990250
H	-3.670331	1.721760	-2.811385

H	-3.106903	0.112704	-2.347286
H	-3.968213	1.136000	-1.170504
C	-2.217379	1.269610	1.337982
H	-3.055340	0.565382	1.258794
H	-1.639770	0.952996	2.215454
C	-2.744260	2.691040	1.522766
H	-3.457058	2.706596	2.354069
H	-1.942793	3.394769	1.763079
H	-3.268947	3.052372	0.632380
C	2.405970	-1.061792	-1.832591
H	1.782964	-0.521411	-2.554319
H	2.275897	-2.126340	-2.061303
C	3.871334	-0.655099	-1.957104
H	4.238533	-0.917347	-2.954908
H	4.003033	0.423250	-1.828866
H	4.502568	-1.170674	-1.225518
C	2.661117	-1.602378	1.065427
H	3.677312	-1.200053	0.995053
H	2.262004	-1.302985	2.041513
C	2.674065	-3.125279	0.931826
H	3.275393	-3.566726	1.732715
H	1.662743	-3.543636	1.004173
H	3.105843	-3.443516	-0.022941
H	-0.851245	-1.784761	-2.061034
C	-0.894755	-2.054238	1.704885
C	-3.229361	-1.899265	-0.389723
O	-0.904102	-2.297582	2.808948
O	-4.295984	-2.185176	-0.635126

$B7^{VI}$

	Coordinates (Angstroms)		
	X	Y	Z
C	2.042422	-2.186161	0.318383
C	1.100526	-1.174253	0.493897
C	1.599265	0.226738	0.607106
C	2.970547	0.356022	1.120726
C	3.909958	-0.545032	0.426760
C	3.420781	-1.944205	0.367955
H	1.704944	-3.212824	0.196727
H	3.108623	0.544514	2.187894
H	4.478218	-0.161330	-0.422986
H	4.118532	-2.776001	0.410294
P	-0.701763	-1.375760	0.455342
P	0.729812	1.489244	-0.330764
Co	-1.418387	0.818051	-0.230139
C	-1.161626	-1.848803	2.180288
H	-2.243582	-2.028737	2.186143
H	-0.673549	-2.807842	2.390995
C	-1.029324	-2.932868	-0.468692
H	-0.537277	-3.759587	0.057438
H	-2.108684	-3.105557	-0.379774
C	-0.780521	-0.814402	3.236505
H	-1.305157	0.133964	3.084501
H	-1.043462	-1.187623	4.231674
H	0.297097	-0.614357	3.228689
C	-0.615733	-2.901565	-1.937977
H	-0.825928	-3.869061	-2.404970

H	-1.170660	-2.141394	-2.495533
H	0.453820	-2.699819	-2.056038
C	1.173127	3.087445	0.450452
H	2.268811	3.137345	0.447734
H	0.813190	3.875930	-0.220858
C	1.541930	1.593853	-1.986392
H	0.926495	2.265091	-2.597567
H	2.513898	2.079307	-1.840104
C	1.721531	0.241006	-2.671590
H	0.772974	-0.292683	-2.790554
H	2.146859	0.384368	-3.669833
H	2.400415	-0.403975	-2.104954
C	0.623343	3.279008	1.859934
H	1.013816	4.208632	2.286348
H	-0.469619	3.342124	1.857579
H	0.915350	2.456654	2.522489
C	-1.773993	0.535782	-2.012761
O	-2.032186	0.408269	-3.114974
H	-1.061497	1.234312	1.163093
C	-3.066217	0.678968	0.544783
O	-4.052065	0.554194	1.102525

$C3^{IV}$

Coordinates (Angstroms)

	X	Y	Z
C	-4.692724	0.015888	-0.882253
C	-3.599800	0.873241	-0.880459

C	-2.339427	0.427143	-0.462039
C	-2.180242	-0.906910	-0.049612
C	-3.290650	-1.761620	-0.056979
C	-4.537400	-1.305706	-0.466864
H	-5.663507	0.376668	-1.208303
H	-3.729642	1.900599	-1.210284
H	-3.181898	-2.796566	0.257142
H	-5.386866	-1.981983	-0.465681
P	-0.536540	-1.550197	0.475538
P	-0.911728	1.580365	-0.462632
C	-0.873242	-2.325273	2.114960
H	-1.578037	-3.153079	1.974512
H	0.074631	-2.762170	2.451324
C	-0.295312	-3.008389	-0.624890
H	0.621414	-3.506465	-0.288181
H	-1.117875	-3.714884	-0.463187
C	-1.411718	-1.344013	3.153390
H	-0.714509	-0.519402	3.333342
H	-2.369025	-0.915632	2.838471
H	-1.570148	-1.855790	4.108070
C	-0.195687	-2.625219	-2.099972
H	-1.136517	-2.196806	-2.461480
H	0.600109	-1.892172	-2.273585
H	0.026564	-3.508723	-2.707053
C	-0.822235	2.168645	-2.205428
H	-1.753598	2.694131	-2.447600
H	-0.014221	2.909339	-2.243203
C	-0.564788	1.040698	-3.201927
H	0.360899	0.502218	-2.969098
H	-1.386762	0.317274	-3.205782

H	-0.468875	1.446255	-4.214332
C	-1.528674	3.064045	0.440063
H	-0.727300	3.811222	0.390034
H	-2.386636	3.478160	-0.102259
C	-1.900776	2.776806	1.892822
H	-2.696884	2.027908	1.961938
H	-1.040996	2.413274	2.464686
H	-2.257836	3.690515	2.378609
Co	0.970106	0.321300	0.332044
C	3.786862	-0.494083	-0.492570
C	3.354254	-1.831630	-1.104257
H	2.424860	-2.191017	-0.649096
H	3.189722	-1.737997	-2.184450
H	4.121325	-2.599090	-0.946876
C	5.107096	-0.054148	-1.157840
H	4.962062	0.139850	-2.227507
H	5.508412	0.855200	-0.697320
H	5.863048	-0.842627	-1.057764
C	4.019862	-0.688098	1.014211
H	4.282561	0.250345	1.515252
H	3.123919	-1.099237	1.499260
H	4.838937	-1.396629	1.186564
C	2.715875	0.560821	-0.762954
H	2.270763	0.452694	-1.762324
C	3.020624	2.006465	-0.430463
H	3.674853	2.451018	-1.196223
H	3.519741	2.120428	0.537875
C	1.290068	0.906840	2.188132
O	1.595820	1.263612	3.223646
H	2.110103	2.623623	-0.413864

$C3^{VI}$

	Coordinates (Angstroms)		
	X	Y	Z
C	3.128893	1.665662	-0.021401
C	2.034994	0.992168	-0.465395
C	2.205680	-0.475064	-0.685549
C	3.551555	-0.931936	-1.110709
C	4.618641	-0.233800	-0.643688
C	4.422091	1.029599	0.004917
H	3.067160	2.710637	0.271892
H	3.665052	-1.826711	-1.715791
H	5.632813	-0.576318	-0.831688
H	5.278489	1.590037	0.363769
P	0.340374	1.646943	-0.591681
P	1.096956	-1.567615	0.253138
Co	-0.897444	-0.193680	0.432150
C	0.130145	1.958411	-2.397062
H	-0.828224	2.475266	-2.523214
H	0.918076	2.648786	-2.718913
C	0.374992	3.332488	0.139094
H	1.212101	3.894730	-0.290539
H	-0.542355	3.824888	-0.204774
C	0.157683	0.675140	-3.224163
H	-0.606289	-0.034613	-2.887194
H	-0.034399	0.898992	-4.278492
H	1.133418	0.181282	-3.159818

C	0.429934	3.327239	1.666257
H	0.535859	4.348389	2.046273
H	-0.489538	2.910465	2.090393
H	1.275633	2.741230	2.042173
C	1.049314	-3.120157	-0.738224
H	2.064982	-3.524501	-0.818517
H	0.465823	-3.836300	-0.146916
C	2.024396	-2.099622	1.767725
H	1.339796	-2.746170	2.330083
H	2.873065	-2.717256	1.451937
C	2.506317	-0.938294	2.632452
H	1.688599	-0.261639	2.903157
H	2.945125	-1.319519	3.560258
H	3.272090	-0.351156	2.115820
C	0.426911	-2.936034	-2.119967
H	0.350902	-3.900953	-2.631683
H	-0.581765	-2.514419	-2.049522
H	1.030263	-2.270690	-2.746533
C	-1.002010	0.149313	2.387921
O	-1.137723	0.273513	3.509084
C	-2.669541	-0.987941	-0.236263
C	-2.860522	-2.095421	0.781718
H	-1.923460	-2.637987	0.973198
H	-3.237749	-1.725534	1.742007
C	-3.780368	0.053276	-0.399101
H	-3.577430	-2.846313	0.414790
H	-2.339338	-1.384829	-1.206730
C	-3.836873	1.002573	0.810505
H	-4.653322	1.726247	0.699202
H	-3.998314	0.461182	1.750133

H	-2.898365	1.569878	0.900442
C	-5.140176	-0.656202	-0.549332
H	-5.930222	0.075326	-0.758752
H	-5.119759	-1.377940	-1.374881
H	-5.416882	-1.193907	0.364348
C	-3.514842	0.880926	-1.663213
H	-4.299594	1.632349	-1.811338
H	-2.557950	1.409299	-1.589725
H	-3.484763	0.245160	-2.556548

$C4^{IV}$

Coordinates (Angstroms)

	X	Y	Z
C	5.055432	0.117588	0.126174
C	4.023289	-0.811239	0.157955
C	2.686475	-0.398672	0.076511
C	2.392874	0.969056	-0.032720
C	3.442250	1.896765	-0.066989
C	4.763814	1.476654	0.011536
H	6.086632	-0.215959	0.191959
H	4.258476	-1.867974	0.255889
H	3.227044	2.957270	-0.165820
H	5.566213	2.207594	-0.016562
P	0.649966	1.535507	-0.171492
P	1.329618	-1.634987	0.147632
C	0.522305	2.871788	1.092606
H	1.276226	3.635286	0.868558

H	-0.457518	3.343800	0.953461
C	0.642860	2.492455	-1.754272
H	-0.407669	2.720556	-1.971903
H	1.153506	3.448914	-1.590579
C	0.679802	2.370736	2.525140
H	-0.117297	1.672164	2.796682
H	1.642170	1.867340	2.669899
H	0.633612	3.209318	3.227511
C	1.282975	1.749625	-2.926735
H	2.360331	1.627633	-2.778797
H	0.854732	0.752014	-3.068265
H	1.130901	2.308642	-3.855573
C	1.827684	-2.899652	-1.101484
H	2.768828	-3.358311	-0.776904
H	1.062227	-3.684452	-1.070950
C	1.971955	-2.345062	-2.516644
H	1.028158	-1.941259	-2.895002
H	2.724853	-1.551058	-2.560122
H	2.284534	-3.140286	-3.201218
C	1.643116	-2.510704	1.750147
H	0.742954	-3.101129	1.959813
H	2.465038	-3.222585	1.609446
C	1.959223	-1.577483	2.920532
H	2.944539	-1.116615	2.803287
H	1.230393	-0.766739	3.022707
H	1.960039	-2.142029	3.858597
Co	-0.736506	-0.415526	-0.062537
C	-1.217060	-0.583974	1.812611
C	-1.167769	-0.644965	-1.956359
O	-1.472817	-0.802964	2.900178

O	-1.485905	-0.776475	-3.040781
C	-4.597518	-0.177898	-0.039168
C	-4.042905	-1.559417	-0.443314
H	-3.922929	-1.634542	-1.530651
H	-3.059308	-1.743575	0.015779
H	-4.719958	-2.361461	-0.124501
C	-4.863538	-0.156051	1.471258
H	-3.953980	-0.343195	2.050547
H	-5.274055	0.807475	1.793731
H	-5.589350	-0.932837	1.737356
C	-5.933130	0.050016	-0.779641
H	-6.369059	1.019532	-0.512031
H	-5.789491	0.030795	-1.866419
H	-6.657986	-0.731576	-0.519192
C	-3.624121	0.893275	-0.465177
H	-3.454120	0.979672	-1.538757
C	-3.198003	2.035961	0.391194
H	-2.437318	2.642875	-0.111133
H	-2.790518	1.710152	1.359223
H	-4.039221	2.708663	0.632187

$C4^{VI}$

Coordinates (Angstroms)		
X	Y	Z

C	2.858211	-2.189179	-0.566710
C	2.030855	-1.119010	-0.681962
C	2.613920	0.219672	-0.377396

C	4.065720	0.390581	-0.637117
C	4.858326	-0.702028	-0.497066
C	4.272965	-2.004337	-0.354193
H	2.483462	-3.203468	-0.679634
H	4.471616	1.369839	-0.873603
H	5.938603	-0.616439	-0.580611
H	4.911977	-2.875501	-0.260325
P	0.234192	-1.162431	-0.962878
P	1.734956	1.218084	0.856474
Co	-0.601979	0.624644	0.431479
C	-0.270623	-2.914945	-0.728251
H	-1.302546	-2.981749	-1.094463
H	0.336999	-3.545966	-1.387809
C	0.080841	-0.925201	-2.792765
H	0.306777	-1.881456	-3.279409
H	-0.970205	-0.692770	-3.002115
C	-0.185963	-3.399568	0.718079
H	-0.857622	-2.834462	1.372088
H	-0.477720	-4.452992	0.779273
H	0.829162	-3.309996	1.118322
C	0.995249	0.167989	-3.347173
H	0.788750	0.325366	-4.410729
H	0.856604	1.127901	-2.838736
H	2.049415	-0.111455	-3.246859
C	2.434633	0.767760	2.519563
H	3.433671	1.209431	2.605778
H	1.793846	1.264778	3.258536
C	2.427673	2.910937	0.618528
H	2.013664	3.531603	1.422419
H	3.510584	2.864555	0.781806

C	2.110694	3.520397	-0.744719
H	1.036085	3.684620	-0.870747
H	2.605104	4.491764	-0.849418
H	2.455335	2.880338	-1.564884
C	2.500219	-0.735454	2.784134
H	2.762506	-0.920256	3.830964
H	1.546090	-1.237102	2.589058
H	3.259360	-1.211776	2.156510
C	-1.058829	1.871049	-1.001524
O	-1.356713	2.556605	-1.858868
C	-3.826506	0.737095	0.808026
C	-4.072267	2.159055	0.429044
H	-3.297984	2.823032	0.838159
H	-4.111549	2.310256	-0.654660
C	-4.289681	-0.434465	-0.023535
H	-5.030372	2.522469	0.837127
C	-3.763968	-0.345129	-1.466246
H	-4.098797	-1.211471	-2.049305
H	-4.112184	0.556570	-1.981104
H	-2.666702	-0.341809	-1.474633
C	-5.833914	-0.455286	-0.050284
H	-6.195325	-1.311950	-0.633163
H	-6.244765	-0.537282	0.962793
H	-6.234216	0.456796	-0.507689
C	-3.774925	-1.738024	0.602024
H	-4.135776	-2.611118	0.045516
H	-2.678271	-1.763838	0.589414
H	-4.103904	-1.841104	1.643100
C	-0.931606	-0.171615	2.187660
O	-1.135065	-0.535798	3.245892

H	-3.667345	0.546239	1.870269

$C5^{IV}$

	Coordinates (Angstroms)		
	X	Y	Z

C	-4.814678	0.794222	1.154448
C	-3.829124	-0.171833	1.314564
C	-2.583980	-0.037075	0.686705
C	-2.334715	1.092838	-0.110889
C	-3.335691	2.060843	-0.263978
C	-4.567010	1.914564	0.362392
H	-5.775514	0.673882	1.645450
H	-4.033829	-1.042649	1.932335
H	-3.153164	2.937212	-0.880142
H	-5.333513	2.672822	0.233950
P	-0.718083	1.307107	-0.957731
P	-1.297079	-1.331304	0.897615
C	-1.176273	1.530518	-2.729438
H	-1.738892	2.466055	-2.831140
H	-0.234215	1.659327	-3.275762
C	-0.178842	2.993617	-0.450368
H	0.725667	3.220413	-1.027060
H	-0.941469	3.719719	-0.753918
C	-1.976868	0.362920	-3.303191
H	-1.439917	-0.586346	-3.209332
H	-2.942317	0.255181	-2.798135
H	-2.171592	0.529310	-4.367528

C	0.097548	3.094428	1.047998
H	-0.813940	2.920842	1.630041
H	0.851164	2.367091	1.369846
H	0.470869	4.092474	1.299055
C	-1.074178	-1.432155	2.721988
H	-2.053215	-1.567325	3.196530
H	-0.492484	-2.340602	2.916445
C	-0.357658	-0.207807	3.286568
H	0.640824	-0.099937	2.847713
H	-0.919851	0.712509	3.092474
H	-0.234282	-0.302603	4.370212
C	-2.172448	-2.901780	0.498943
H	-1.443814	-3.704900	0.661507
H	-2.980210	-3.048957	1.225723
C	-2.716043	-2.953523	-0.927187
H	-3.443847	-2.155566	-1.109232
H	-1.915667	-2.861763	-1.668494
H	-3.217998	-3.910853	-1.101078
Co	0.611299	-0.595824	-0.328700
C	0.642182	-1.723260	-1.909590
C	2.442058	-1.149476	0.461874
O	0.758466	-2.422394	-2.801184
O	2.158699	-2.142045	1.074477
C	4.047509	0.825707	0.499999
C	3.543766	1.054742	1.932172
H	2.461444	0.887638	2.007740
H	4.037744	0.380338	2.642259
H	3.738839	2.084932	2.250281
C	5.544082	1.161576	0.443461
H	6.118277	0.536421	1.137249

H	5.958226	1.024623	-0.561314
H	5.701957	2.209264	0.724044
C	3.281080	1.738063	-0.463635
H	3.710578	1.722792	-1.471006
H	2.227762	1.436136	-0.539567
H	3.305058	2.773266	-0.104994
C	3.855767	-0.673619	0.143082
C	4.106792	-1.041701	-1.326585
H	5.131578	-0.782898	-1.607167
H	3.422619	-0.515905	-2.000404
H	4.522152	-1.269200	0.780929
H	3.980368	-2.117885	-1.483215

$C5^{VI}$

Coordinates (Angstroms)

	X	Y	Z
C	-3.817337	-1.066494	0.119201
C	-2.625000	-0.635057	-0.370544
C	-2.442148	0.845233	-0.466219
C	-3.661002	1.650030	-0.728080
C	-4.831384	1.185577	-0.222680
C	-4.907331	-0.144255	0.312545
H	-3.995979	-2.119216	0.323261
H	-3.593995	2.598693	-1.252544
H	-5.741485	1.775408	-0.294069
H	-5.847872	-0.514161	0.705997
P	-1.151255	-1.655130	-0.688465

P	-1.002164	1.540420	0.396569
Co	0.583096	-0.261651	0.198751
C	-1.139089	-1.877397	-2.519308
H	-0.244535	-2.466140	-2.754713
H	-2.014645	-2.473629	-2.802398
C	-1.540381	-3.338914	-0.064867
H	-2.512352	-3.646218	-0.467538
H	-0.793149	-4.003653	-0.514557
C	-1.116876	-0.552247	-3.278477
H	-0.275934	0.073328	-2.961492
H	-1.010198	-0.734569	-4.352735
H	-2.044736	0.009897	-3.124831
C	-1.507310	-3.460177	1.457665
H	-1.850273	-4.453957	1.763732
H	-0.491076	-3.329039	1.842689
H	-2.154388	-2.719848	1.940313
C	-0.696878	3.144186	-0.455617
H	-1.611611	3.746794	-0.419331
H	0.053917	3.672745	0.144545
C	-1.576820	2.091123	2.073036
H	-0.674650	2.410355	2.609052
H	-2.213539	2.974138	1.946975
C	-2.318558	1.009839	2.854495
H	-1.741928	0.081688	2.924476
H	-2.518674	1.355154	3.874020
H	-3.278114	0.773091	2.384653
C	-0.213490	2.970899	-1.893344
H	-0.004021	3.945524	-2.345940
H	0.706531	2.375595	-1.937779
H	-0.967633	2.470051	-2.510032

C	0.772994	-0.783586	2.049485
O	0.888672	-1.045348	3.152398
C	3.455191	0.873687	-0.458335
C	2.917060	1.890799	0.549022
H	2.124224	2.491050	0.091484
H	2.503119	1.404898	1.440522
C	4.559047	-0.099820	0.077486
H	3.706665	2.576825	0.864806
H	3.882006	1.410389	-1.316159
C	4.005454	-1.075850	1.123559
H	4.811428	-1.722618	1.488212
H	3.590787	-0.550345	1.990330
H	3.226798	-1.728906	0.707493
C	5.675577	0.740979	0.716662
H	6.515609	0.090380	0.984960
H	6.049507	1.502728	0.022205
H	5.342100	1.241076	1.631425
C	5.158270	-0.894250	-1.092037
H	5.978732	-1.524493	-0.731656
H	4.423014	-1.552493	-1.566196
H	5.559936	-0.224587	-1.861636
C	2.292568	0.054725	-1.041088
O	2.237421	-0.405266	-2.141243

$C6^{IV}$

Coordinates (Angstroms)		
X	Y	Z

C	-5.122554	0.448172	-0.912013
C	-3.978817	1.216926	-0.736260
C	-2.754006	0.617210	-0.415143
C	-2.689239	-0.779117	-0.276983
C	-3.848711	-1.544670	-0.456428
C	-5.058103	-0.937729	-0.769653
H	-6.064679	0.928614	-1.157790
H	-4.042092	2.296251	-0.849936
H	-3.802802	-2.625786	-0.349246
H	-5.950166	-1.541684	-0.904856
P	-1.102478	-1.612156	0.124269
P	-1.254773	1.652692	-0.167379
C	-1.514192	-2.631847	1.608464
H	-2.181137	-3.444066	1.295585
H	-0.576665	-3.094445	1.939444
C	-0.931245	-2.881112	-1.207738
H	0.055791	-3.340251	-1.074336
H	-1.675597	-3.667594	-1.035837
C	-2.155055	-1.838072	2.745500
H	-1.531856	-0.997122	3.066033
H	-3.129878	-1.437935	2.449214
H	-2.307785	-2.486830	3.613934
C	-1.079052	-2.319547	-2.621614
H	-2.093449	-1.946621	-2.794729
H	-0.379166	-1.501334	-2.813523
H	-0.881204	-3.106204	-3.357208
C	-1.111947	2.584742	-1.749275
H	-2.054763	3.112563	-1.935115
H	-0.338006	3.346347	-1.596775
C	-0.752115	1.684884	-2.929236

H	0.220612	1.203791	-2.780837
H	-1.504083	0.901834	-3.078624
H	-0.694807	2.271649	-3.851999
C	-1.812226	2.946425	1.020549
H	-0.967435	3.633572	1.147930
H	-2.624299	3.518499	0.556981
C	-2.257427	2.385466	2.368910
H	-3.085719	1.677646	2.256113
H	-1.438190	1.871496	2.881628
H	-2.596349	3.197073	3.020876
Co	0.494052	0.137250	0.378176
C	0.692685	0.253999	2.304122
C	2.514416	0.654683	0.039812
O	0.980857	0.320185	3.405410
O	2.568182	1.821486	-0.212879
C	4.976070	-0.042280	-0.375048
C	5.551408	1.306798	0.078639
H	4.900643	2.144197	-0.188669
H	5.705210	1.324833	1.164574
H	6.523363	1.475794	-0.398888
C	5.982377	-1.143554	-0.001371
H	6.088112	-1.240257	1.085918
H	5.694875	-2.118703	-0.407339
H	6.966602	-0.892863	-0.412908
C	4.781500	-0.037858	-1.897217
H	4.368483	-0.986923	-2.256821
H	4.117462	0.771455	-2.220741
H	5.747136	0.109628	-2.393814
C	3.633642	-0.331053	0.368200
C	3.113369	-1.768919	0.260102

H	3.769183	-2.454799	0.800899
H	3.046251	-2.103457	-0.779162
H	3.791064	-0.118368	1.439505
H	2.113937	-1.853837	0.706723
H	1.850139	-0.719806	-2.610097
H	1.503670	-0.614778	-1.958380

$C6^{VI}$

	Coordinates (Angstroms)		
	X	Y	Z

C	3.859951	1.027647	0.196023
C	2.701822	0.573487	-0.353241
C	2.503038	-0.906815	-0.341539
C	3.721509	-1.748377	-0.432421
C	4.859136	-1.256816	0.119441
C	4.918252	0.113545	0.542302
H	4.036903	2.090190	0.342099
H	3.674141	-2.738566	-0.876534
H	5.760492	-1.862129	0.168674
H	5.833305	0.505887	0.972251
P	1.262483	1.580554	-0.827401
P	1.004270	-1.518729	0.483743
Co	-0.538066	0.289787	0.123524
C	1.316307	1.648312	-2.669500
H	0.525862	2.346606	-2.969612
H	2.274141	2.083915	-2.975843
C	1.669526	3.308081	-0.349735

H	2.679069	3.541407	-0.708186
H	0.981864	3.945236	-0.918186
C	1.098763	0.288872	-3.328711
H	0.149275	-0.157784	-3.012709
H	1.068433	0.396093	-4.417934
H	1.905035	-0.410526	-3.082924
C	1.527438	3.583923	1.146127
H	1.898801	4.586285	1.382580
H	0.477101	3.539821	1.450751
H	2.091769	2.866804	1.752471
C	0.707128	-3.150289	-0.324262
H	1.524635	-3.829580	-0.057027
H	-0.205635	-3.556866	0.127257
C	1.502526	-2.019770	2.197111
H	0.586301	-2.361259	2.693634
H	2.173531	-2.882572	2.116369
C	2.172718	-0.903539	2.994136
H	1.557378	0.001096	3.035309
H	2.350289	-1.232835	4.023047
H	3.138734	-0.633215	2.556488
C	0.563874	-3.057562	-1.841766
H	0.278469	-4.029706	-2.256455
H	-0.201883	-2.331679	-2.136774
H	1.503572	-2.753074	-2.314224
C	-0.733253	1.023429	1.895224
O	-0.863866	1.423781	2.954182
C	-3.503123	-0.599894	-0.688557
C	-2.864839	-1.932392	-0.301042
H	-2.072343	-2.192344	-1.009112
H	-2.425729	-1.895390	0.703336

C	-4.626159	-0.081870	0.276635
H	-3.600707	-2.739270	-0.325659
H	-3.945776	-0.690826	-1.690010
C	-4.047764	0.421334	1.606273
H	-4.860620	0.637563	2.308558
H	-3.394231	-0.320929	2.078919
H	-3.484736	1.352118	1.470955
C	-5.599577	-1.237526	0.555624
H	-6.472505	-0.854274	1.095722
H	-5.955533	-1.696337	-0.374251
H	-5.145155	-2.018560	1.173918
C	-5.402228	1.055100	-0.401050
H	-6.191207	1.418024	0.267397
H	-4.758314	1.906107	-0.645295
H	-5.876734	0.710076	-1.327278
C	-2.403806	0.454269	-0.833931
O	-2.461448	1.501537	-1.406922
H	-2.359301	-1.189514	-3.907343
H	-2.037127	-1.323074	-3.251606

TSA4-5^{IV}

Coordinates (Angstroms)		
X	Y	Z

C	3.428583	2.424667	-0.561541
C	2.543438	1.364790	-0.335797
C	3.019383	0.038593	-0.372467
C	4.369644	-0.190431	-0.662743

C	5.236824	0.871006	-0.901710
C	4.768167	2.181130	-0.843955
H	3.069887	3.449693	-0.522924
H	4.756776	-1.203526	-0.702880
H	6.280616	0.674144	-1.126543
H	5.444383	3.011587	-1.022504
P	1.853774	-1.323914	0.034090
P	0.769494	1.688203	0.002669
Co	-0.344716	-0.381672	-0.267411
C	2.244794	-1.706472	1.800874
C	3.676550	-2.126994	2.118757
H	1.538544	-2.487849	2.105777
H	1.975092	-0.806539	2.367711
H	3.775295	-2.330085	3.190647
H	3.961463	-3.037880	1.581338
H	4.392180	-1.339576	1.861640
C	2.430767	-2.794016	-0.910187
C	1.637655	-4.043885	-0.522648
H	3.499942	-2.966342	-0.750804
H	2.289154	-2.564701	-1.972461
H	1.931712	-4.886646	-1.156447
H	1.823070	-4.329290	0.518312
H	0.559756	-3.892254	-0.646249
C	0.783754	2.319038	1.734686
C	-0.578848	2.827721	2.202071
H	1.538658	3.110601	1.809407
H	1.119125	1.486737	2.364782
H	-0.530766	3.106904	3.259590
H	-0.892659	3.712658	1.638654
H	-1.357648	2.063054	2.096187

C	0.342841	3.156537	-1.035077
C	-1.142688	3.202384	-1.397413
H	0.944354	3.095945	-1.948414
H	0.645042	4.067361	-0.505735
H	-1.364415	4.111521	-1.966282
H	-1.420754	2.343059	-2.018307
H	-1.783695	3.202411	-0.508978
C	-0.990877	-0.802829	1.468629
O	-1.242119	-1.092468	2.544235
C	-1.343523	-1.710728	-1.466428
O	-1.627797	-2.641591	-2.086982
C	-2.971482	-0.380484	-1.372459
C	-4.005106	-1.028049	-0.507029
H	-3.146488	-0.313517	-2.445084
H	-2.449705	0.488225	-0.961891
H	-4.537776	-1.793124	-1.082777
H	-3.522916	-1.536655	0.340022
C	-5.034920	-0.019701	0.081428
C	-4.346445	0.929057	1.072021
H	-3.573600	1.537924	0.587639
H	-5.076790	1.620790	1.507987
H	-3.881103	0.373278	1.895173
C	-6.107403	-0.827446	0.822095
H	-6.848478	-0.158638	1.275811
H	-6.636633	-1.502725	0.139334
H	-5.664581	-1.432447	1.622669
C	-5.688204	0.789592	-1.046333
H	-4.958371	1.427526	-1.560603
H	-6.144308	0.128686	-1.793534
H	-6.474165	1.442110	-0.648226

TSC2-3^{IV}

	Coordinates (Angstroms)		
	X	Y	Z
C	4.853887	0.908304	0.370450
C	4.025331	-0.112860	-0.077346
C	2.635258	-0.023448	0.067508
C	2.074042	1.116814	0.670593
C	2.921340	2.138446	1.119761
C	4.299208	2.036384	0.973552
H	5.929797	0.824425	0.251876
H	4.463763	-0.993830	-0.539182
H	2.501697	3.025676	1.586475
H	4.941757	2.836525	1.328291
P	0.252086	1.305120	0.831768
P	1.561251	-1.408423	-0.469844
C	-0.023948	1.711466	2.604620
H	0.560959	2.598976	2.872692
H	-1.082291	1.983847	2.695872
C	-0.072931	2.893892	-0.044420
H	-1.133740	3.127527	0.101368
H	0.499439	3.691234	0.444174
C	0.307370	0.539744	3.527554
H	-0.307255	-0.337630	3.294101
H	1.360944	0.251441	3.443623
H	0.116264	0.810809	4.570853
C	0.265112	2.824288	-1.532433

H	1.331948	2.632563	-1.689118
H	-0.299969	2.033680	-2.038863
H	0.021365	3.773226	-2.020741
C	2.007696	-1.717579	-2.224198
H	3.084933	-1.905189	-2.301595
H	1.494841	-2.644202	-2.509201
C	1.586998	-0.564930	-3.134894
H	0.509271	-0.374837	-3.066264
H	2.113186	0.360067	-2.875358
H	1.818293	-0.799183	-4.179016
C	2.221655	-2.861934	0.445535
H	1.548057	-3.695376	0.212629
H	3.211310	-3.122120	0.052830
C	2.285574	-2.627956	1.955280
H	3.038607	-1.874823	2.208201
H	1.324470	-2.286780	2.356580
H	2.551436	-3.556165	2.470892
Co	-0.781367	-0.821598	-0.041225
H	-0.957125	-2.417748	-0.786502
C	-1.295717	-2.226549	1.307194
O	-1.533965	-3.159534	1.918212
C	-3.777557	-0.020733	-0.639696
C	-3.426746	0.819937	0.601253
H	-2.782972	0.256099	1.290527
H	-2.896081	1.735875	0.316550
H	-4.333848	1.110203	1.144562
C	-4.688411	0.818077	-1.556602
H	-4.183837	1.736391	-1.880431
H	-4.972136	0.253821	-2.452511
H	-5.605832	1.105580	-1.028948

C	-4.531966	-1.278783	-0.198900
H	-4.875089	-1.867541	-1.057072
H	-3.911176	-1.925712	0.432329
H	-5.416127	-0.998491	0.384507
C	-2.519669	-0.350154	-1.434889
H	-2.019431	0.508469	-1.888665
C	-2.119879	-1.610958	-1.844359
H	-1.417927	-1.707342	-2.668139
H	-2.752154	-2.476500	-1.671798

TSC4-5^{IV}

Coordinates (Angstroms)

	X	Y	Z
C	-5.093537	-0.590320	-0.640411
C	-3.942137	-1.296524	-0.314475
C	-2.714860	-0.637351	-0.170199
C	-2.655327	0.754117	-0.353654
C	-3.821867	1.455586	-0.684173
C	-5.032752	0.790326	-0.827712
H	-6.038441	-1.113734	-0.750147
H	-3.998148	-2.372069	-0.167099
H	-3.784379	2.531408	-0.834208
H	-5.929429	1.346220	-1.084691
P	-1.058826	1.645084	-0.177304
P	-1.195479	-1.578276	0.262638
C	-0.835097	2.459405	-1.815805
H	-1.725799	3.053568	-2.053137

H	0.001904	3.159916	-1.707369
C	-1.429649	3.045488	0.955505
H	-0.536158	3.681380	0.961807
H	-2.244773	3.641069	0.528394
C	-0.548974	1.445415	-2.922719
H	0.350347	0.855440	-2.701673
H	-1.385223	0.749530	-3.050934
H	-0.386266	1.954075	-3.878256
C	-1.773856	2.590433	2.371933
H	-2.651020	1.934237	2.379144
H	-0.938286	2.052191	2.831634
H	-1.999114	3.457392	3.001494
C	-1.656171	-2.419998	1.840494
H	-2.396279	-3.200138	1.626205
H	-0.749506	-2.920585	2.200546
C	-2.195741	-1.458953	2.900106
H	-1.511005	-0.625546	3.087425
H	-3.159591	-1.037547	2.597522
H	-2.341993	-1.987159	3.847805
C	-1.171245	-2.950507	-0.967124
H	-0.288651	-3.557508	-0.732883
H	-2.049287	-3.589361	-0.817789
C	-1.114286	-2.447719	-2.409262
H	-2.037628	-1.925476	-2.681284
H	-0.277863	-1.758023	-2.567519
H	-0.988195	-3.287222	-3.100399
Co	0.589788	0.022102	0.237562
C	2.054270	-1.030126	-0.843488
C	3.677211	0.431515	-1.002308
H	3.871683	0.180240	-2.046688

C	2.931373	1.715210	-0.807826
H	3.611239	2.572836	-0.906749
H	2.152704	1.837553	-1.567830
H	2.470321	1.785205	0.188183
C	4.785301	0.008999	-0.054286
C	5.376685	-1.341034	-0.485127
H	4.654490	-2.155696	-0.372055
H	5.702792	-1.316513	-1.531588
H	6.247844	-1.584559	0.133446
C	5.895511	1.082880	-0.159116
H	6.767400	0.764610	0.424144
H	6.216905	1.225888	-1.197279
H	5.561917	2.048269	0.235721
C	4.316226	-0.083564	1.403535
H	3.581544	-0.886937	1.530178
H	5.167835	-0.311459	2.054501
H	3.873435	0.854618	1.755643
O	2.343429	-1.978533	-1.433221
C	1.022636	-0.024127	2.078238
O	1.235658	-0.102705	3.198076

TSC6-1^{IV}

	Coordinates (Angstroms)		
	X	Y	Z

C	5.023827	0.477172	-1.288731
C	4.012384	-0.474000	-1.231508
C	2.793550	-0.188263	-0.604137

C	2.598404	1.078965	-0.028180
C	3.625366	2.029307	-0.089524
C	4.830258	1.732905	-0.714669
H	5.962445	0.241455	-1.781039
H	4.170216	-1.449296	-1.684336
H	3.483001	3.010826	0.355505
H	5.616930	2.480123	-0.755223
P	1.013648	1.494629	0.800552
P	1.459947	-1.452886	-0.550657
C	1.503697	1.931621	2.519445
H	2.293861	2.691215	2.494836
H	0.623632	2.389859	2.986266
C	0.494363	3.092708	0.053731
H	-0.417401	3.394623	0.583050
H	1.258135	3.848976	0.269322
C	1.949265	0.699608	3.305680
H	1.158224	-0.060498	3.333816
H	2.841710	0.244985	2.862035
H	2.189584	0.968995	4.339257
C	0.236477	2.993620	-1.448462
H	1.147671	2.720491	-1.991350
H	-0.531161	2.244591	-1.672819
H	-0.109464	3.957462	-1.835789
C	1.197680	-1.872178	-2.327111
H	2.129629	-2.279744	-2.737504
H	0.453111	-2.676950	-2.348446
C	0.719211	-0.682027	-3.157559
H	-0.221961	-0.276650	-2.770484
H	1.461021	0.123862	-3.162887
H	0.551942	-0.989914	-4.194863

C	2.285910	-2.950341	0.131358
H	1.534285	-3.748948	0.105828
H	3.105469	-3.256186	-0.529692
C	2.790583	-2.738677	1.557909
H	3.572564	-1.972625	1.592451
H	1.980825	-2.429586	2.229155
H	3.214455	-3.667712	1.952723
Co	-0.360378	-0.451284	0.624466
C	-1.019213	-1.987872	1.516868
C	-3.126591	-1.041602	-1.114991
O	-1.269899	-2.969020	2.043099
O	-3.042423	-1.973302	-1.850426
C	-4.362879	1.030790	-0.230061
C	-3.917487	1.690443	-1.545281
H	-2.855478	1.517192	-1.757628
H	-4.500462	1.313263	-2.394390
H	-4.064731	2.775229	-1.494005
C	-5.802478	1.476176	0.068619
H	-6.474558	1.220569	-0.759068
H	-6.195437	1.014337	0.980954
H	-5.838019	2.562858	0.207285
C	-3.453590	1.496469	0.919462
H	-3.833960	1.169420	1.893424
H	-2.425046	1.125182	0.812963
H	-3.408751	2.591704	0.933496
C	-4.360788	-0.515460	-0.403022
C	-4.487008	-1.317849	0.901889
H	-5.403722	-1.034232	1.426975
H	-3.644334	-1.132090	1.574514
H	-5.196627	-0.789432	-1.060796

H	-4.535718	-2.391280	0.695657
H	-1.977438	-0.370996	-0.836078
H	-1.175256	0.246943	-0.763845

IM1

	Coordinates (Angstroms)		
	X	Y	Z

Co	-0.853744	-0.010285	0.076337
P	0.802976	-1.539351	-0.052072
O	-2.142823	1.415712	-0.039783
C	-3.402770	1.252725	-0.159388
C	-4.051297	0.021541	-0.316086
H	-5.129495	0.031376	-0.420195
C	-4.207442	2.524210	-0.132047
H	-4.081412	3.008450	0.843148
H	-5.270817	2.349248	-0.307964
H	-3.823498	3.215546	-0.889858
C	2.422651	-0.703123	0.044370
C	3.631141	-1.397163	0.157795
H	3.636028	-2.479329	0.241837
C	4.835819	-0.701731	0.164385
H	5.771814	-1.243904	0.255627
P	0.802747	1.526518	-0.147648
C	2.427574	0.698975	-0.038226
C	3.644988	1.386480	-0.060137
H	3.664890	2.466294	-0.165295
C	4.842943	0.686796	0.043584
H	5.784880	1.226249	0.032783

O	-2.139357	-1.394135	-0.322084
C	-3.397004	-1.212050	-0.431588
C	-4.193981	-2.455050	-0.723467
H	-4.052558	-3.177531	0.087983
H	-5.260403	-2.251012	-0.839424
H	-3.814993	-2.917870	-1.641080
C	0.848224	-2.829880	1.251590
H	1.728228	-3.461163	1.083875
H	1.007678	-2.307828	2.202383
C	-0.421184	-3.679897	1.305307
H	-0.584577	-4.216877	0.365279
H	-0.333640	-4.422191	2.105074
H	-1.306133	-3.066935	1.499457
C	0.714922	-2.408262	-1.667183
H	0.792411	-1.628128	-2.434171
H	-0.308836	-2.795963	-1.722251
C	1.736490	-3.515913	-1.909556
H	1.671156	-4.302122	-1.150291
H	1.551293	-3.979347	-2.884215
H	2.758623	-3.124803	-1.916502
C	0.678007	2.814959	1.155704
H	0.846157	2.301031	2.109755
H	-0.381240	3.098827	1.140086
C	0.860564	2.394838	-1.764975
H	1.776149	2.997510	-1.787133
H	0.975444	1.613351	-2.525072
C	1.566036	4.052295	1.043585
H	1.463729	4.543290	0.070447
H	1.272471	4.775852	1.811147
H	2.620780	3.814092	1.204358

C	-0.366280	3.255995	-2.059889
H	-1.278615	2.654146	-2.084963
H	-0.499748	4.038853	-1.305611
H	-0.245152	3.743447	-3.032618
C	-1.049619	-0.078221	2.116121
O	-1.305827	-0.106266	3.220454

IM2

	Coordinates (Angstroms)		
	X	Y	Z

Co	0.028676	-1.669619	0.656104
P	-1.644248	-0.215359	0.207266
C	-0.717172	1.328389	-0.159378
C	-1.404801	2.489794	-0.530120
H	-2.480464	2.464980	-0.670191
C	-0.729031	3.689001	-0.730237
H	-1.281984	4.579108	-1.014185
P	1.649421	-0.166355	0.248148
C	0.689543	1.371520	-0.042065
C	1.352021	2.591370	-0.219770
H	2.428224	2.649327	-0.094843
C	0.649534	3.744773	-0.554055
H	1.181262	4.681645	-0.688176
C	-2.735953	-0.471471	-1.246485
H	-3.345542	0.422842	-1.413095
H	-2.078238	-0.581206	-2.116342
C	-3.624460	-1.704191	-1.081638

H	-4.334769	-1.582350	-0.256764
H	-4.200865	-1.876682	-1.995739
H	-3.030570	-2.605144	-0.886288
C	-2.761473	0.131833	1.630067
H	-2.107093	0.456642	2.446295
H	-3.150185	-0.850996	1.924181
C	-3.911009	1.115977	1.430038
H	-4.550098	0.840927	0.584493
H	-4.538034	1.125814	2.328091
H	-3.547647	2.135375	1.273348
C	2.631797	-0.444070	-1.288781
H	1.898370	-0.488701	-2.102772
H	3.041748	-1.456298	-1.185738
C	2.858161	0.216155	1.569671
H	3.483875	1.061717	1.264517
H	2.277134	0.533395	2.441967
C	3.744018	0.545702	-1.625785
H	4.479864	0.625287	-0.819064
H	4.272042	0.204903	-2.522626
H	3.348231	1.543179	-1.836087
C	3.723204	-0.997653	1.910101
H	3.108087	-1.847414	2.228757
H	4.328297	-1.315948	1.053995
H	4.406546	-0.751555	2.728811
H	0.020781	-0.788125	1.873903
C	0.055498	-2.568108	-0.949154
O	0.074993	-3.076178	-1.970865

IM3

	Coordinates (Angstroms)		
	X	Y	Z
C	-1.298722	1.268261	-0.109664
C	-2.367864	2.167111	-0.194856
H	-3.373031	1.806171	-0.388162
C	-2.153451	3.531243	-0.029373
H	-2.989069	4.221248	-0.092478
C	-0.870933	4.008191	0.228653
H	-0.703106	5.070228	0.377835
C	0.202847	3.125480	0.282649
H	1.198545	3.513892	0.469346
C	0.005789	1.753545	0.093191
C	0.506893	-1.950868	1.607032
C	1.855986	-2.409436	-0.847542
Co	0.402571	-1.542348	-0.184207
O	0.619255	-2.174307	2.718497
O	2.773944	-2.899497	-1.312121
P	-1.586781	-0.532817	-0.188251
P	1.397984	0.567727	0.023019
C	-2.658986	-0.826823	-1.642954
H	-3.594909	-0.272049	-1.518588
H	-2.134065	-0.402245	-2.504995
C	-2.932657	-2.315084	-1.855079
H	-3.521313	-2.460156	-2.765980
H	-1.996360	-2.874996	-1.967122
H	-3.494472	-2.746148	-1.019607
C	-2.594412	-0.975909	1.290108
H	-2.653366	-2.071257	1.273786

H	-1.984620	-0.710452	2.161212
C	-3.988571	-0.367744	1.417148
H	-4.487237	-0.795765	2.292879
H	-3.944477	0.715625	1.559689
H	-4.613053	-0.581832	0.543910
C	2.344821	0.987688	-1.501039
H	1.647538	0.829679	-2.331641
H	3.110932	0.208070	-1.592114
C	2.989228	2.367876	-1.586327
H	3.568335	2.441921	-2.512933
H	2.238600	3.163222	-1.601961
H	3.673835	2.552521	-0.751642
C	2.497900	0.985736	1.431213
H	2.766656	2.046817	1.393004
H	1.916287	0.832168	2.347223
C	3.755746	0.115229	1.438125
H	4.359316	0.339257	2.323347
H	3.509093	-0.952788	1.463062
H	4.376498	0.300641	0.555134
H	0.178712	-1.250579	-1.639849

IM4

	Coordinates (Angstroms)		
	X	Y	Z

C	-1.474917	1.141040	-0.022733
C	-2.649893	1.899321	-0.030057
H	-3.607834	1.425762	-0.218087

C	-2.597584	3.269768	0.204992
H	-3.514528	3.850925	0.201979
C	-1.375893	3.892471	0.452994
H	-1.338868	4.959134	0.651126
C	-0.197864	3.152513	0.430885
H	0.752057	3.647814	0.608375
C	-0.238927	1.778763	0.172066
C	0.842628	-1.899138	1.624640
C	2.220456	-2.146509	-0.794478
Co	0.655600	-1.384948	-0.224790
O	0.933047	-2.250131	2.702623
O	3.169739	-2.664948	-1.151695
P	-1.466224	-0.680430	-0.212094
P	1.270416	0.769114	-0.020823
H	-0.009959	-2.706420	-0.584287
C	-2.467481	-1.025855	-1.708351
H	-3.431567	-0.518731	-1.589640
H	-1.952623	-0.549126	-2.549805
C	-2.674667	-2.515639	-1.971043
H	-3.284434	-2.649089	-2.869967
H	-1.719950	-3.027331	-2.128692
H	-3.190969	-3.006318	-1.138904
C	-2.387068	-1.371977	1.221533
H	-2.205813	-2.452200	1.185464
H	-1.878574	-0.995251	2.116416
C	-3.882875	-1.078529	1.299895
H	-4.308659	-1.615113	2.153979
H	-4.079401	-0.013259	1.449855
H	-4.414605	-1.409947	0.402349
C	2.058718	1.313439	-1.591501

H	1.369859	1.011999	-2.389707
H	2.950855	0.684784	-1.700451
C	2.423733	2.789358	-1.720153
H	2.929897	2.955139	-2.676886
H	1.536053	3.428542	-1.698904
H	3.103734	3.111390	-0.924572
C	2.403100	1.244672	1.336254
H	2.622260	2.315052	1.254630
H	1.857220	1.091317	2.274047
C	3.691616	0.422786	1.320626
H	4.351505	0.747883	2.130791
H	3.483454	-0.643408	1.465453
H	4.236017	0.541508	0.377697

IM5

Coordinates (Angstroms)

	X	Y	Z
C	1.718667	1.040698	0.089371
C	2.963361	1.669834	0.208606
H	3.866561	1.078570	0.317482
C	3.060748	3.057064	0.187373
H	4.032836	3.531103	0.280532
C	1.914727	3.833752	0.035625
H	1.989763	4.916053	-0.001421
C	0.669445	3.223190	-0.062810
H	-0.215375	3.840179	-0.181413
C	0.556790	1.828393	-0.013137

C	-0.888350	-1.650556	-1.718615
C	-0.755652	-1.404250	1.901506
Co	-0.827973	-1.237472	0.068252
O	-0.841002	-1.964287	-2.812936
O	-0.620901	-1.576971	3.019633
P	1.548602	-0.782171	0.004356
P	-1.083419	1.018613	-0.063808
H	-0.598427	-2.738201	0.160841
C	2.600707	-1.432267	1.364985
H	3.616103	-1.032565	1.270245
H	2.191927	-1.033168	2.300249
C	2.624480	-2.960784	1.390178
H	3.214642	-3.310953	2.242812
H	1.615791	-3.379013	1.484327
H	3.075910	-3.370516	0.480340
C	2.374136	-1.308558	-1.558505
H	2.140406	-2.375398	-1.661028
H	1.845207	-0.795368	-2.370717
C	3.878526	-1.082750	-1.682235
H	4.236722	-1.519972	-2.620317
H	4.126001	-0.017251	-1.697800
H	4.431338	-1.555993	-0.864134
C	-2.066168	1.641429	1.365122
H	-1.470073	1.424584	2.258928
H	-2.940308	0.979618	1.410233
C	-2.510819	3.101291	1.360935
H	-3.183782	3.275420	2.206938
H	-1.664280	3.784593	1.470004
H	-3.054341	3.362973	0.447287
C	-1.888303	1.683117	-1.574011

H	-1.896132	2.777168	-1.513058
H	-1.241056	1.412339	-2.416046
C	-3.302286	1.143973	-1.786837
H	-3.744951	1.606139	-2.674631
H	-3.296727	0.060498	-1.948477
H	-3.957017	1.363194	-0.936402
C	-3.132903	-1.709426	0.201121
O	-4.118826	-2.266720	0.212326

IM6

Coordinates (Angstroms)

	X	Y	Z
C	0.735587	1.548419	0.087082
C	1.448996	2.745536	0.217079
H	2.522381	2.729032	0.379182
C	0.790149	3.967315	0.133400
H	1.350700	4.891429	0.234016
C	-0.584164	4.004197	-0.091795
H	-1.096344	4.957319	-0.178836
C	-1.306070	2.819447	-0.192689
H	-2.378255	2.860703	-0.355940
C	-0.659750	1.583882	-0.080293
C	0.018609	-2.014591	-1.828239
C	-0.084980	-2.083208	1.747035
Co	0.035143	-1.715648	-0.031809
O	-0.079618	-2.218796	-2.944976
O	-0.239239	-2.336712	2.846843

P	1.590963	-0.065284	0.050779
P	-1.572015	-0.002458	-0.055856
H	-0.994117	-2.827219	-0.084291
C	2.735644	-0.075053	1.482654
H	3.391693	0.800634	1.432857
H	2.117468	0.037008	2.380290
C	3.553899	-1.364607	1.545332
H	4.167722	-1.374737	2.451263
H	2.904369	-2.248444	1.570342
H	4.224122	-1.457071	0.684259
C	2.639650	-0.063335	-1.463164
H	3.049962	-1.078536	-1.530911
H	1.942397	0.045495	-2.302239
C	3.754345	0.973330	-1.562595
H	4.332228	0.791877	-2.474786
H	3.354836	1.989659	-1.622134
H	4.446946	0.918745	-0.716026
C	-2.574418	0.026252	1.491055
H	-1.851147	0.116809	2.310619
H	-3.012062	-0.976341	1.572012
C	-3.658013	1.092339	1.624086
H	-4.196769	0.944479	2.566025
H	-3.233174	2.100213	1.641877
H	-4.390161	1.037846	0.811809
C	-2.772883	0.084911	-1.442246
H	-3.354239	1.010255	-1.362905
H	-2.187483	0.152938	-2.366361
C	-3.698680	-1.131236	-1.475274
H	-4.369861	-1.066740	-2.337395
H	-3.132673	-2.065919	-1.557296

H	-4.318292	-1.188357	-0.573918

IM7

	Coordinates (Angstroms)		
	X	Y	Z

C	4.529641	-0.502989	-0.232519
C	5.806126	-1.051019	-0.395810
H	5.926984	-2.105681	-0.618573
C	6.934087	-0.247497	-0.269738
H	7.920640	-0.680046	-0.402054
C	6.794456	1.107612	0.017143
H	7.672237	1.740448	0.100344
C	5.530421	1.655108	0.210927
H	5.443944	2.710403	0.445168
C	4.388537	0.853138	0.106987
C	1.227271	0.433862	-1.755116
C	1.084762	-0.725707	1.591064
Co	1.282244	-0.178434	-0.085367
O	1.268176	0.808474	-2.836506
O	1.013878	-1.120843	2.663736
P	3.024132	-1.501256	-0.485812
P	2.718816	1.511701	0.474336
H	0.554247	-1.429229	-0.463793
C	3.218261	-2.968260	0.592012
H	4.189442	-3.416971	0.354775
H	3.284812	-2.603988	1.622741
C	2.100446	-3.997049	0.437994

H	2.281414	-4.836747	1.115735
H	1.124375	-3.570019	0.686694
H	2.050249	-4.392451	-0.581857
C	3.024335	-2.129956	-2.215925
H	2.011902	-2.520895	-2.371193
H	3.127760	-1.256036	-2.867147
C	4.067168	-3.182667	-2.586267
H	3.872432	-3.528292	-3.606510
H	5.080742	-2.773953	-2.566313
H	4.028135	-4.055053	-1.927079
C	2.715457	1.919531	2.271533
H	2.992390	0.992543	2.786923
H	1.672940	2.125705	2.532649
C	3.604297	3.070121	2.735948
H	3.447077	3.226946	3.807914
H	4.665276	2.853081	2.585346
H	3.362482	4.007564	2.225746
C	2.624141	3.105167	-0.431249
H	3.443830	3.741591	-0.082177
H	2.824923	2.887340	-1.485819
C	1.287064	3.824999	-0.266774
H	1.312006	4.772500	-0.813420
H	0.463112	3.226374	-0.667847
H	1.075012	4.050459	0.783519
C	-4.536233	0.005423	-0.209359
C	-5.898866	0.176888	-0.466976
H	-6.270460	1.108514	-0.878281
C	-6.794246	-0.853663	-0.197784
H	-7.849780	-0.717882	-0.410543
C	-6.336362	-2.054510	0.337271

H	-7.033534	-2.862232	0.535848
C	-4.988082	-2.216394	0.643255
H	-4.654676	-3.145290	1.093908
C	-4.081883	-1.185456	0.382649
C	-1.388239	-0.591698	-1.825196
C	-0.814105	1.385386	1.046308
Co	-1.290330	0.360499	-0.306982
O	-1.466435	-1.134291	-2.826890
O	-0.631312	2.109250	1.919309
P	-3.293650	1.272800	-0.639914
P	-2.345581	-1.210667	0.952701
H	-0.869172	1.525449	-1.142098
C	-3.681510	2.758920	0.356927
H	-4.749601	2.968893	0.225254
H	-3.540832	2.485896	1.408507
C	-2.839643	3.978735	-0.019260
H	-3.068503	4.803205	0.662361
H	-1.766077	3.775729	0.049568
H	-3.053881	4.315438	-1.038189
C	-3.524478	1.747845	-2.403161
H	-2.628981	2.331924	-2.644761
H	-3.462531	0.824666	-2.989087
C	-4.785448	2.525347	-2.780005
H	-4.666983	2.915049	-3.796067
H	-5.674437	1.889979	-2.775673
H	-4.962528	3.378267	-2.117884
C	-2.490731	-0.708903	2.721925
H	-2.954346	0.284630	2.704461
H	-1.475673	-0.577307	3.111016
C	-3.281583	-1.645465	3.631511

H	-3.353976	-1.200571	4.629008
H	-4.300020	-1.802613	3.263232
H	-2.793439	-2.618955	3.736835
C	-1.788920	-2.956300	0.976647
H	-0.847747	-2.970389	1.537151
H	-2.503541	-3.532389	1.573480
C	-1.615285	-3.590005	-0.400592
H	-1.382920	-4.653308	-0.286836
H	-2.529641	-3.509954	-0.998328
H	-0.792074	-3.130724	-0.956317

TS1-2

Coordinates (Angstroms)

	X	Y	Z

Co	-0.808372	0.053875	0.192226
P	0.698911	-1.615232	0.053841
O	-2.153976	1.445484	0.239668
C	-3.381891	1.457577	-0.077627
C	-4.195327	0.360652	-0.443233
H	-5.251032	0.582952	-0.542884
C	-4.024647	2.817986	0.009654
H	-3.867997	3.232888	1.010926
H	-5.093801	2.793907	-0.209029
H	-3.529300	3.488040	-0.702254
C	2.373955	-0.890628	-0.026180
C	3.510191	-1.707322	0.021435
H	3.412400	-2.776588	0.180631

C	4.776946	-1.156517	-0.139425
H	5.651935	-1.797912	-0.101152
P	1.009690	1.535569	-0.158574
C	2.517658	0.498099	-0.204930
C	3.796428	1.031576	-0.395531
H	3.921357	2.093986	-0.575434
C	4.919033	0.210645	-0.363242
H	5.905336	0.640533	-0.507904
O	-2.642776	-1.453463	-0.642261
C	-3.843998	-0.979152	-0.590149
C	-4.920683	-2.018983	-0.715381
H	-4.790922	-2.763971	0.078021
H	-5.924491	-1.595438	-0.646455
H	-4.809847	-2.541915	-1.671776
C	0.709961	-2.828290	1.427029
H	1.503287	-3.561598	1.247688
H	0.981104	-2.282613	2.337777
C	-0.642385	-3.525339	1.581809
H	-0.897721	-4.106166	0.689428
H	-0.609795	-4.213182	2.432250
H	-1.449539	-2.804926	1.755671
C	0.444149	-2.577066	-1.493022
H	0.518077	-1.848404	-2.307602
H	-0.603031	-2.898963	-1.458630
C	1.372404	-3.763418	-1.734960
H	1.327854	-4.496240	-0.922721
H	1.068840	-4.272899	-2.655286
H	2.411261	-3.444801	-1.860988
C	1.231957	2.782998	1.181747
H	1.451512	2.213945	2.093292

H	0.231900	3.211638	1.322816
C	1.036294	2.471557	-1.738049
H	2.001061	2.981396	-1.842641
H	0.974118	1.725341	-2.538369
C	2.259471	3.896075	0.989533
H	2.106734	4.437282	0.050089
H	2.170804	4.620871	1.806032
H	3.282774	3.510616	1.003973
C	-0.123270	3.462853	-1.837783
H	-1.087247	2.954531	-1.732993
H	-0.062743	4.232934	-1.060961
H	-0.104596	3.966168	-2.809602
H	-1.000457	-0.105906	-1.441199
H	-1.749541	-0.662209	-1.155050
C	-0.747924	0.079576	2.041398
O	-0.740900	0.194199	3.172177

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