

Supporting Information

for

Is the Polarization of the C=C Bond Imperative for the Bifunctional Outer-Sphere C=C Hydrogenation?

Xinliang Ai,^{a+} Xiaofeng Xie,^{a+} Xueqing Song,^a Longfei Li^{a*} and Henry F. Schaefer, III^{b*}

^a College of Pharmacy, Key Laboratory of Pharmaceutical Quality Control of Hebei Province, Key Laboratory of Medicinal Chemistry and Molecular Diagnosis of Ministry of Education, Hebei University, Baoding 071002, Hebei, P. R. China

^b Center for Computational Quantum Chemistry, University of Georgia, Athens, Georgia 30602, United States

+ These authors contributed equally to this work.

*Email: lilongfei@hbu.edu.cn (L.L.); ccq@uga.edu (H.F.S.)

Table S1. The computed potential energies (E , a.u.) and relative potential energies (ΔE , kcal/mol) at the ω B97X-D/BS-II level. The relative Gibbs free energies (ΔG , 298K) are in kcal/mol.	S2
Table S2. The imaginary frequencies (in cm^{-1}) of transition states at the ω B97X-D/BS-I level....	S4
Figure S1. The pathways for the bifunctional outer-sphere C=C hydrogenations by the Mn pincer complex A1.....	S7
Figure S2. The comparisons between triplet states and singlet states of Mn pincer complexes in the outer-sphere C=C hydrogenation.....	S9
Figure S3. The energy barriers of hydrogen addition processes (ΔG^\ddagger in kcal/mol), the LUMO and HOMO energies for alkene derivatives. $\text{BPI}_{\text{C}(1)=\text{C}(2)}$ denotes the bond polarity index of C(1)=C(2) bond, and Per denotes the percentage of ionic portion in total NRT bond order.	S10
Figure S4. The energy profiles for the asymmetric outer-sphere bifunctional hydrogenation of (1-chlorovinyl)benzene catalyzed by designed Mn complex. The relative Gibbs free energies (ΔG) are in kcal/mol.	S12
Figure S5. The predicted enantiomeric excess (ee) for (1-fluorovinyl)benzene, (1-chlorovinyl)benzene, the corresponding equation. The relative Gibbs free energies (ΔG) are in kcal/mol.	S13
Cartesian coordinates of all stationary points optimized at ω B97X-D/BS-I level in toluene solvent.	S14

Energy summary.

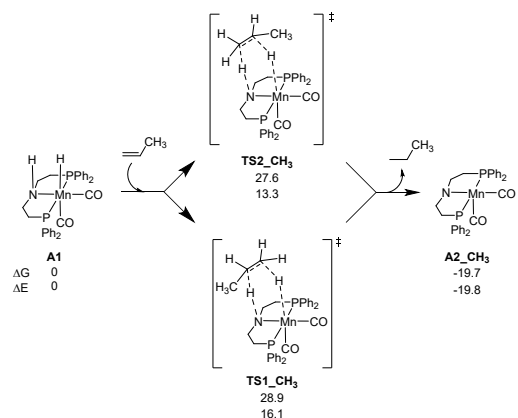
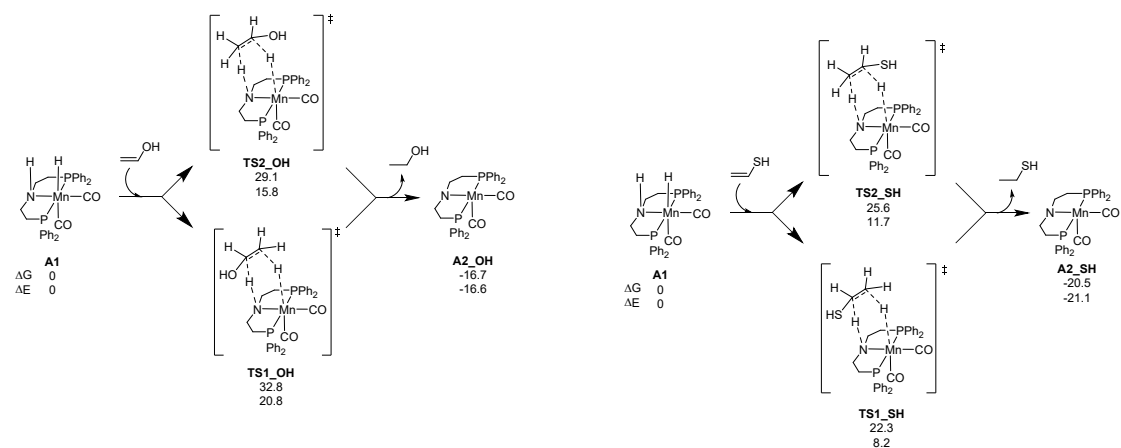
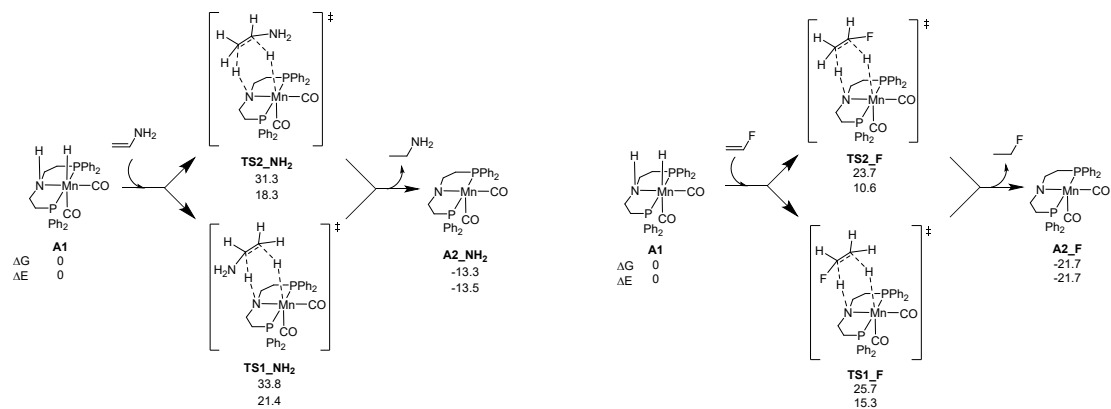
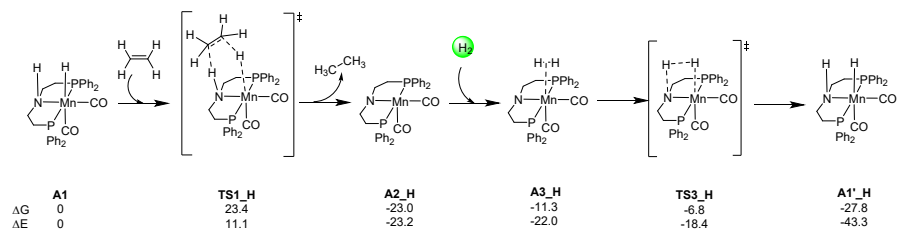
Table S1. The computed potential energies (E , a.u.) and relative potential energies (ΔE , kcal/mol) at the ω B97X-D/BS-II level. The relative Gibbs free energies (ΔG , 298K) are in kcal/mol.

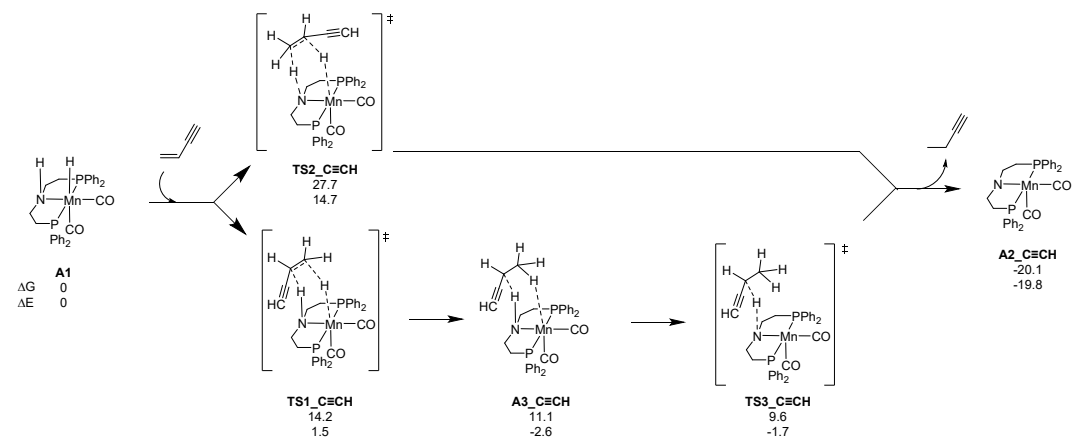
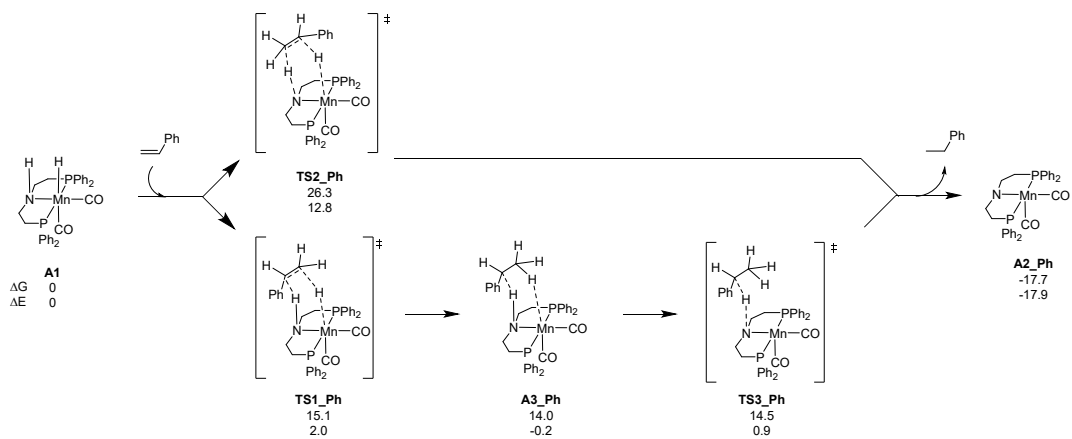
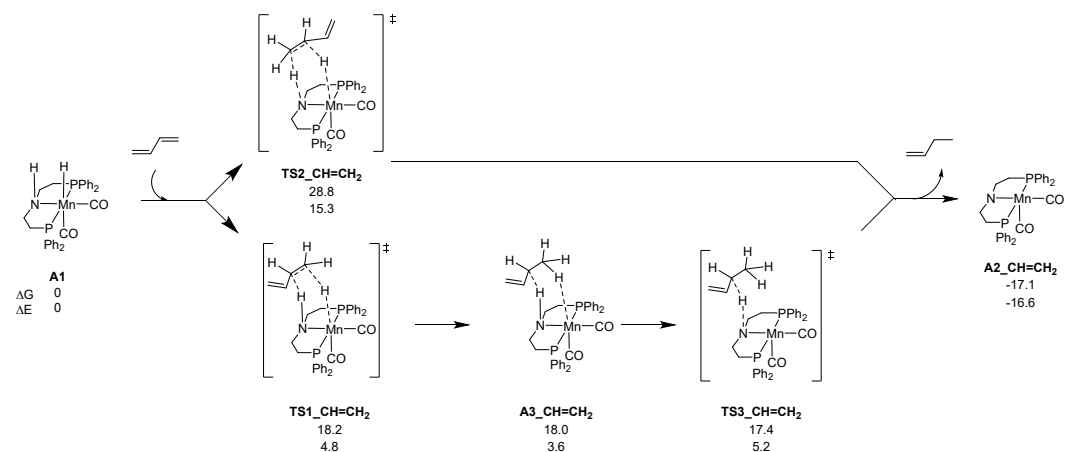
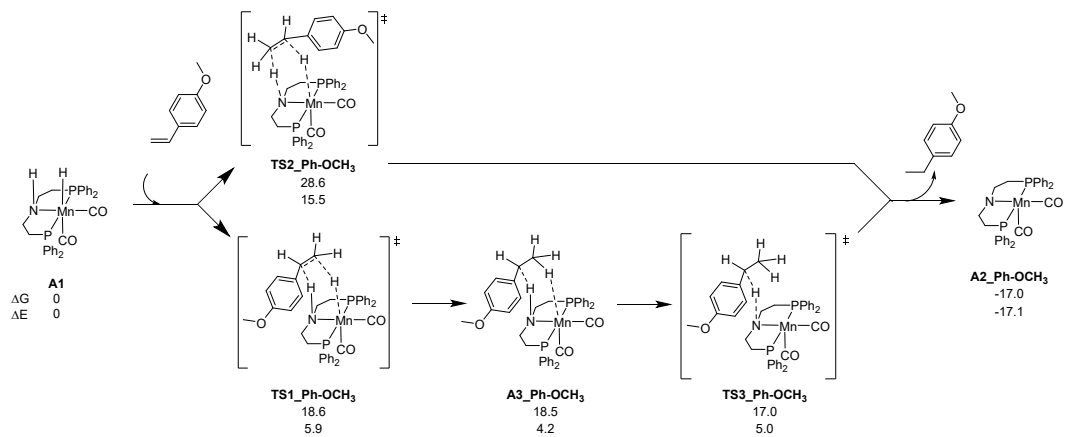
Complex	E	ΔE	G	ΔG
A1	-2153.5931	0.0	-2153.1291	0.0
A1_triplet	-2153.5446	30.4	-2153.0898	24.6
TS1_H	-2232.1632	11.1	-2231.6508	23.4
TS2_CH ₃	-2271.4813	13.3	-2270.9399	27.6
TS1_CH ₃	-2271.4770	16.1	-2270.9379	28.9
TS2_Ph	-2463.2141	12.8	-2462.6256	26.3
TS1_Ph	-2463.2313	2.0	-2462.6434	15.1
TS2_F	-2331.4114	10.6	-2330.9070	23.7
TS1_F	-2331.4040	15.3	-2330.9037	25.7
TS2_NH ₂	-2287.5205	18.3	-2286.9914	31.3
TS1_NH ₂	-2287.5154	21.4	-2286.9874	33.8
TS2_SH	-2630.3704	11.7	-2629.8590	25.6
TS1_SH	-2630.3761	8.2	-2629.8643	22.3
TS2_OH	-2307.3889	15.8	-2306.8716	29.1
TS1_OH	-2307.3808	20.8	-2306.8657	32.8
TS2_CHO	-2345.4936	10.9	-2344.9736	23.8
TS1_CHO	-2345.5195	-5.3	-2344.9994	7.7
TS2_CH=CH ₂	-2309.5590	15.3	-2309.0147	28.8
TS1_CH=CH ₂	-2309.5756	4.8	-2309.0316	18.2
TS2_C≡CH	-2308.2994	14.7	-2307.7794	27.7
TS1_C≡CH	-2308.3205	1.5	-2307.8009	14.2
TS2_Ph-NO ₂	-2667.7322	9.2	-2667.1437	23.8
TS1_Ph-NO ₂	-2667.7519	-3.2	-2667.1648	10.5
TS2_Ph-OCH ₃	-2577.7394	15.5	-2577.1225	28.6
TS1_Ph-OCH ₃	-2577.7545	5.9	-2577.1384	18.6
A2_NH ₂	-2152.3848	-13.5	-2151.9439	-13.3
A2_OH	-2152.3848	-16.6	-2151.9439	-16.7
A2_CH ₃	-2152.3848	-19.8	-2151.9439	-19.7
A2_F	-2152.3848	-21.7	-2151.9439	-21.7
A2_H	-2152.3848	-23.2	-2151.9439	-23.0
A2_H_triplet	-2152.3540	-3.9	-2151.9204	-8.2
A2_SH	-2152.3848	-21.1	-2151.9439	-20.5
A2_Ph-OCH ₃	-2152.3848	-17.1	-2151.9439	-17.0
A2_CH=CH ₂	-2152.3848	-16.6	-2151.9439	-17.1
A2_Ph	-2152.3848	-17.9	-2151.9439	-17.7
A2_C≡CH	-2152.3848	-19.8	-2151.9439	-20.1
A2_Ph-NO ₂	-2152.3848	-18.7	-2151.9439	-19.7
A2_CHO	-2152.3848	-18.4	-2151.9439	-19.0
A3_H	-2153.5591	-22.0	-2153.1029	-11.3
A3_Ph-OCH ₃	-2577.7573	4.2	-2577.1386	18.5
A3_CH=CH ₂	-2309.5777	3.6	-2309.0319	18.0
A3_Ph	-2463.2348	-0.2	-2462.6453	14.0
A3_C≡CH	-2308.3271	-2.6	-2307.8058	11.1
A3_Ph-NO ₂	-2667.7687	-13.8	-2667.1774	2.6
A3_CHO	-2345.5480	-23.3	-2345.0253	-8.6

TS3_H	-2153.5534	-18.4	-2153.0957	-6.8
TS3_Ph-OCH₃	-2577.7560	5.0	-2577.1409	17.0
TS3_CH=CH₂	-2309.5750	5.2	-2309.0329	17.4
TS3_Ph	-2463.2331	0.9	-2462.6445	14.5
TS3_C≡CH	-2308.3256	-1.7	-2307.8082	9.6
TS3_Ph-NO₂	-2667.7581	-7.1	-2667.1714	6.4
TS3_CHO	-2345.5256	-9.2	-2345.0066	3.2
B1	-1927.4090	0.0	-1926.9328	0.0
TSB1-2_a	-2336.2876	6.7	-2335.6968	19.8
TSB1-2_b	-2336.2855	8.1	-2335.6929	22.3
TSB1-2_c	-2336.2750	14.6	-2335.6850	27.3
TSB1-2_d	-2336.2743	15.1	-2335.6819	29.2
B2	-1926.1950	-14.9	-1925.7425	-15.4
B3	-1927.3709	-14.8	-1926.9009	-3.4
C1	-1927.4090	0.0	-1926.9328	0.0
TSB3-1	-1927.3644	-10.7	-1926.8956	-0.1
TSC1-2_a	-2696.6586	2.6	-2696.0694	15.8
TSC1-2_b	-2696.6563	4.0	-2696.0662	17.9
TSC1-2_c	-2696.6352	17.3	-2696.0464	30.3
TSC1-2_d	-2696.6331	18.7	-2696.0415	33.3
C2	-1926.1950	-16.8	-1925.7425	-17.0
C3	-1927.3709	-16.6	-1926.9009	-5.0
TSC3-1	-1927.3644	-12.6	-1926.8956	-1.7
C1'	-1927.4090	-40.6	-1926.9328	-25.0

Table S2. The imaginary frequencies (in cm^{-1}) of transition states at the $\omega\text{B97X-D/BS-I}$ level.

Complex	Imaginary frequencies (in cm^{-1})
TS1_H	508.69 <i>i</i>
TS2_CH ₃	501.19 <i>i</i>
TS1_CH ₃	539.27 <i>i</i>
TS2_Ph	620.05 <i>i</i>
TS1_Ph	779.71 <i>i</i>
TS2_F	747.34 <i>i</i>
TS1_F	775.27 <i>i</i>
TS2_NH ₂	449.18 <i>i</i>
TS1_NH ₂	606.81 <i>i</i>
TS2_SH	537.77 <i>i</i>
TS1_SH	676.68 <i>i</i>
TS2_OH	524.38 <i>i</i>
TS1_OH	746.05 <i>i</i>
TS2_CHO	485.85 <i>i</i>
TS1_CHO	439.80 <i>i</i>
TS2_CH=CH ₂	567.67 <i>i</i>
TS1_CH=CH ₂	732.41 <i>i</i>
TS2_C≡CH	706.60 <i>i</i>
TS1_C≡CH	759.00 <i>i</i>
TS2_Ph-NO ₂	576.19 <i>i</i>
TS1_Ph-NO ₂	906.08 <i>i</i>
TS2_Ph-OCH ₃	604.76 <i>i</i>
TS1_Ph-OCH ₃	705.04 <i>i</i>
TS3_H	944.82 <i>i</i>
TS3_Ph-OCH ₃	713.91 <i>i</i>
TS3_CH=CH ₂	948.08 <i>i</i>
TS3_Ph	804.17 <i>i</i>
TS3_C≡CH	818.57 <i>i</i>
TS3_Ph-NO ₂	1430.80 <i>i</i>
TS3_CHO	1270.45 <i>i</i>
TSB1-2_a	784.38 <i>i</i>
TSB1-2_b	717.65 <i>i</i>
TSB1-2_c	619.52 <i>i</i>
TSB1-2_d	558.72 <i>i</i>
TSC1-2_a	804.08 <i>i</i>
TSC1-2_b	798.48 <i>i</i>
TSC1-2_c	948.87 <i>i</i>
TSC1-2_d	918.53 <i>i</i>
TSB3-1	1083.12 <i>i</i>
TSC3-1	1083.12 <i>i</i>





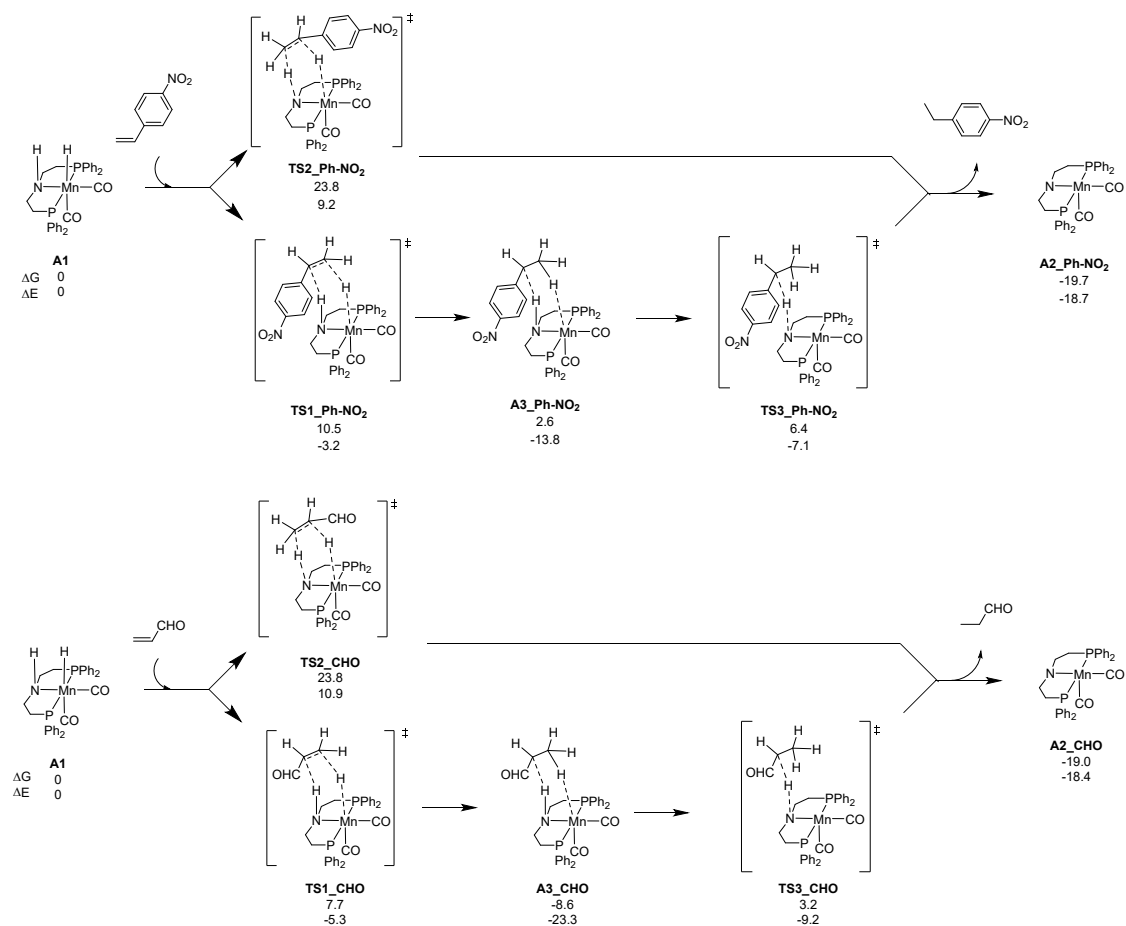


Figure S1. The pathways for the bifunctional outer-sphere C=C hydrogenations by the Mn pincer complex **A1**.

The pathway for catalytic bifunctional hydrogenation of ethylene is shown in Figure S1. Through the transition state **TS1_H**, the hydride and hydrogen in **A1** move to the C=C bond in a concerted manner. The energy barrier for the step is 23.4 kcal/mol. The optimized geometric structure of **TS1_H** is shown in Figure 2 in the main text, indicating no elongation of the N-H bond in Mn pincer complex (1.069 Å). The generated complex **A2_H** undergoes the hydrogen addition over the transition state **TS3_H** with an energy barrier of 16.2 kcal/mol. After that, the catalytic Mn pincer complex **A1** is regenerated.

The pathways for the bifunctional hydrogenations of alkene derivatives with various substituents are shown in Figure S1. The hydrogen activation steps are same with the step via **TS1_H**, and thus omitted in Figure S1 for clarity. The hydride transfer through the transition states **TS2** will generate the instable anionic RCH₂CH₂⁻ moiety,

which will abstract the amine proton spontaneously. Therefore, the bifunctional outer-sphere C=C hydrogenations through **TS2** is mediated in a concerted manner. In contrast, the hydride transfer through the transition state **TS1** will generate the anionic RCH⁻CH₃ moiety. For -NH₂, -OH, -CH₃, -F, -SH substituents, the anionic RCH⁻CH₃ moiety are destabilized by the “push” effect, and concerted manners are predicted. For -Ph-OCH₃, -CH=CH₂, -Ph, -C≡CH, -Ph-NO₂ and -CHO substituents, the RCH⁻CH₃ moiety are stabilized by the “pull” effects, and stepwise manners are predicted.

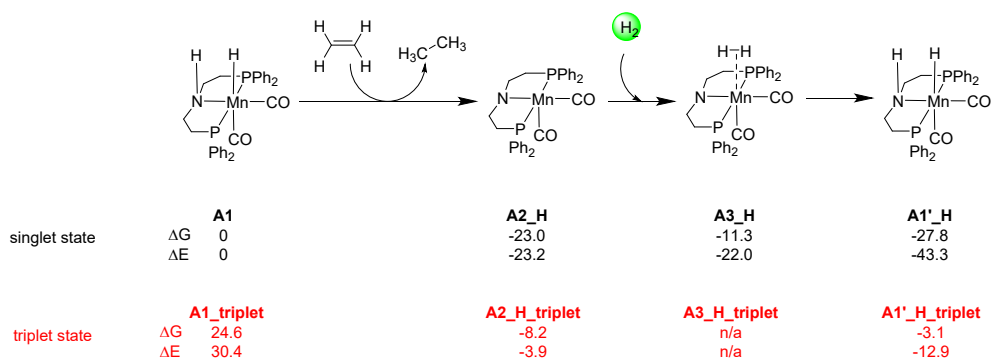


Figure S2. The comparisons between triplet states and singlet states of Mn pincer complexes in the outer-sphere C=C hydrogenation.

The triplet states and singlet states of Mn pincer complexes involved in the outer-sphere C=C hydrogenation are compared in Figure S2. The energies are relative to the singlet structure **A1**. The n/a denotes the structure **A1_H_triplet** cannot be located in the structure optimizations. The energies of Mn pincer complexes in singlet states are lower than those in triplet states, suggesting the Mn pincer complexes have singlet ground states.

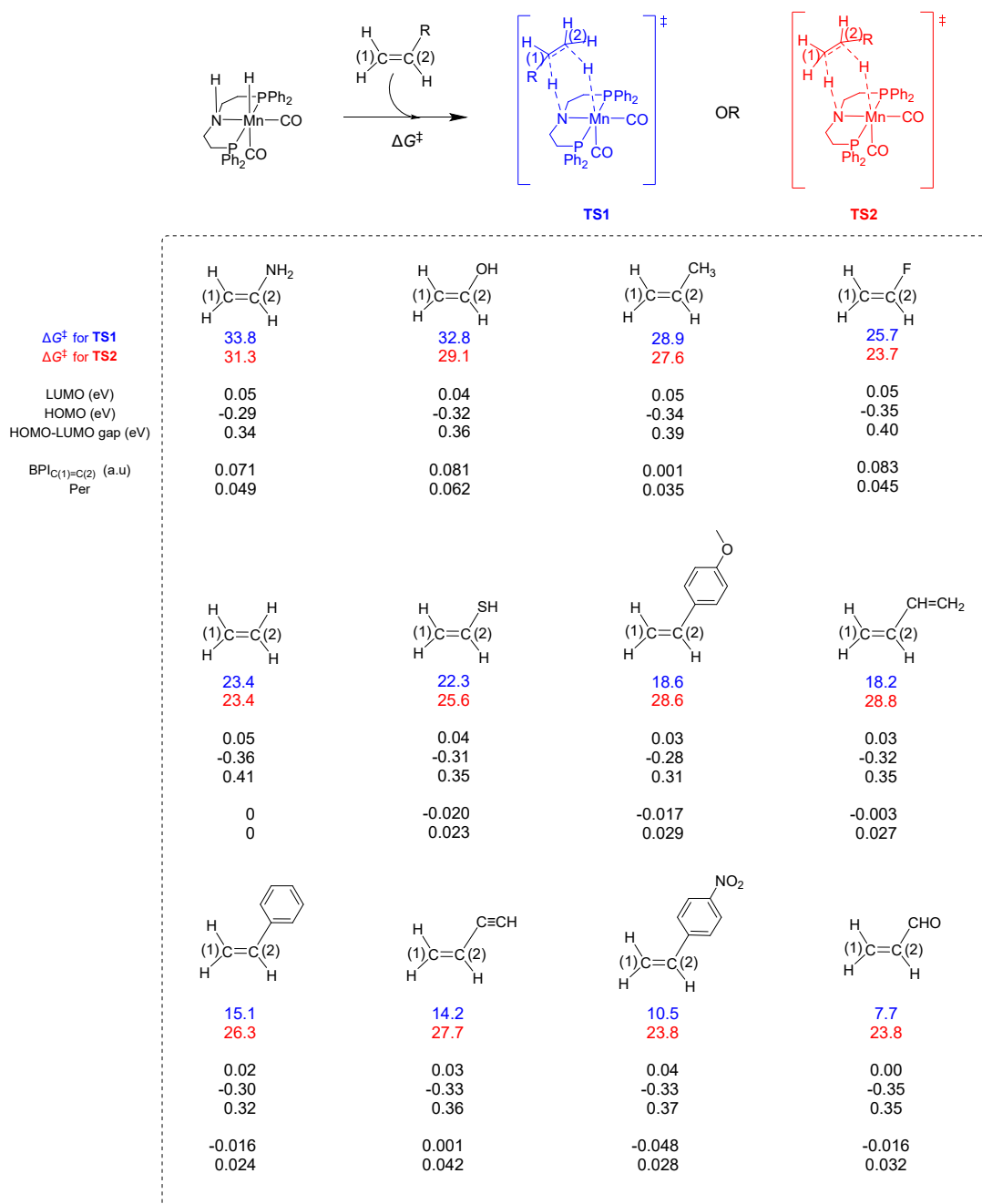


Figure S3. The energy barriers of hydrogen addition processes (ΔG^\ddagger in kcal/mol), the LUMO and HOMO energies for alkene derivatives. BPI_{C(1)=C(2)} denotes the bond polarity index of C(1)=C(2) bond, and Per denotes the percentage of ionic portion in total NRT bond order.

The BPI between atoms A and B in a molecule is defined as

$$\text{BPI}_{AB} = (\text{EI}_A - \text{EI}_A^{\text{ref}}) - (\text{EI}_B - \text{EI}_B^{\text{ref}})$$

where EI^{ref} is reference EI value derived from calculation of homonuclear species.¹

EI_A can be regarded as average energy per valence electron of atom A. The bond polarity index of C(1)=C(2) bonds (BPI_{C(1)=C(2)}) is computed with the Multiwfn

software developed by Lu.² It is suggested the C(1)=C(2) bonds with -NH₂ and -OH substituents own high values of BPI, while the C(1)=C(2) bonds with -C≡CH and -Ph-NO₂, -CHO substituents own low values of BPI. This suggests the polarization of C=C bonds is not the controlling factor for the outer-sphere bifunctional C=C bond hydrogenations.

The natural resonance theory (NRT) provides an analysis of molecular electron density in terms of resonance structures and weights.³ It also measures bond order and valency that are closely related to classical resonance theory concepts. Herein, the NRT bond order is computed using the NBO program, and the bond polarity of C(1)=C(2) bond is measured by percentage of ionic portion in total bond order (Per in Figure S3). It is suggested the C(1)=C(2) bonds with -NH₂ and -OH substituents own high values of Per, while the C(1)=C(2) bonds with -Ph-NO₂ and -CHO substituents own low values of Per. This suggests the polarization of C=C bonds is not the controlling factor for the outer-sphere bifunctional C=C bond hydrogenations.

The asymmetric outer-sphere bifunctional hydrogenation of (1-chlorovinyl)benzene catalyzed by designed Mn complex.

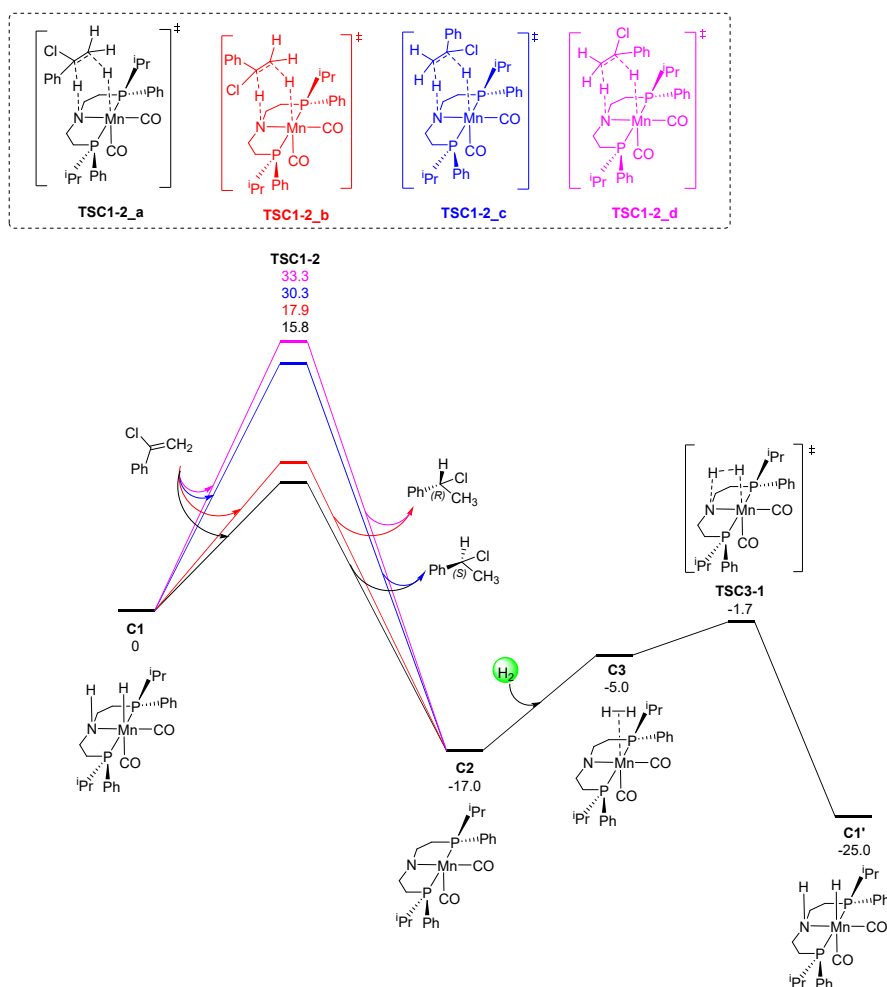
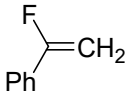
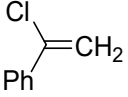


Figure S4. The energy profiles for the asymmetric outer-sphere bifunctional hydrogenation of (1-chlorovinyl)benzene catalyzed by designed Mn complex. The relative Gibbs free energies (ΔG) are in kcal/mol.

The (1-chlorovinyl)benzene molecule is selected as the prochiral alkene model. The energy profiles including four possible pathways are shown in Figure S4. The hydride and hydrogen can transfer to the C=C bond in a stepwise or concerted manner, and the (1-chloroethyl)benzene is produced. The hydride transfer step is the chiral determining step. The pathway via six-membered transition state **TSC1-2_a** is most favorable with an energy barrier of 15.8 kcal/mol, which is 2.1 kcal/mol lower than that for the second-lowest transition state **TSC1-2_b**. The generated intermediate **C2** can undergo the hydrogen activation to regenerate the starting species **C1** through the transition state **TSC3-1** with an energy barrier of 15.3 kcal/mol.

The predicted enantiomeric excess (ee) for alkenes.

			
(1-fluorovinyl)benzene		(1-chlorovinyl)benzene	
T (°C)	ee	T (°C)	ee
25	97.1%	25	94.3%
50	96.0%	50	96.3%
80	94.4%	80	90.4%

$$ee = \frac{1 - e^{-\Delta\Delta G^\ddagger/RT}}{1 + e^{-\Delta\Delta G^\ddagger/RT}} * 100$$

Figure S5. The predicted enantiomeric excess (ee) for (1-fluorovinyl)benzene, (1-chlorovinyl)benzene, the corresponding equation. The relative Gibbs free energies (ΔG) are in kcal/mol.

According to the computed Gibbs free energy differences ($\Delta\Delta G^\ddagger$), the enantiomeric excess (ee) are predicted for (1-fluorovinyl)benzene and (1-chlorovinyl)benzene. The results with various temperatures and the corresponding equation⁴ are shown in Figure S5.

Cartesian coordinates of all stationary points optimized at ω B97X-D/BS-I level in toluene solvent.

A1

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.00005000	-0.149175000	0.182439000
P	-2.222216000	0.053546000	0.456359000
O	0.000019000	0.322610000	-2.708952000
C	-0.000015000	0.105959000	-1.573006000
N	0.000005000	-0.084158000	2.353889000
C	-1.235794000	-0.631581000	2.929533000
C	1.235812000	-0.631564000	2.929533000
C	2.422724000	0.091724000	2.306008000
C	-2.422720000	0.091693000	2.306017000
H	3.364995000	-0.343280000	2.640727000
H	-2.422638000	1.141516000	2.615561000
H	2.422625000	1.141549000	2.615544000
P	2.222210000	0.053563000	0.456352000
C	-0.000016000	-1.937463000	0.134962000
O	0.000034000	-3.096038000	0.097822000
H	-3.364981000	-0.343328000	2.640738000
C	3.105869000	1.575574000	-0.094814000
C	2.638848000	2.815135000	0.351081000
C	4.181116000	1.545946000	-0.982193000
C	3.249820000	3.992701000	-0.054644000
H	1.771369000	2.859069000	1.001186000
C	4.783961000	2.728338000	-1.402918000
H	4.554926000	0.601146000	-1.358896000
C	4.326478000	3.952611000	-0.935575000
H	2.874612000	4.944698000	0.305155000
H	5.612973000	2.686904000	-2.101083000
H	4.797900000	4.872750000	-1.263180000
C	3.375963000	-1.267184000	-0.101806000
C	4.623164000	-1.481859000	0.491405000
C	3.011690000	-2.048267000	-1.198092000
C	5.476806000	-2.465564000	0.009928000
H	4.949221000	-0.866841000	1.323448000
C	3.869141000	-3.027884000	-1.687816000
H	2.050467000	-1.889222000	-1.673132000
C	5.100275000	-3.241859000	-1.081842000
H	6.440221000	-2.621744000	0.482983000
H	3.569539000	-3.625993000	-2.541261000
H	5.768028000	-4.008863000	-1.458870000
C	-3.105880000	1.575562000	-0.094790000
C	-4.181124000	1.545940000	-0.982172000
C	-2.638866000	2.815119000	0.351122000
C	-4.783975000	2.728333000	-1.402884000
H	-4.554929000	0.601143000	-1.358889000
C	-3.249843000	3.992687000	-0.054589000
H	-1.771390000	2.859049000	1.001231000
C	-4.326499000	3.952603000	-0.935523000
H	-5.612984000	2.686904000	-2.101052000
H	-2.874642000	4.944681000	0.305224000
H	-4.797926000	4.872744000	-1.263117000
C	-3.375963000	-1.267197000	-0.101816000
C	-4.623188000	-1.481854000	0.491350000
C	-3.011654000	-2.048299000	-1.198077000
C	-5.476822000	-2.465556000	0.009852000
H	-4.949274000	-0.866823000	1.323372000
C	-3.869096000	-3.027915000	-1.687822000
H	-2.050407000	-1.889275000	-1.673077000
C	-5.100256000	-3.241869000	-1.081893000
H	-6.440257000	-2.621720000	0.482871000
H	-3.569465000	-3.626040000	-2.541246000
H	-5.768002000	-4.008872000	-1.458937000
H	1.248358000	-0.516649000	4.021596000
H	1.270277000	-1.700823000	2.702047000
H	-1.270246000	-1.700840000	2.702044000
H	-1.248338000	-0.516670000	4.021596000
H	-0.000001000	0.916807000	2.531007000
H	-0.000020000	1.453222000	0.285464000

A1_triplet

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.000239000	0.182733000	-0.185629000
P	-2.287924000	0.140310000	0.480403000
O	-0.004627000	1.562323000	-2.927231000
C	-0.002948000	0.946861000	-1.962932000
N	0.000435000	-0.096081000	2.553577000
C	-1.237515000	-0.757719000	2.914300000
C	1.241945000	-0.750503000	2.915243000
C	2.403399000	0.046375000	2.321472000
C	-2.403317000	0.034389000	2.322678000
H	3.372428000	-0.346108000	2.639508000
H	-2.358082000	1.068805000	2.679357000
H	2.351803000	1.081888000	2.674043000
P	2.287845000	0.144214000	0.478931000
C	0.000481000	-1.615719000	-0.379315000
O	0.000807000	-2.769945000	-0.478934000
H	-3.370116000	-0.365068000	2.638762000
C	3.436941000	1.526138000	0.093883000
C	2.919882000	2.740319000	-0.354817000
C	4.818789000	1.391210000	0.256876000
C	3.770236000	3.807224000	-0.630707000
H	1.847885000	2.843876000	-0.484585000
C	5.665545000	2.457016000	-0.015502000
H	5.237576000	0.445513000	0.586121000
C	5.141642000	3.667566000	-0.460983000
H	3.357450000	4.745339000	-0.985409000
H	6.736095000	2.341171000	0.114016000
H	5.804961000	4.497162000	-0.680899000
C	3.237829000	-1.299464000	-0.140003000
C	3.697698000	-2.335575000	0.669614000
C	3.426153000	-1.388866000	-1.522827000
C	4.345860000	-3.433870000	0.110772000
H	3.550543000	-2.305006000	1.743155000
C	4.079099000	-2.478472000	-2.078899000
H	3.055167000	-0.598892000	-2.169532000
C	4.541481000	-3.506207000	-1.261343000
H	4.695150000	-4.234436000	0.753865000
H	4.220442000	-2.532180000	-3.152730000
H	5.044085000	-4.363197000	-1.695955000
C	-3.439090000	1.522257000	0.101764000
C	-4.820282000	1.385770000	0.269180000
C	-2.924572000	2.737708000	-0.346311000
C	-5.668927000	2.451252000	0.001612000
H	-5.237102000	0.439085000	0.598119000
C	-3.776860000	3.804337000	-0.617428000
H	-1.853065000	2.842479000	-0.479173000
C	-5.147550000	3.663091000	-0.443430000
H	-6.738941000	2.334236000	0.134457000
H	-3.366111000	4.743517000	-0.971681000
H	-5.812357000	4.492487000	-0.659578000
C	-3.236100000	-1.301478000	-0.145499000
C	-3.684120000	-2.347884000	0.657498000
C	-3.433558000	-1.379110000	-1.527784000
C	-4.329823000	-3.444683000	0.092916000
H	-3.529584000	-2.326744000	1.730238000
C	-4.083830000	-2.467425000	-2.089485000
H	-3.072197000	-0.580804000	-2.169672000
C	-4.534456000	-3.505497000	-1.278459000
H	-4.670005000	-4.253265000	0.730840000
H	-4.232254000	-2.511835000	-3.162801000
H	-5.035077000	-4.361362000	-1.717551000
H	1.380725000	-0.845581000	4.004099000
H	1.222417000	-1.764922000	2.501583000
H	-1.212752000	-1.771178000	2.498575000
H	-1.375535000	-0.855679000	4.003004000
H	-0.002411000	0.864454000	2.878879000
H	-0.000634000	1.759381000	0.213443000

A2_H

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.000006000	0.075396000	0.249149000
P	-2.261115000	0.104810000	0.512820000
O	0.000009000	1.674243000	-2.224040000
C	-0.000032000	1.059314000	-1.244868000
N	0.000046000	-0.187524000	2.142950000
C	-1.190937000	-0.549450000	2.910197000
C	1.191057000	-0.549478000	2.910141000
C	2.422188000	0.141105000	2.340246000
C	-2.422076000	0.141162000	2.340355000
H	3.365679000	-0.272390000	2.704796000
H	-2.397497000	1.202611000	2.603733000
H	2.397656000	1.202550000	2.603641000
P	2.261137000	0.104789000	0.512716000
C	-0.000025000	-1.400629000	-0.725676000
O	0.000035000	-2.400189000	-1.300793000
H	-3.365563000	-0.272296000	2.704960000
C	3.308888000	1.511419000	-0.025198000
C	2.714918000	2.768615000	-0.144742000
C	4.681440000	1.384588000	-0.246149000
C	3.477802000	3.881023000	-0.478984000
H	1.648352000	2.878113000	0.023530000
C	5.443147000	2.496689000	-0.584502000
H	5.159199000	0.414736000	-0.159296000
C	4.843117000	3.745660000	-0.702024000
H	3.003068000	4.851247000	-0.574286000
H	6.507986000	2.385471000	-0.757525000
H	5.438450000	4.611744000	-0.970064000
C	3.173702000	-1.359822000	-0.092458000
C	3.640086000	-2.365101000	0.752085000
C	3.326689000	-1.507176000	-1.474284000
C	4.261972000	-3.493381000	0.225030000
H	3.517981000	-2.282263000	1.825907000
C	3.955150000	-2.627030000	-1.997718000
H	2.948501000	-0.741065000	-2.144831000
C	4.425062000	-3.624012000	-1.147397000
H	4.618203000	-4.270164000	0.892789000
H	4.071401000	-2.727985000	-3.070999000
H	4.909590000	-4.503440000	-1.557022000
C	-3.308874000	1.511441000	-0.025075000
C	-4.681423000	1.384607000	-0.246040000
C	-2.714908000	2.768640000	-0.144599000
C	-5.443132000	2.496708000	-0.584386000
H	-5.159179000	0.414750000	-0.159204000
C	-3.477793000	3.881049000	-0.478834000
H	-1.648343000	2.878140000	0.023680000
C	-4.843106000	3.745683000	-0.701887000
H	-6.507969000	2.385488000	-0.757421000
H	-3.003062000	4.851276000	-0.574120000
H	-5.438441000	4.611768000	-0.969922000
C	-3.173725000	-1.359803000	-0.092281000
C	-3.640155000	-2.365022000	0.752308000
C	-3.326722000	-1.507210000	-1.474100000
C	-4.262093000	-3.493298000	0.225304000
H	-3.518045000	-2.282141000	1.826126000
C	-3.955236000	-2.627058000	-1.997483000
H	-2.948500000	-0.741145000	-2.144681000
C	-4.425191000	-3.623981000	-1.147117000
H	-4.618358000	-4.270035000	0.893097000
H	-4.071494000	-2.728054000	-3.070759000
H	-4.909760000	-4.503405000	-1.556703000
H	1.073371000	-0.254309000	3.963229000
H	1.337595000	-1.642568000	2.912539000
H	-1.337502000	-1.642536000	2.912603000
H	-1.073197000	-0.254282000	3.963279000

A2_H_triplet

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.000026000	-0.310811000	0.162882000
P	-2.272482000	0.159514000	0.548411000
O	0.000375000	0.580978000	-2.668742000
C	0.000196000	0.234412000	-1.561502000
N	-0.000035000	-0.394108000	2.153114000
C	-1.203785000	-0.790994000	2.852523000
C	1.203551000	-0.791653000	2.852434000
C	2.375115000	0.075823000	2.378806000
C	-2.374976000	0.076848000	2.378671000
H	3.348982000	-0.265614000	2.739739000
H	-2.222130000	1.102578000	2.725841000
H	2.222750000	1.101497000	2.726352000
P	2.272600000	0.159165000	0.548567000
C	-0.000024000	-2.134525000	-0.518390000
O	-0.000051000	-3.172615000	-0.990459000
H	-3.348979000	-0.264007000	2.739783000
C	3.171824000	1.673338000	0.065222000
C	2.448733000	2.758402000	-0.426917000
C	4.556401000	1.782377000	0.217100000
C	3.098772000	3.943117000	-0.757243000
H	1.374933000	2.669918000	-0.555038000
C	5.203710000	2.965166000	-0.112189000
H	5.130319000	0.938127000	0.585727000
C	4.474858000	4.047246000	-0.598891000
H	2.529810000	4.781695000	-1.143103000
H	6.278384000	3.044749000	0.009190000
H	4.982829000	4.969922000	-0.857536000
C	3.317724000	-1.194554000	-0.104136000
C	3.789710000	-2.236698000	0.692316000
C	3.553083000	-1.232326000	-1.482526000
C	4.496211000	-3.292441000	0.122739000
H	3.606359000	-2.239775000	1.760278000
C	4.264930000	-2.280320000	-2.046634000
H	3.177402000	-0.436282000	-2.118068000
C	4.737133000	-3.315560000	-1.244085000
H	4.855575000	-4.098317000	0.753319000
H	4.444082000	-2.294993000	-3.116013000
H	5.285311000	-4.139908000	-1.686643000
C	-3.171650000	1.673556000	0.064531000
C	-4.556237000	1.782644000	0.216280000
C	-2.448530000	2.758461000	-0.427917000
C	-5.203527000	2.965326000	-0.113431000
H	-5.130181000	0.938507000	0.585125000
C	-3.098550000	3.943068000	-0.758668000
H	-1.374724000	2.669940000	-0.555958000
C	-4.474646000	4.047250000	-0.600435000
H	-6.278209000	3.044944000	0.007850000
H	-2.529566000	4.781519000	-1.144771000
H	-4.982601000	4.969840000	-0.859416000
C	-3.317761000	-1.194364000	-0.103731000
C	-3.790569000	-2.235697000	0.693291000
C	-3.552582000	-1.233023000	-1.482187000
C	-4.497319000	-3.291530000	0.124191000
H	-3.607659000	-2.238045000	1.761329000
C	-4.264687000	-2.281092000	-2.045827000
H	-3.176289000	-0.437604000	-2.118150000
C	-4.737691000	-3.315530000	-1.242713000
H	-4.857314000	-4.096777000	0.755215000
H	-4.443425000	-2.296468000	-3.115264000
H	-5.286074000	-4.139943000	-1.684894000
H	1.087464000	-0.651824000	3.938878000
H	1.455250000	-1.860937000	2.708976000
H	-1.455935000	-1.860207000	2.709323000
H	-1.087640000	-0.650947000	3.938934000

A3_H

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.001761000	0.155148000	0.230824000
P	-2.260281000	0.136561000	0.534178000
O	0.047723000	0.619333000	-2.673596000
C	0.022235000	0.468310000	-1.527858000
N	-0.002110000	-0.097973000	2.308703000

C	-1.184023000	-0.709101000	2.870902000
C	1.184287000	-0.697086000	2.875003000
C	2.425883000	0.029885000	2.363794000
C	-2.431043000	0.008141000	2.359528000
H	3.363634000	-0.435207000	2.677373000
H	-2.432086000	1.037401000	2.730622000
H	2.418438000	1.060662000	2.730763000
P	2.255872000	0.151545000	0.538022000
C	0.005268000	-1.613344000	-0.045516000
O	0.006038000	-2.750469000	-0.200214000
H	-3.362973000	-0.468329000	2.673039000
C	3.316877000	1.569942000	0.063420000
C	2.770703000	2.663311000	-0.604782000
C	4.679648000	1.574220000	0.375797000
C	3.568996000	3.749977000	-0.950794000
H	1.718090000	2.666116000	-0.863311000
C	5.475164000	2.658370000	0.033960000
H	5.122915000	0.720517000	0.878795000
C	4.919765000	3.749253000	-0.629951000
H	3.132854000	4.594526000	-1.472734000
H	6.531503000	2.651618000	0.279354000
H	5.543246000	4.594561000	-0.900163000
C	3.177970000	-1.258560000	-0.181454000
C	3.553139000	-2.372300000	0.566870000
C	3.430787000	-1.246566000	-1.555940000
C	4.182198000	-3.451668000	-0.046545000
H	3.350129000	-2.415060000	1.630793000
C	4.061184000	-2.321467000	-2.165445000
H	3.136655000	-0.389524000	-2.154060000
C	4.438850000	-3.428262000	-1.410722000
H	4.467103000	-4.314025000	0.546255000
H	4.253647000	-2.297426000	-3.232387000
H	4.926710000	-4.271316000	-1.887416000
C	-3.316587000	1.559868000	0.062045000
C	-4.605010000	1.695286000	0.586966000
C	-2.846937000	2.515365000	-0.836494000
C	-5.401231000	2.773109000	0.226367000
H	-4.989676000	0.952891000	1.278918000
C	-3.648901000	3.591237000	-1.206570000
H	-1.852495000	2.418344000	-1.257120000
C	-4.923936000	3.722857000	-0.672984000
H	-6.397028000	2.872145000	0.644311000
H	-3.274540000	4.325150000	-1.911685000
H	-5.548667000	4.562453000	-0.957621000
C	-3.184769000	-1.269648000	-0.191569000
C	-3.551439000	-2.389838000	0.551495000
C	-3.446204000	-1.249055000	-1.564132000
C	-4.180823000	-3.466931000	-0.065367000
H	-3.340952000	-2.439665000	1.613700000
C	-4.076859000	-2.321969000	-2.177090000
H	-3.157958000	-0.387669000	-2.158899000
C	-4.446151000	-3.435093000	-1.427785000
H	-4.458895000	-4.334466000	0.523118000
H	-4.275883000	-2.291201000	-3.242667000
H	-4.934137000	-4.276538000	-1.907180000
H	1.169207000	-0.631142000	3.976456000
H	1.274199000	-1.780307000	2.641280000
H	-1.263842000	-1.792690000	2.634921000
H	-1.172268000	-0.645556000	3.972551000
H	0.038744000	1.711507000	1.087110000
H	-0.105098000	1.947394000	0.350924000

B1

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.069690000	-0.111767000	0.058343000
P	-1.967616000	0.671945000	0.626179000
O	0.183533000	0.938102000	-2.671160000
C	0.127807000	0.517024000	-1.592259000
N	0.127208000	-0.650656000	2.173051000
C	-1.205328000	-0.959460000	2.707570000
C	1.146825000	-1.662920000	2.482617000
C	2.489325000	-1.177760000	1.947702000

C	-2.129059000	0.216503000	2.419433000
H	3.263144000	-1.940407000	2.062954000
H	-1.802706000	1.088598000	2.997242000
H	2.812129000	-0.293873000	2.506604000
P	2.252035000	-0.658865000	0.178857000
C	-0.554745000	-1.696119000	-0.473872000
O	-1.010050000	-2.688937000	-0.866291000
H	-3.150480000	-0.008750000	2.727072000
C	3.566749000	0.610132000	-0.051997000
C	4.882943000	0.367552000	0.353988000
C	3.265350000	1.829121000	-0.656259000
C	5.872856000	1.322493000	0.161839000
H	5.142466000	-0.572812000	0.831264000
C	4.258425000	2.781939000	-0.861852000
H	2.243397000	2.037091000	-0.949047000
C	5.562066000	2.531838000	-0.452823000
H	6.887704000	1.122982000	0.488810000
H	4.008933000	3.723292000	-1.339252000
H	6.334744000	3.277042000	-0.608326000
C	-3.476003000	0.005617000	-0.195788000
C	-4.699230000	-0.193214000	0.448749000
C	-3.392832000	-0.273045000	-1.562306000
C	-5.804920000	-0.662606000	-0.250940000
H	-4.807759000	0.021453000	1.505639000
C	-4.499836000	-0.730133000	-2.266838000
H	-2.449390000	-0.141748000	-2.079629000
C	-5.708730000	-0.929673000	-1.611787000
H	-6.744866000	-0.816293000	0.268173000
H	-4.411068000	-0.939835000	-3.327047000
H	-6.571730000	-1.296055000	-2.156988000
H	1.205453000	-1.844929000	3.564091000
H	0.846747000	-2.596725000	1.998848000
H	-1.566314000	-1.865098000	2.211502000
H	-1.161035000	-1.158467000	3.786796000
H	0.430398000	0.225005000	2.591520000
H	0.551066000	1.344482000	0.569308000
C	-2.290806000	2.504637000	0.645916000
H	-1.474298000	2.874723000	1.276577000
C	2.989351000	-2.061094000	-0.807461000
H	4.066759000	-2.042559000	-0.609336000
C	2.760605000	-1.799656000	-2.296352000
H	3.263067000	-2.565196000	-2.896192000
H	1.693848000	-1.829547000	-2.537126000
H	3.149997000	-0.825086000	-2.604848000
C	2.448975000	-3.428439000	-0.391905000
H	2.933499000	-4.209495000	-0.986810000
H	2.648333000	-3.651394000	0.659738000
H	1.373804000	-3.508729000	-0.562263000
C	-3.629508000	2.908223000	1.261669000
H	-3.677847000	3.997275000	1.363936000
H	-4.465941000	2.600014000	0.627944000
H	-3.781022000	2.479296000	2.256713000
C	-2.119423000	3.096539000	-0.751474000
H	-2.272027000	4.180110000	-0.718794000
H	-1.119477000	2.907905000	-1.145776000
H	-2.851536000	2.682071000	-1.452552000

C1

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.069690000	-0.111767000	0.058343000
P	-1.967616000	0.671945000	0.626179000
O	0.183533000	0.938102000	-2.671160000
C	0.127807000	0.517024000	-1.592259000
N	0.127208000	-0.650656000	2.173051000
C	-1.205328000	-0.959460000	2.707570000
C	1.146825000	-1.662920000	2.482617000
C	2.489325000	-1.177776000	1.947702000
C	-2.129059000	0.216503000	2.419433000
H	3.263144000	-1.940407000	2.062954000
H	-1.802706000	1.088598000	2.997242000
H	2.812129000	-0.293873000	2.506604000
P	2.252035000	-0.658865000	0.178857000

C	-0.554745000	-1.696119000	-0.473872000
O	-1.010050000	-2.688937000	-0.866291000
H	-3.150480000	-0.008750000	2.727072000
C	3.566749000	0.610132000	-0.051997000
C	4.882943000	0.367552000	0.353988000
C	3.265350000	1.829121000	-0.656259000
C	5.872856000	1.322493000	0.161839000
H	5.142466000	-0.572812000	0.831264000
C	4.258425000	2.781939000	-0.861852000
H	2.243397000	2.037091000	-0.949047000
C	5.562066000	2.531838000	-0.452823000
H	6.887704000	1.122982000	0.488810000
H	4.008933000	3.723292000	-1.339252000
H	6.334744000	3.277042000	-0.608326000
C	-3.476003000	0.005617000	-0.195788000
C	-4.699230000	-0.193214000	0.448749000
C	-3.392832000	-0.273045000	-1.562306000
C	-5.804920000	-0.662606000	-0.250940000
H	-4.807759000	0.021453000	1.505639000
C	-4.499836000	-0.730133000	-2.266838000
H	-2.449390000	-0.141748000	-2.079629000
C	-5.708730000	-0.929673000	-1.611787000
H	-6.744866000	-0.816293000	0.268173000
H	-4.411068000	-0.939835000	-3.327047000
H	-6.571730000	-1.296055000	-2.156988000
H	1.205453000	-1.844929000	3.564091000
H	0.846747000	-2.596725000	1.998848000
H	-1.566314000	-1.865098000	2.211502000
H	-1.161035000	-1.158467000	3.786796000
H	0.430398000	0.225005000	2.591520000
H	0.551066000	1.344482000	0.569308000
C	-2.290806000	2.504637000	0.645916000
H	-1.474298000	2.874723000	1.276577000
C	2.989351000	-2.061094000	-0.807461000
H	4.066759000	-2.042559000	-0.609336000
C	2.760605000	-1.799656000	-2.296352000
H	3.263067000	-2.565196000	-2.896192000
H	1.693848000	-1.829547000	-2.537126000
H	3.149997000	-0.825086000	-2.604848000
C	2.448975000	-3.428439000	-0.391905000
H	2.933499000	-4.209495000	-0.986810000
H	2.648333000	-3.651394000	0.659738000
H	1.373804000	-3.508729000	-0.562263000
C	-3.629508000	2.908223000	1.261669000
H	-3.677847000	3.997275000	1.363936000
H	-4.465941000	2.600014000	0.627944000
H	-3.781022000	2.479296000	2.256713000
C	-2.119423000	3.096539000	-0.751474000
H	-2.272027000	4.180110000	-0.718794000
H	-1.119477000	2.907905000	-1.145776000
H	-2.851536000	2.682071000	-1.452552000

CI'

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.069690000	-0.111767000	0.058343000
P	-1.967616000	0.671945000	0.626179000
O	0.183533000	0.938102000	-2.671160000
C	0.127807000	0.517024000	-1.592259000
N	0.127208000	-0.650656000	2.173051000
C	-1.205328000	-0.959460000	2.707570000
C	1.146825000	-1.662920000	2.482617000
C	2.489325000	-1.177760000	1.947702000
C	-2.129059000	0.216503000	2.419433000
H	3.263144000	-1.940407000	2.062954000
H	-1.802706000	1.088598000	2.997242000
H	2.812129000	-0.293873000	2.506604000
P	2.252035000	-0.658865000	0.178857000
C	-0.554745000	-1.696119000	-0.473872000
O	-1.010050000	-2.688937000	-0.866291000
H	-3.150480000	-0.008750000	2.727072000
C	3.566749000	0.610132000	-0.051997000
C	4.882943000	0.367552000	0.353988000

C	3.26535000	1.82912100	-0.65625900
C	5.87285600	1.32249300	0.16183900
H	5.14246600	-0.57281200	0.83126400
C	4.25842500	2.78193900	-0.86185200
H	2.24339700	2.03709100	-0.94904700
C	5.56206600	2.53183800	-0.45282300
H	6.88770400	1.12298200	0.48881000
H	4.00893300	3.72329200	-1.33925200
H	6.33474400	3.27704200	-0.60832600
C	-3.47600300	0.00561700	-0.19578800
C	-4.69923000	-0.19321400	0.44874900
C	-3.39283200	-0.27304500	-1.56230600
C	-5.80492000	-0.66260600	-0.25094000
H	-4.80775900	0.02145300	1.50563900
C	-4.49983600	-0.73013300	-2.26683800
H	-2.44939000	-0.14174800	-2.07962900
C	-5.70873000	-0.92967300	-1.61178700
H	-6.74486600	-0.81629300	0.26817300
H	-4.41106800	-0.93983500	-3.32704700
H	-6.57173000	-1.29605500	-2.15698800
H	1.20545300	-1.84492900	3.56409100
H	0.84674700	-2.59672500	1.99884800
H	-1.56631400	-1.86509800	2.21150200
H	-1.16103500	-1.15846700	3.78679600
H	0.43039800	0.22500500	2.59152000
H	0.55106600	1.34448200	0.56930800
C	-2.29080600	2.50463700	0.64591600
H	-1.47429800	2.87472300	1.27657700
C	2.98935100	-2.06109400	-0.80746100
H	4.06675900	-2.04255900	-0.60933600
C	2.76060500	-1.79965600	-2.29635200
H	3.26306700	-2.56519600	-2.89619200
H	1.69384800	-1.82954700	-2.53712600
H	3.14999700	-0.82508600	-2.60484800
C	2.44897500	-3.42843900	-0.39190500
H	2.93349900	-4.20949500	-0.98681000
H	2.64833300	-3.65139400	0.65973800
H	1.37380400	-3.50872900	-0.56226300
C	-3.62950800	2.90822300	1.26166900
H	-3.67784700	3.99727500	1.36393600
H	-4.46594100	2.60001400	0.62794400
H	-3.78102200	2.47929600	2.25671300
C	-2.11942300	3.09653900	-0.75147400
H	-2.27202700	4.18011000	-0.71879400
H	-1.11947700	2.90790500	-1.14577600
H	-2.85153600	2.68207100	-1.45255200

B2

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.09309400	0.06951700	0.02071000
P	-2.01508400	0.90777800	0.30025200
O	0.96773900	2.31767400	-1.64560200
C	0.63056500	1.41609800	-1.00380600
N	-0.07741400	-0.31678200	1.88111200
C	-1.24455900	0.00790900	2.69866000
C	0.80980900	-1.20583500	2.63206200
C	2.24221100	-1.09143500	2.12878700
C	-1.98744300	1.19694100	2.10524900
H	2.86050300	-1.95309500	2.39734600
H	-1.39415100	2.10625200	2.24752900
H	2.70680400	-0.19925000	2.55549700
P	2.18908900	-0.82621600	0.30501500
C	-0.29378000	-0.84289600	-1.44375100
O	-0.56223700	-1.45688400	-2.38923300
H	-2.96534400	1.35803600	2.56303300
C	3.68342300	0.21630900	0.04125000
C	4.90853100	-0.26470100	-0.42345300
C	3.58609300	1.56715900	0.38751100
C	6.00234400	0.58591200	-0.54941100
H	5.02881000	-1.30696600	-0.69311200
C	4.67871500	2.41522500	0.26962300
H	2.64379000	1.95919500	0.75684000

C	5.89089000	1.926889000	-0.205577000
H	6.944035000	0.194649000	-0.919018000
H	4.579086000	3.460806000	0.539479000
H	6.743494000	2.589385000	-0.307164000
C	-3.455864000	-0.195842000	0.004190000
C	-4.395557000	-0.500304000	0.991475000
C	-3.624924000	-0.750413000	-1.268369000
C	-5.473930000	-1.333599000	0.714275000
H	-4.296073000	-0.093100000	1.989875000
C	-4.706956000	-1.574546000	-1.549054000
H	-2.905575000	-0.542983000	-2.050423000
C	-5.634417000	-1.870553000	-0.556702000
H	-6.190423000	-1.561722000	1.495911000
H	-4.819078000	-1.993356000	-2.543002000
H	-6.475495000	-2.520245000	-0.772761000
H	0.792703000	-0.951696000	3.701989000
H	0.460449000	-2.246972000	2.561403000
H	-1.927166000	-0.854852000	2.778131000
H	-0.936288000	0.251340000	3.726027000
C	-2.535600000	2.525476000	-0.445389000
H	-1.693343000	3.184286000	-0.201127000
C	2.632786000	-2.476442000	-0.417050000
H	3.606072000	-2.745901000	0.008706000
C	2.745302000	-2.427967000	-1.943137000
H	3.160573000	-3.371301000	-2.312262000
H	1.766520000	-2.296198000	-2.406452000
H	3.390504000	-1.619832000	-2.295336000
C	1.616121000	-3.530659000	0.029632000
H	1.846549000	-4.489611000	-0.444720000
H	1.632995000	-3.685168000	1.111281000
H	0.597496000	-3.253518000	-0.256686000
C	-3.811425000	3.097177000	0.171185000
H	-4.045181000	4.063406000	-0.287115000
H	-4.664004000	2.432840000	-0.001229000
H	-3.713794000	3.257204000	1.248028000
C	-2.648729000	2.432853000	-1.968043000
H	-2.754098000	3.435177000	-2.393939000
H	-1.769927000	1.969310000	-2.422869000
H	-3.531599000	1.857134000	-2.260674000

C2

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.093094000	0.069517000	0.020710000
P	-2.015084000	0.907778000	0.300252000
O	0.967739000	2.317674000	-1.645602000
C	0.630565000	1.416098000	-1.003806000
N	-0.077414000	-0.316782000	1.881112000
C	-1.244559000	0.007909000	2.698660000
C	0.809809000	-1.205835000	2.632062000
C	2.242211000	-1.091435000	2.128787000
C	-1.987443000	1.196941000	2.105249000
H	2.860503000	-1.953095000	2.397346000
H	-1.394151000	2.106252000	2.247529000
H	2.706804000	-0.199250000	2.555497000
P	2.189089000	-0.826216000	0.305015000
C	-0.293780000	-0.842896000	-1.443751000
O	-0.562237000	-1.456884000	-2.389233000
H	-2.965344000	1.358036000	2.563033000
C	3.683423000	0.216309000	0.041250000
C	4.908531000	-0.264701000	-0.423453000
C	3.586093000	1.567159000	0.387511000
C	6.002344000	0.585912000	-0.549411000
H	5.028810000	-1.306966000	-0.693112000
C	4.678715000	2.415225000	0.269623000
H	2.643790000	1.959195000	0.756840000
C	5.890890000	1.926889000	-0.205577000
H	6.944035000	0.194649000	-0.919018000
H	4.579086000	3.460806000	0.539479000
H	6.743494000	2.589385000	-0.307164000
C	-3.455864000	-0.195842000	0.004190000
C	-4.395557000	-0.500304000	0.991475000
C	-3.624924000	-0.750413000	-1.268369000

C	-5.473930000	-1.333599000	0.714275000
H	-4.296073000	-0.093100000	1.989875000
C	-4.706956000	-1.574546000	-1.549054000
H	-2.905575000	-0.542983000	-2.050423000
C	-5.634417000	-1.870553000	-0.556702000
H	-6.190423000	-1.561722000	1.495911000
H	-4.819078000	-1.993356000	-2.543002000
H	-6.475495000	-2.520245000	-0.772761000
H	0.792703000	-0.951696000	3.701989000
H	0.460449000	-2.246972000	2.561403000
H	-1.927166000	-0.854852000	2.778131000
H	-0.936288000	0.251340000	3.726027000
C	-2.535600000	2.525476000	-0.445389000
H	-1.693343000	3.184286000	-0.201127000
C	2.632786000	-2.476442000	-0.417050000
H	3.606072000	-2.745901000	0.008706000
C	2.745302000	-2.427967000	-1.943137000
H	3.160573000	-3.371301000	-2.312262000
H	1.766520000	-2.296198000	-2.406452000
H	3.390504000	-1.619832000	-2.295336000
C	1.616121000	-3.530659000	0.029632000
H	1.846549000	-4.489611000	-0.444720000
H	1.632995000	-3.685168000	1.111281000
H	0.597496000	-3.253518000	-0.256686000
C	-3.811425000	3.097177000	0.171185000
H	-4.045181000	4.063406000	-0.287115000
H	-4.664004000	2.432840000	-0.001229000
H	-3.713794000	3.257204000	1.248028000
C	-2.648729000	2.432853000	-1.968043000
H	-2.754098000	3.435177000	-2.393939000
H	-1.769927000	1.969310000	-2.422869000
H	-3.531599000	1.857134000	-2.260674000

B3

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.093540000	-0.029751000	0.097025000
O	0.114294000	0.865291000	-2.702924000
C	0.114576000	0.547629000	-1.589615000
N	0.120509000	-0.630522000	2.100775000
C	-1.167672000	-0.977439000	2.653947000
C	1.094739000	-1.645549000	2.432801000
C	2.477865000	-1.207398000	1.956976000
H	2.789244000	-0.323364000	2.520691000
P	2.284975000	-0.687826000	0.200361000
C	-0.533317000	-1.615674000	-0.418640000
O	-0.983270000	-2.628124000	-0.730563000
H	1.134519000	-1.807576000	3.523690000
H	0.854206000	-2.635795000	1.990772000
H	-1.598090000	-1.902392000	2.212635000
H	-1.087741000	-1.173550000	3.736936000
H	0.630151000	1.657827000	0.455384000
H	0.661850000	1.291012000	1.149747000
H	3.237178000	-1.983666000	2.085569000
C	3.592899000	0.581122000	-0.048470000
C	4.853736000	0.434928000	0.537928000
C	3.352348000	1.697439000	-0.848758000
C	5.845293000	1.385553000	0.333589000
H	5.066286000	-0.425720000	1.164449000
C	4.346470000	2.647530000	-1.060616000
H	2.382486000	1.830009000	-1.313451000
C	5.593063000	2.494758000	-0.467822000
H	6.816121000	1.260740000	0.800710000
H	4.142222000	3.508488000	-1.687656000
H	6.366979000	3.237542000	-0.627517000
C	2.974103000	-2.080551000	-0.826034000
H	4.054412000	-2.062793000	-0.640783000
C	2.724910000	-1.802118000	-2.308170000
H	3.220460000	-2.561351000	-2.921249000
H	1.655685000	-1.832831000	-2.537437000
H	3.110003000	-0.824966000	-2.613468000
C	2.440506000	-3.452503000	-0.415109000
H	1.365443000	-3.539891000	-0.580696000

H	2.928262000	-4.225165000	-1.018158000
H	2.641976000	-3.678658000	0.634362000
P	-2.013086000	0.670469000	0.673164000
C	-2.145841000	0.172227000	2.440285000
H	-1.818472000	1.036781000	3.027058000
H	-3.161050000	-0.080790000	2.749856000
C	-2.350740000	2.501021000	0.700377000
H	-1.548798000	2.881429000	1.345114000
C	-3.696934000	2.869452000	1.322166000
H	-3.832334000	2.428538000	2.313667000
H	-3.772216000	3.956071000	1.431984000
H	-4.525872000	2.543636000	0.687306000
C	-2.192311000	3.115539000	-0.689203000
H	-2.346433000	4.197949000	-0.638729000
H	-1.198685000	2.936735000	-1.105976000
H	-2.930507000	2.709927000	-1.388482000
C	-3.471624000	-0.014359000	-0.205369000
C	-3.374599000	-0.231085000	-1.582042000
C	-4.687726000	-0.279306000	0.428289000
C	-4.464497000	-0.695554000	-2.308150000
H	-2.437647000	-0.042835000	-2.093080000
C	-5.776210000	-0.751927000	-0.295118000
H	-4.800490000	-0.114138000	1.493155000
C	-5.667627000	-0.959528000	-1.665310000
H	-4.367130000	-0.859612000	-3.375540000
H	-6.711818000	-0.956346000	0.213887000
H	-6.517229000	-1.330020000	-2.228371000

C3

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.093540000	-0.029751000	0.097025000
O	0.114294000	0.865291000	-2.702924000
C	0.114576000	0.547629000	-1.589615000
N	0.120509000	-0.630522000	2.100775000
C	-1.167672000	-0.977439000	2.653947000
C	1.094739000	-1.645549000	2.432801000
C	2.477865000	-1.207398000	1.956976000
H	2.789244000	-0.323364000	2.520691000
P	2.284975000	-0.687826000	0.200361000
C	-0.533317000	-1.615674000	-0.418640000
O	-0.983270000	-2.628124000	-0.730563000
H	1.134519000	-1.807576000	3.523690000
H	0.854206000	-2.635795000	1.990772000
H	-1.598090000	-1.902392000	2.212635000
H	-1.087741000	-1.173550000	3.736936000
H	0.630151000	1.657827000	0.455384000
H	0.661850000	1.291012000	1.149747000
H	3.237178000	-1.983666000	2.085569000
C	3.592899000	0.581122000	-0.048470000
C	4.853736000	0.434928000	0.537928000
C	3.352348000	1.697439000	-0.848758000
C	5.845293000	1.385553000	0.333589000
H	5.066286000	-0.425720000	1.164449000
C	4.346470000	2.647530000	-1.060616000
H	2.382486000	1.830009000	-1.313451000
C	5.593063000	2.494758000	-0.467822000
H	6.816121000	1.260740000	0.800710000
H	4.142222000	3.508488000	-1.687656000
H	6.366979000	3.237542000	-0.627517000
C	2.974103000	-2.080551000	-0.826034000
H	4.054412000	-2.062793000	-0.640783000
C	2.724910000	-1.802118000	-2.308170000
H	3.220460000	-2.561351000	-2.921249000
H	1.655685000	-1.832831000	-2.537437000
H	3.110003000	-0.824966000	-2.613468000
C	2.440506000	-3.452503000	-0.415109000
H	1.365443000	-3.539891000	-0.580696000
H	2.928262000	-4.225165000	-1.018158000
H	2.641976000	-3.678658000	0.634362000
P	-2.013086000	0.670469000	0.673164000
C	-2.145841000	0.172227000	2.440285000
H	-1.818472000	1.036781000	3.027058000

H	-3.161050000	-0.080790000	2.749856000
C	-2.350740000	2.501021000	0.700377000
H	-1.548798000	2.881429000	1.345114000
C	-3.696934000	2.869452000	1.322166000
H	-3.832334000	2.428538000	2.313667000
H	-3.772216000	3.956071000	1.431984000
H	-4.525872000	2.543636000	0.687306000
C	-2.192311000	3.115539000	-0.689203000
H	-2.346433000	4.197949000	-0.638729000
H	-1.198685000	2.936735000	-1.105976000
H	-2.930507000	2.709927000	-1.388482000
C	-3.471624000	-0.014359000	-0.205369000
C	-3.374599000	-0.231085000	-1.582042000
C	-4.687726000	-0.279306000	0.428289000
C	-4.464497000	-0.695554000	-2.308150000
H	-2.437647000	-0.042835000	-2.093080000
C	-5.776210000	-0.751927000	-0.295118000
H	-4.800490000	-0.114138000	1.493155000
C	-5.667627000	-0.959528000	-1.665310000
H	-4.367130000	-0.859612000	-3.375540000
H	-6.711818000	-0.956346000	0.213887000
H	-6.517229000	-1.330020000	-2.228371000

TSB3-1

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.021154000	-0.038899000	0.124497000
O	0.124168000	1.174957000	-2.547051000
C	0.087589000	0.718724000	-1.483577000
N	0.034924000	-0.673592000	2.149128000
C	-1.266975000	-1.020469000	2.669475000
C	1.036793000	-1.668090000	2.452022000
C	2.405494000	-1.190425000	1.979029000
H	2.697110000	-0.305728000	2.552644000
P	2.219593000	-0.662382000	0.221105000
C	-0.509289000	-1.616398000	-0.525839000
O	-0.850525000	-2.654142000	-0.893923000
H	1.082190000	-1.860684000	3.536172000
H	0.801963000	-2.639853000	1.973908000
H	-1.660251000	-1.942583000	2.198767000
H	-1.211923000	-1.221598000	3.751697000
C	-2.249236000	0.119193000	2.427570000
C	2.773537000	-2.117476000	-0.798136000
H	2.088408000	-2.913998000	-0.483147000
C	4.209726000	-2.570572000	-0.543594000
H	4.927968000	-1.822389000	-0.890641000
H	4.408338000	-2.769862000	0.512484000
H	4.405631000	-3.497439000	-1.092092000
C	2.544876000	-1.835447000	-2.284178000
H	2.810058000	-2.716627000	-2.876443000
H	1.504189000	-1.587514000	-2.500885000
H	3.171762000	-1.005782000	-2.627324000
H	0.375536000	0.669564000	1.650326000
H	0.515254000	1.350203000	1.007554000
H	3.171785000	-1.956038000	2.117489000
P	-2.101936000	0.620978000	0.657360000
H	-3.263294000	-0.151225000	2.724528000
H	-1.948774000	0.990553000	3.019031000
C	3.559800000	0.566282000	-0.028173000
C	4.735947000	0.535315000	0.726680000
C	3.419601000	1.548480000	-1.009862000
C	5.743830000	1.466236000	0.507479000
H	4.871541000	-0.218836000	1.494143000
C	4.431126000	2.475317000	-1.235789000
H	2.511816000	1.599677000	-1.598160000
C	5.593796000	2.437952000	-0.475951000
H	6.648398000	1.431799000	1.105002000
H	4.304476000	3.232609000	-2.001669000
H	6.379300000	3.166209000	-0.645888000
C	-2.496793000	2.439386000	0.705820000
H	-1.707735000	2.833110000	1.357923000
C	-3.858043000	2.757684000	1.322937000
H	-3.990091000	2.299903000	2.307232000

H	-3.964958000	3.840034000	1.447462000
H	-4.672478000	2.418926000	0.676146000
C	-2.349466000	3.081134000	-0.672235000
H	-1.342201000	2.957922000	-1.073463000
H	-3.059103000	2.653836000	-1.388301000
H	-2.554835000	4.154192000	-0.605476000
C	-3.532324000	-0.101171000	-0.237374000
C	-4.754795000	-0.387924000	0.374185000
C	-3.402898000	-0.323697000	-1.610447000
C	-5.818505000	-0.888101000	-0.367435000
H	-4.892191000	-0.218742000	1.435746000
C	-4.468704000	-0.814047000	-2.355131000
H	-2.458152000	-0.120722000	-2.102144000
C	-5.678542000	-1.099579000	-1.734259000
H	-6.759462000	-1.109574000	0.124318000
H	-4.347718000	-0.981076000	-3.419645000
H	-6.509112000	-1.489985000	-2.312099000

TSC3-1

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.021154000	-0.038899000	0.124497000
O	0.124168000	1.174957000	-2.547051000
C	0.087589000	0.718724000	-1.483577000
N	0.034924000	-0.673592000	2.149128000
C	-1.266975000	-1.020469000	2.669475000
C	1.036793000	-1.668090000	2.452022000
C	2.405494000	-1.190425000	1.979029000
H	2.697110000	-0.305728000	2.552644000
P	2.219593000	-0.662382000	0.221105000
C	-0.509289000	-1.616398000	-0.525839000
O	-0.850525000	-2.654142000	-0.893923000
H	1.082190000	-1.860684000	3.536172000
H	0.801963000	-2.639853000	1.973908000
H	-1.660251000	-1.942583000	2.198767000
H	-1.211923000	-1.221598000	3.751697000
C	-2.249236000	0.119193000	2.427570000
C	2.773537000	-2.117476000	-0.798136000
H	2.088408000	-2.913998000	-0.483147000
C	4.209726000	-2.570572000	-0.543594000
H	4.927968000	-1.822389000	-0.890641000
H	4.408338000	-2.769862000	0.512484000
H	4.405631000	-3.497439000	-1.092092000
C	2.544876000	-1.835447000	-2.284178000
H	2.810058000	-2.716627000	-2.876443000
H	1.504189000	-1.587514000	-2.500885000
H	3.171762000	-1.005782000	-2.627324000
H	0.375536000	0.669564000	1.650326000
H	0.515254000	1.350203000	1.007554000
H	3.171785000	-1.956038000	2.117489000
P	-2.101936000	0.620978000	0.657360000
H	-3.263294000	-0.151225000	2.724528000
H	-1.948774000	0.990553000	3.019031000
C	3.559800000	0.566282000	-0.028173000
C	4.735947000	0.535315000	0.726680000
C	3.419601000	1.548480000	-1.009862000
C	5.743830000	1.466236000	0.507479000
H	4.871541000	-0.218836000	1.494143000
C	4.431126000	2.475317000	-1.235789000
H	2.511816000	1.599677000	-1.598160000
C	5.593796000	2.437952000	-0.475951000
H	6.648398000	1.431799000	1.105002000
H	4.304476000	3.232609000	-2.001669000
H	6.379300000	3.166209000	-0.645888000
C	-2.496793000	2.439386000	0.705820000
H	-1.707735000	2.833110000	1.357923000
C	-3.858043000	2.757684000	1.322937000
H	-3.990091000	2.299903000	2.307232000
H	-3.964958000	3.840034000	1.447462000
H	-4.672478000	2.418926000	0.676146000
C	-2.349466000	3.081134000	-0.672235000
H	-1.342201000	2.957922000	-1.073463000
H	-3.059103000	2.653836000	-1.388301000

H	-2.554835000	4.154192000	-0.605476000
C	-3.532324000	-0.101171000	-0.237374000
C	-4.754795000	-0.387924000	0.374185000
C	-3.402898000	-0.323697000	-1.610447000
C	-5.818505000	-0.888101000	-0.367435000
H	-4.892191000	-0.218742000	1.435746000
C	-4.468704000	-0.814047000	-2.355131000
H	-2.458152000	-0.120722000	-2.102144000
C	-5.678542000	-1.099579000	-1.734259000
H	-6.759462000	-1.109574000	0.124318000
H	-4.347718000	-0.981076000	-3.419645000
H	-6.509112000	-1.489985000	-2.312099000

TSB1-2_a

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.590001000	-0.593671000	-0.039175000
P	2.322675000	0.864300000	0.255003000
O	1.187213000	-2.381072000	2.206048000
C	0.954608000	-1.672600000	1.320069000
N	-0.024199000	0.862540000	-1.494061000
C	1.102168000	1.604698000	-2.091750000
C	-0.924856000	0.327360000	-2.534327000
C	-2.089980000	-0.397661000	-1.880376000
C	1.986129000	2.181659000	-0.996910000
H	-2.696501000	-0.917479000	-2.625492000
H	1.445546000	2.970948000	-0.467900000
H	-2.735708000	0.323334000	-1.374281000
P	-1.409133000	-1.543256000	-0.595654000
C	1.571511000	-1.565864000	-1.157684000
O	2.265456000	-2.195448000	-1.836839000
H	2.884252000	2.630962000	-1.421117000
C	-2.772428000	-1.661412000	0.629821000
C	-4.106878000	-1.713296000	0.217493000
C	-2.488499000	-1.711549000	1.993206000
C	-5.132857000	-1.796410000	1.148958000
H	-4.352534000	-1.670194000	-0.838872000
C	-3.514568000	-1.801613000	2.928606000
H	-1.459499000	-1.663752000	2.329440000
C	-4.838154000	-1.838575000	2.508479000
H	-6.164264000	-1.824916000	0.814507000
H	-3.277546000	-1.836623000	3.986240000
H	-5.638779000	-1.899219000	3.237399000
C	4.018970000	0.234099000	-0.064719000
C	4.961779000	0.881923000	-0.863373000
C	4.383597000	-0.960775000	0.562407000
C	6.235408000	0.348738000	-1.031872000
H	4.718607000	1.811837000	-1.363660000
C	5.659461000	-1.486337000	0.407620000
H	3.660105000	-1.496076000	1.167186000
C	6.589053000	-0.833298000	-0.393495000
H	6.952503000	0.862662000	-1.662801000
H	5.921423000	-2.414538000	0.903253000
H	7.582078000	-1.248602000	-0.525611000
H	-1.293158000	1.137299000	-3.175723000
H	-0.336214000	-0.355153000	-3.153708000
H	1.666414000	0.902221000	-2.712348000
H	0.731231000	2.405673000	-2.743321000
H	-0.572110000	1.524760000	-0.937955000
H	-0.300760000	0.441316000	1.048938000
C	-1.447407000	2.530047000	0.970923000
C	-1.031274000	1.459571000	1.739757000
C	2.541760000	1.854767000	1.814535000
H	1.632407000	2.463176000	1.843696000
C	-1.532695000	-3.236428000	-1.368008000
H	-2.607029000	-3.433336000	-1.461352000
H	-1.812872000	0.800468000	2.100262000
H	-0.255932000	1.642590000	2.476406000
F	-0.476619000	3.508110000	0.726616000
C	-0.909837000	-3.313967000	-2.761276000
H	0.168045000	-3.147792000	-2.735345000
H	-1.075708000	-4.312769000	-3.177544000
H	-1.351961000	-2.596181000	-3.457417000

C	-0.923607000	-4.272076000	-0.422679000
H	-1.070539000	-5.279757000	-0.823641000
H	0.152186000	-4.111063000	-0.306661000
H	-1.380624000	-4.238029000	0.570352000
C	3.745250000	2.794987000	1.774647000
H	3.742304000	3.436620000	2.661643000
H	4.686522000	2.238173000	1.767962000
H	3.730547000	3.448853000	0.897920000
C	2.567525000	0.953450000	3.046684000
H	2.625197000	1.562273000	3.954508000
H	1.671073000	0.332691000	3.111478000
H	3.438677000	0.290544000	3.040227000
C	-2.634979000	2.665578000	0.178644000
C	-3.747461000	1.818834000	0.385848000
C	-2.743238000	3.633964000	-0.842021000
C	-4.879972000	1.918460000	-0.402265000
H	-3.721559000	1.072937000	1.171931000
C	-3.886095000	3.722337000	-1.625203000
H	-1.919211000	4.315845000	-1.016012000
C	-4.962907000	2.864074000	-1.423703000
H	-5.711512000	1.246564000	-0.214123000
H	-3.934409000	4.476012000	-2.405009000
H	-5.853416000	2.939134000	-2.037307000

TSBI-2_b

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.209012000	-0.834966000	-0.053608000
P	1.984845000	-0.279695000	0.256654000
O	-0.515321000	-2.477476000	2.355640000
C	-0.393721000	-1.824372000	1.407222000
N	-0.054139000	0.583289000	-1.654366000
C	1.303052000	0.676669000	-2.225535000
C	-1.079656000	0.418066000	-2.702831000
C	-2.464413000	0.354528000	-2.071056000
C	2.313898000	0.917755000	-1.114682000
H	-3.221567000	0.096308000	-2.814715000
H	2.176245000	1.920742000	-0.700147000
H	-2.718527000	1.330083000	-1.653719000
P	-2.405540000	-0.848658000	-0.667502000
C	0.249244000	-2.247949000	-1.026996000
O	0.585612000	-3.181624000	-1.621927000
H	3.329573000	0.869312000	-1.507725000
C	-3.696545000	-0.241675000	0.490106000
C	-4.846658000	0.400599000	0.025574000
C	-3.551589000	-0.449223000	1.861888000
C	-5.823355000	0.834246000	0.913313000
H	-4.985458000	0.575323000	-1.036262000
C	-4.532936000	-0.024768000	2.750975000
H	-2.659251000	-0.930189000	2.243890000
C	-5.668907000	0.620940000	2.278787000
H	-6.705465000	1.340935000	0.537450000
H	-4.402161000	-0.192185000	3.814360000
H	-6.429811000	0.961295000	2.972452000
C	3.257845000	-1.599400000	0.120414000
C	4.496319000	-1.416722000	-0.497895000
C	2.990812000	-2.829247000	0.727365000
C	5.439521000	-2.437634000	-0.514223000
H	4.744214000	-0.471803000	-0.966783000
C	3.936848000	-3.846329000	0.723122000
H	2.031183000	-2.998603000	1.202195000
C	5.163399000	-3.653957000	0.098829000
H	6.394401000	-2.279077000	-1.003475000
H	3.710187000	-4.793026000	1.200792000
H	5.900762000	-4.449057000	0.087458000
H	-1.028678000	1.245020000	-3.421915000
H	-0.851654000	-0.507685000	-3.238908000
H	1.510973000	-0.265808000	-2.740544000
H	1.353969000	1.486379000	-2.963767000
H	-0.237686000	1.472899000	-1.185553000
H	-0.608916000	0.630737000	0.860747000
C	-0.844174000	2.957724000	0.416257000
C	-0.974659000	1.917129000	1.325905000

C	2.535254000	0.650719000	1.766580000
H	1.880668000	1.524574000	1.748006000
C	-3.254849000	-2.378188000	-1.313859000
H	-4.309231000	-2.099070000	-1.422897000
H	-1.988070000	1.638419000	1.597867000
H	-0.296014000	1.930187000	2.173139000
F	-1.892148000	3.062039000	-0.510619000
C	-2.732752000	-2.829974000	-2.677469000
H	-1.678497000	-3.108502000	-2.638699000
H	-3.291329000	-3.712661000	-3.004698000
H	-2.859070000	-2.063621000	-3.446459000
C	-3.146920000	-3.495901000	-0.276237000
H	-3.715134000	-4.371204000	-0.605945000
H	-2.106414000	-3.804146000	-0.138833000
H	-3.542250000	-3.191154000	0.696830000
C	3.982192000	1.134228000	1.706108000
H	4.185629000	1.797191000	2.553437000
H	4.685277000	0.298374000	1.763709000
H	4.191767000	1.697759000	0.792801000
C	2.250075000	-0.140308000	3.040923000
H	2.546501000	0.445887000	3.916715000
H	1.189091000	-0.378583000	3.140281000
H	2.814734000	-1.077820000	3.067831000
C	0.319635000	3.713675000	0.055208000
C	0.469535000	4.286125000	-1.226573000
C	1.381147000	3.899063000	0.968882000
C	1.638829000	4.941573000	-1.585065000
H	-0.337159000	4.197095000	-1.944692000
C	2.545893000	4.547627000	0.597030000
H	1.275117000	3.545222000	1.988010000
C	2.697030000	5.065120000	-0.688771000
H	1.726174000	5.360766000	-2.582672000
H	3.341987000	4.664144000	1.325625000
H	3.609220000	5.575575000	-0.975619000

TSB1-2_c

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.093281000	-0.694425000	0.053973000
P	-2.189113000	0.155754000	0.458831000
O	0.027349000	0.055080000	-2.778943000
C	-0.011350000	-0.225142000	-1.656103000
N	-0.100097000	-0.946282000	2.147658000
C	-1.432293000	-1.177913000	2.733393000
C	0.904529000	-1.875695000	2.692455000
C	2.264056000	-1.607086000	2.057533000
C	-2.361233000	-0.059993000	2.284492000
H	2.992155000	-2.363236000	2.361094000
H	-2.023068000	0.882046000	2.728235000
H	2.636427000	-0.630288000	2.377603000
P	2.038700000	-1.520624000	0.226402000
C	-0.817085000	-2.262011000	-0.352023000
O	-1.318981000	-3.266051000	-0.630458000
H	-3.382926000	-0.229800000	2.624138000
C	3.512605000	-0.611671000	-0.381653000
C	4.722125000	-0.639559000	0.314790000
C	3.449823000	0.079002000	-1.590826000
C	5.838190000	0.023437000	-0.179411000
H	4.800724000	-1.168661000	1.258514000
C	4.568067000	0.735936000	-2.091040000
H	2.521383000	0.113766000	-2.147643000
C	5.763832000	0.713135000	-1.384449000
H	6.767729000	0.003583000	0.379239000
H	4.499849000	1.271326000	-3.031707000
H	6.634737000	1.232279000	-1.769275000
C	-3.612720000	-0.712134000	-0.316882000
C	-4.773780000	-1.074136000	0.366858000
C	-3.532204000	-0.985402000	-1.685548000
C	-5.825936000	-1.694296000	-0.298864000
H	-4.876894000	-0.876747000	1.427141000
C	-4.586345000	-1.593043000	-2.354322000
H	-2.632829000	-0.730505000	-2.234949000
C	-5.736531000	-1.951711000	-1.661038000

H	-6.718527000	-1.973843000	0.250287000
H	-4.502133000	-1.795204000	-3.416308000
H	-6.557953000	-2.434662000	-2.178858000
H	0.971280000	-1.763992000	3.782701000
H	0.569453000	-2.895082000	2.483508000
H	-1.798332000	-2.153157000	2.398778000
H	-1.369384000	-1.199022000	3.829392000
H	0.175520000	0.010236000	2.464386000
H	0.601771000	0.860403000	0.597643000
C	0.752346000	1.856690000	2.747457000
C	1.104884000	1.919769000	1.409042000
H	-0.101563000	2.398596000	3.128865000
H	1.428297000	1.395384000	3.456745000
F	2.448807000	1.593010000	1.187652000
C	-2.627340000	1.941536000	0.212971000
H	-1.827975000	2.462152000	0.747721000
C	2.495926000	-3.229081000	-0.380185000
H	3.577198000	-3.302637000	-0.216403000
C	2.225152000	-3.332951000	-1.881855000
H	2.571643000	-4.300160000	-2.259261000
H	1.156577000	-3.252394000	-2.099202000
H	2.745632000	-2.553840000	-2.445193000
C	1.822374000	-4.363220000	0.391947000
H	2.150697000	-5.323167000	-0.019438000
H	2.089672000	-4.358310000	1.451732000
H	0.734906000	-4.330077000	0.308124000
C	-3.971764000	2.335704000	0.821873000
H	-4.122212000	3.414249000	0.708960000
H	-4.800809000	1.832305000	0.315280000
H	-4.033392000	2.106052000	1.889192000
C	-2.549277000	2.334393000	-1.260789000
H	-2.679267000	3.415693000	-1.361720000
H	-1.586008000	2.075483000	-1.702418000
H	-3.340316000	1.848553000	-1.841072000
C	0.708234000	3.063115000	0.511224000
C	0.078976000	4.202427000	1.007365000
C	1.014795000	3.001705000	-0.846878000
C	-0.273180000	5.242321000	0.153089000
H	-0.130183000	4.285380000	2.067275000
C	0.688183000	4.048303000	-1.696913000
H	1.512117000	2.120617000	-1.233087000
C	0.031304000	5.169624000	-1.200862000
H	-0.773195000	6.118091000	0.552695000
H	0.933429000	3.981230000	-2.751238000
H	-0.237725000	5.983370000	-1.865673000

TSBI-2_d

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.456498000	0.504924000	-0.013127000
P	2.289723000	-0.828086000	0.363428000
O	0.005921000	-0.211016000	-2.822544000
C	0.177131000	0.052882000	-1.708946000
N	0.572460000	0.850673000	2.074150000
C	1.880863000	0.555559000	2.682856000
C	0.034483000	2.153450000	2.507529000
C	-1.397280000	2.272200000	1.999843000
C	2.372719000	-0.803905000	2.204939000
H	-1.817745000	3.260707000	2.194606000
H	1.687990000	-1.586217000	2.543869000
H	-2.008819000	1.532454000	2.521455000
P	-1.406431000	1.826573000	0.205714000
C	1.498254000	1.857172000	-0.490628000
O	2.211322000	2.708916000	-0.811720000
H	3.357912000	-1.031396000	2.613432000
C	-3.093214000	1.174421000	-0.102423000
C	-4.167628000	1.460960000	0.741863000
C	-3.331948000	0.451472000	-1.272621000
C	-5.451772000	1.034749000	0.422551000
H	-4.014472000	2.022185000	1.657158000
C	-4.618760000	0.047717000	-1.604085000
H	-2.510037000	0.190709000	-1.928263000
C	-5.681201000	0.336373000	-0.756571000

H	-6.274172000	1.257382000	1.093927000
H	-4.785086000	-0.511354000	-2.517554000
H	-6.684086000	0.009189000	-1.008643000
C	3.918378000	-0.206430000	-0.222925000
C	5.052686000	-0.103715000	0.583217000
C	4.023345000	0.151584000	-1.570288000
C	6.259647000	0.345537000	0.057027000
H	5.011181000	-0.372228000	1.632268000
C	5.230288000	0.585707000	-2.100898000
H	3.147901000	0.102505000	-2.209489000
C	6.352894000	0.685842000	-1.286424000
H	7.129073000	0.424629000	0.700744000
H	5.291153000	0.856136000	-3.149228000
H	7.294154000	1.034889000	-1.696645000
H	0.052513000	2.229662000	3.602627000
H	0.672858000	2.945190000	2.105722000
H	2.579106000	1.344695000	2.385829000
H	1.804277000	0.570414000	3.777759000
H	-0.107470000	0.151602000	2.431950000
H	-0.521147000	-0.865312000	0.631717000
C	-1.643639000	-1.177687000	2.689520000
C	-1.248368000	-1.712620000	1.474694000
H	-1.034999000	-1.330454000	3.572191000
H	-2.611913000	-0.709436000	2.796166000
C	2.374813000	-2.629297000	-0.090697000
H	1.437889000	-3.022301000	0.307349000
C	-1.558438000	3.473101000	-0.670484000
H	-2.588187000	3.793980000	-0.475606000
F	-0.199850000	-2.651334000	1.635247000
C	-0.612385000	4.544968000	-0.127789000
H	0.434862000	4.295717000	-0.302642000
H	-0.810833000	5.490962000	-0.641778000
H	-0.751186000	4.724233000	0.940987000
C	-1.379089000	3.292063000	-2.177875000
H	-1.548755000	4.244574000	-2.689488000
H	-0.364543000	2.960929000	-2.416846000
H	-2.081893000	2.565171000	-2.592596000
C	3.543321000	-3.359969000	0.569414000
H	3.496057000	-4.426002000	0.325110000
H	4.505567000	-2.979874000	0.212287000
H	3.521689000	-3.274388000	1.658958000
C	2.379905000	-2.830259000	-1.605997000
H	3.317688000	-2.488015000	-2.053634000
H	2.276217000	-3.896131000	-1.831273000
H	1.557071000	-2.306757000	-2.098123000
C	-2.222256000	-2.246626000	0.456123000
C	-1.757547000	-2.626115000	-0.801808000
C	-3.561521000	-2.455328000	0.771419000
C	-2.612520000	-3.200253000	-1.731122000
H	-0.713305000	-2.467191000	-1.045747000
C	-4.424408000	-3.016834000	-0.162863000
H	-3.928553000	-2.187982000	1.755043000
C	-3.953124000	-3.395724000	-1.413675000
H	-2.232412000	-3.492840000	-2.704062000
H	-5.468836000	-3.162572000	0.090985000
H	-4.626842000	-3.839748000	-2.138916000

TSC1-2_a

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.628266000	-0.647040000	-0.042722000
P	2.390909000	0.781910000	0.168237000
O	1.207574000	-2.336690000	2.281237000
C	0.982949000	-1.665697000	1.364494000
N	0.023333000	0.747261000	-1.553281000
C	1.161251000	1.417322000	-2.212371000
C	-0.915608000	0.192472000	-2.549385000
C	-2.075023000	-0.499976000	-1.849273000
C	2.099953000	2.018935000	-1.176445000
H	-2.697680000	-1.039231000	-2.566768000
H	1.623281000	2.882239000	-0.706032000
H	-2.707933000	0.239755000	-1.355914000
P	-1.379277000	-1.608660000	-0.540857000

C	1.586096000	-1.686879000	-1.120550000
O	2.266531000	-2.353679000	-1.777809000
H	3.013263000	2.374229000	-1.653988000
C	-2.725361000	-1.709273000	0.705052000
C	-4.060138000	-1.835797000	0.311445000
C	-2.427248000	-1.679785000	2.066134000
C	-5.072833000	-1.916405000	1.257374000
H	-4.317757000	-1.854728000	-0.742750000
C	-3.439964000	-1.762583000	3.016597000
H	-1.397889000	-1.577359000	2.388256000
C	-4.764609000	-1.876452000	2.613884000
H	-6.105081000	-2.006664000	0.936651000
H	-3.191714000	-1.732447000	4.071803000
H	-5.55263000	-1.934576000	3.353831000
C	4.087761000	0.115596000	-0.075026000
C	5.086190000	0.766748000	-0.801688000
C	4.398965000	-1.096977000	0.545931000
C	6.358083000	0.216110000	-0.912647000
H	4.888078000	1.715326000	-1.286548000
C	5.672505000	-1.642404000	0.446881000
H	3.636236000	-1.630047000	1.101712000
C	6.655085000	-0.988606000	-0.286856000
H	7.118712000	0.733195000	-1.487525000
H	5.891285000	-2.585905000	0.934430000
H	7.646452000	-1.419077000	-0.375996000
H	-1.289606000	0.986643000	-3.207044000
H	-0.352837000	-0.516644000	-3.163104000
H	1.682694000	0.662398000	-2.808105000
H	0.804212000	2.196833000	-2.897241000
H	-0.490107000	1.452170000	-1.015262000
H	-0.226434000	0.468068000	0.981119000
C	-1.540638000	2.509914000	0.800374000
C	-1.058777000	1.506631000	1.621240000
C	2.585504000	1.856607000	1.672310000
H	1.660629000	2.441450000	1.669638000
C	-1.504228000	-3.323699000	-1.264929000
H	-2.578552000	-3.531033000	-1.329975000
H	-1.782389000	0.783073000	1.978420000
H	-0.303410000	1.755256000	2.358816000
C	-0.913149000	-3.439549000	-2.669412000
H	0.162853000	-3.260586000	-2.676702000
H	-1.077088000	-4.453523000	-3.048154000
H	-1.381910000	-2.750852000	-3.377380000
C	-0.870158000	-4.328043000	-0.302137000
H	-1.017713000	-5.347887000	-0.670786000
H	0.206370000	-4.157376000	-0.209517000
H	-1.309527000	-4.267794000	0.697679000
C	3.764778000	2.824083000	1.593123000
H	3.730089000	3.519160000	2.438058000
H	4.719881000	2.293173000	1.636981000
H	3.749244000	3.422499000	0.677364000
C	2.623690000	1.016366000	2.946545000
H	2.683368000	1.670112000	3.822463000
H	1.729678000	0.397015000	3.046653000
H	3.497968000	0.357629000	2.967212000
C	-2.774721000	2.479071000	0.032199000
C	-3.840186000	1.648645000	0.436980000
C	-2.964401000	3.229920000	-1.142979000
C	-5.003931000	1.554153000	-0.308274000
H	-3.759209000	1.069150000	1.349372000
C	-4.133187000	3.128750000	-1.885354000
H	-2.179811000	3.896219000	-1.481966000
C	-5.162628000	2.285110000	-1.482540000
H	-5.797969000	0.901059000	0.038448000
H	-4.237550000	3.716902000	-2.791516000
H	-6.076478000	2.210548000	-2.061067000
Cl	-0.490812000	3.935597000	0.566068000

TSC1-2_b

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.087296000	-0.931346000	-0.018351000
P	2.059209000	-0.194050000	0.268964000

O	-0.258781000	-2.500333000	2.451682000
C	-0.191818000	-1.879137000	1.476559000
N	-0.057457000	0.443835000	-1.662158000
C	1.290151000	0.669477000	-2.219406000
C	-1.033843000	0.119571000	-2.720659000
C	-2.418820000	-0.068300000	-2.116091000
C	2.260354000	1.024680000	-1.103961000
H	-3.119210000	-0.458015000	-2.858133000
H	2.007978000	2.004435000	-0.689577000
H	-2.798485000	0.894780000	-1.772546000
P	-2.268234000	-1.167218000	-0.635001000
C	0.491204000	-2.329082000	-0.951141000
O	0.904654000	-3.245335000	-1.524094000
H	3.277167000	1.095916000	-1.489855000
C	-3.610501000	-0.594155000	0.480979000
C	-4.805125000	-0.071905000	-0.019952000
C	-3.456405000	-0.710362000	1.862293000
C	-5.815793000	0.336322000	0.841116000
H	-4.952104000	0.031797000	-1.090026000
C	-4.471888000	-0.313714000	2.725563000
H	-2.531840000	-1.099942000	2.270804000
C	-5.651691000	0.214517000	2.216665000
H	-6.731402000	0.753665000	0.436644000
H	-4.334142000	-0.411382000	3.796736000
H	-6.439541000	0.535059000	2.889414000
C	3.425863000	-1.413092000	0.096872000
C	4.613025000	-1.156806000	-0.591562000
C	3.279831000	-2.646739000	0.737250000
C	5.623312000	-2.110593000	-0.645125000
H	4.769649000	-0.207208000	-1.089519000
C	4.292359000	-3.596297000	0.694368000
H	2.360488000	-2.874246000	1.265402000
C	5.466417000	-3.331683000	-0.000868000
H	6.536906000	-1.895382000	-1.188702000
H	4.157348000	-4.548317000	1.195545000
H	6.254067000	-4.075873000	-0.043446000
H	-1.055659000	0.912850000	-3.478330000
H	-0.693562000	-0.799646000	-3.206189000
H	1.599195000	-0.253435000	-2.719246000
H	1.267334000	1.469647000	-2.969452000
H	-0.353442000	1.320409000	-1.222130000
H	-0.627903000	0.505058000	0.824519000
C	-1.012423000	2.866025000	0.411216000
C	-1.033096000	1.819105000	1.320411000
C	2.583256000	0.776321000	1.764238000
H	1.849604000	1.584683000	1.785294000
C	-2.991603000	-2.796255000	-1.186762000
H	-4.063106000	-2.603912000	-1.316597000
H	-1.997954000	1.471121000	1.673376000
H	-0.273954000	1.824196000	2.095622000
C	-2.427433000	-3.291108000	-2.518525000
H	-1.362206000	-3.516599000	-2.451240000
H	-2.939478000	-4.214601000	-2.806863000
H	-2.576552000	-2.571680000	-3.327935000
C	-2.808586000	-3.837470000	-0.082476000
H	-3.305584000	-4.772186000	-0.359986000
H	-1.748560000	-4.055271000	0.077543000
H	-3.234008000	-3.504880000	0.868468000
C	3.974229000	1.394353000	1.639804000
H	4.165128000	2.050745000	2.495159000
H	4.751681000	0.624969000	1.634242000
H	4.078627000	1.998125000	0.734444000
C	2.439486000	-0.044211000	3.043663000
H	2.682158000	0.576368000	3.912202000
H	1.423298000	-0.422037000	3.174136000
H	3.124337000	-0.898085000	3.050166000
C	0.134572000	3.686329000	0.059872000
C	0.319158000	4.238907000	-1.221569000
C	1.148333000	3.927378000	1.009142000
C	1.475805000	4.932791000	-1.548507000
H	-0.450686000	4.106372000	-1.973150000
C	2.305374000	4.613302000	0.674943000
H	1.012807000	3.589655000	2.030117000
C	2.488785000	5.112461000	-0.611706000
H	1.588156000	5.335139000	-2.550247000
H	3.065066000	4.773945000	1.433042000
H	3.392719000	5.651803000	-0.871147000

Cl -2.500957000 3.140550000 -0.535570000

TSC1-2_c

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.037412000	-0.653480000	0.030751000
P	-2.207409000	0.092767000	0.325441000
O	0.055185000	-0.159482000	-2.859217000
C	0.029691000	-0.343856000	-1.716235000
N	-0.034195000	-0.677567000	2.129878000
C	-1.357212000	-0.841025000	2.758145000
C	0.984403000	-1.528976000	2.769216000
C	2.338933000	-1.303838000	2.105101000
C	-2.320618000	0.177042000	2.163190000
H	3.085230000	-2.000545000	2.494904000
H	-1.997043000	1.186858000	2.434082000
H	2.687373000	-0.286298000	2.305606000
P	2.104916000	-1.442620000	0.278842000
C	-0.680246000	-2.287315000	-0.205786000
O	-1.120638000	-3.344511000	-0.365867000
H	-3.328251000	0.048258000	2.558998000
C	3.581997000	-0.642599000	-0.459365000
C	4.820219000	-0.672776000	0.184798000
C	3.489382000	-0.043294000	-1.713748000
C	5.937348000	-0.095227000	-0.404858000
H	4.919497000	-1.135509000	1.161271000
C	4.608929000	0.523965000	-2.311213000
H	2.535864000	-0.001668000	-2.224636000
C	5.833369000	0.504900000	-1.655586000
H	6.890088000	-0.112241000	0.113223000
H	4.518292000	0.992448000	-3.284956000
H	6.705041000	0.957891000	-2.115109000
C	-3.532639000	-1.065940000	-0.214113000
C	-4.586167000	-1.482442000	0.599559000
C	-3.484590000	-1.532039000	-1.531606000
C	-5.564561000	-2.342751000	0.110821000
H	-4.661672000	-1.143158000	1.625799000
C	-4.466325000	-2.379370000	-2.025366000
H	-2.663335000	-1.240446000	-2.177496000
C	-5.509408000	-2.790266000	-1.202678000
H	-6.371624000	-2.661470000	0.761613000
H	-4.408022000	-2.729730000	-3.049918000
H	-6.271357000	-3.462297000	-1.582058000
H	1.049713000	-1.300824000	3.841330000
H	0.667687000	-2.570682000	2.669888000
H	-1.706910000	-1.862202000	2.577306000
H	-1.281746000	-0.697701000	3.844243000
H	0.246934000	0.307082000	2.343390000
H	0.637410000	0.995325000	0.434835000
C	0.730928000	2.115299000	2.591086000
C	0.971978000	2.225324000	1.234352000
H	-0.208878000	2.454704000	3.008117000
H	1.511676000	1.822809000	3.280455000
C	-2.894165000	1.727581000	-0.236524000
H	-2.133592000	2.444065000	0.079327000
C	2.560285000	-3.217378000	-0.111768000
H	3.645636000	-3.256164000	0.035816000
C	2.268852000	-3.515041000	-1.583483000
H	2.631356000	-4.515292000	-1.840572000
H	1.196990000	-3.484538000	-1.794034000
H	2.765928000	-2.802983000	-2.247922000
C	1.930893000	-4.255069000	0.817696000
H	2.271597000	-5.253281000	0.523829000
H	2.228416000	-4.107699000	1.859018000
H	0.841521000	-4.256814000	0.764137000
C	-4.220012000	2.090897000	0.430176000
H	-4.547955000	3.074280000	0.077665000
H	-5.005143000	1.370636000	0.180195000
H	-4.137221000	2.146597000	1.518747000
C	-3.007734000	1.788926000	-1.759666000
H	-3.248674000	2.811162000	-2.064579000
H	-2.075544000	1.508319000	-2.254232000
H	-3.804673000	1.134935000	-2.125462000

C	0.231697000	3.218262000	0.376730000
C	-0.462941000	4.276148000	0.959645000
C	0.259886000	3.119480000	-1.014398000
C	-1.155923000	5.188346000	0.168339000
H	-0.456785000	4.394027000	2.036439000
C	-0.408789000	4.040095000	-1.804864000
H	0.805678000	2.302951000	-1.471945000
C	-1.132461000	5.073172000	-1.214946000
H	-1.702124000	5.998766000	0.638955000
H	-0.378193000	3.942237000	-2.884459000
H	-1.667684000	5.786706000	-1.832132000
Cl	2.745893000	2.245870000	0.836643000

TSC1-2_d

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.477055000	0.525791000	0.007633000
P	2.337505000	-0.792697000	0.262016000
O	0.037402000	0.042078000	-2.853441000
C	0.202255000	0.212771000	-1.721333000
N	0.597462000	0.716145000	2.117765000
C	1.917911000	0.391431000	2.689829000
C	0.080100000	1.998159000	2.636131000
C	-1.345198000	2.196438000	2.136404000
C	2.444109000	-0.909056000	2.099059000
H	-1.726757000	3.186076000	2.394438000
H	1.792737000	-1.736597000	2.389858000
H	-1.985689000	1.450691000	2.610166000
P	-1.368545000	1.867168000	0.317859000
C	1.512301000	1.915073000	-0.360200000
O	2.223972000	2.791273000	-0.610722000
H	3.442080000	-1.133384000	2.476815000
C	-3.075413000	1.300510000	-0.040590000
C	-4.143962000	1.552640000	0.821433000
C	-3.331237000	0.692127000	-1.270487000
C	-5.439912000	1.200652000	0.462215000
H	-3.976898000	2.029276000	1.781269000
C	-4.629101000	0.363949000	-1.640199000
H	-2.514041000	0.459823000	-1.942791000
C	-5.685632000	0.614350000	-0.773612000
H	-6.258345000	1.392717000	1.147687000
H	-4.808125000	-0.110245000	-2.598075000
H	-6.697779000	0.345275000	-1.055589000
C	3.954448000	-0.105687000	-0.287789000
C	5.102639000	-0.085821000	0.504964000
C	4.039409000	0.386810000	-1.593509000
C	6.302002000	0.413503000	0.007331000
H	5.079812000	-0.462170000	1.520833000
C	5.237818000	0.873666000	-2.096554000
H	3.155322000	0.400166000	-2.222384000
C	6.373875000	0.890629000	-1.294911000
H	7.182175000	0.425309000	0.641185000
H	5.281052000	1.251942000	-3.111881000
H	7.308700000	1.280039000	-1.682894000
H	0.098226000	2.001628000	3.733650000
H	0.740402000	2.796863000	2.287182000
H	2.592720000	1.220616000	2.454730000
H	1.851898000	0.313222000	3.782308000
H	-0.078988000	0.002483000	2.429417000
H	-0.504994000	-0.945119000	0.576291000
C	-1.961983000	-1.160312000	2.478273000
C	-1.450096000	-1.733223000	1.329653000
H	-1.504622000	-1.308020000	3.447293000
H	-2.863494000	-0.564501000	2.412406000
C	2.442278000	-2.543716000	-0.352977000
H	1.484865000	-2.968142000	-0.046506000
C	-1.471137000	3.572660000	-0.454810000
H	-2.501249000	3.893945000	-0.263517000
C	-0.529869000	4.600928000	0.174234000
H	0.519957000	4.350994000	0.019350000
H	-0.703153000	5.574776000	-0.295011000
H	-0.701351000	4.726968000	1.245694000

C	-1.261929000	3.485436000	-1.966578000
H	-1.414369000	4.469377000	-2.421021000
H	-0.245945000	3.161140000	-2.206952000
H	-1.961214000	2.792991000	-2.441093000
C	3.569646000	-3.345067000	0.295337000
H	3.563058000	-4.368855000	-0.092300000
H	4.549958000	-2.913209000	0.070236000
H	3.459460000	-3.407141000	1.381258000
C	2.521571000	-2.600440000	-1.878853000
H	3.484271000	-2.234048000	-2.246864000
H	2.414499000	-3.638413000	-2.208197000
H	1.729817000	-2.019075000	-2.357354000
C	-2.339062000	-2.156520000	0.185555000
C	-1.810937000	-2.403857000	-1.080023000
C	-3.693491000	-2.393157000	0.405559000
C	-2.617486000	-2.862960000	-2.110220000
H	-0.753781000	-2.235727000	-1.250274000
C	-4.506941000	-2.847035000	-0.626900000
H	-4.107752000	-2.229801000	1.393095000
C	-3.973179000	-3.085118000	-1.886510000
H	-2.186570000	-3.047913000	-3.088304000
H	-5.562409000	-3.015473000	-0.442031000
H	-4.607936000	-3.443646000	-2.690022000
Cl	-0.317786000	-3.133240000	1.748727000

TS1_H

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.006052000	0.061996000	0.122774000
P	2.246088000	-0.095622000	0.378339000
O	-0.042095000	-0.338150000	-2.783878000
C	-0.021824000	-0.194995000	-1.635618000
N	0.006713000	0.039123000	2.214756000
C	1.268622000	0.436469000	2.865490000
C	-1.153957000	0.688033000	2.849824000
C	-2.435539000	0.129534000	2.242388000
C	2.424033000	-0.301720000	2.199891000
H	-3.315064000	0.694631000	2.557368000
H	2.325092000	-1.374642000	2.389029000
H	-2.565987000	-0.906275000	2.567636000
P	-2.237185000	0.067141000	0.404846000
C	0.070271000	1.826723000	-0.072417000
O	0.121131000	2.971621000	-0.208576000
H	3.395106000	0.015028000	2.585656000
C	-3.299907000	-1.337060000	-0.105341000
C	-4.581968000	-1.497603000	0.426739000
C	-2.837709000	-2.248836000	-1.051331000
C	-5.380633000	-2.559619000	0.026466000
H	-4.962202000	-0.786354000	1.153156000
C	-3.642214000	-3.307811000	-1.461402000
H	-1.842074000	-2.133622000	-1.463894000
C	-4.911237000	-3.466086000	-0.920294000
H	-6.371634000	-2.679684000	0.450229000
H	-3.272680000	-4.010926000	-2.199570000
H	-5.537008000	-4.294209000	-1.234745000
C	-3.186385000	1.493898000	-0.248610000
C	-3.313337000	2.676232000	0.479895000
C	-3.703303000	1.436849000	-1.544404000
C	-3.959378000	3.777315000	-0.070832000
H	-2.900614000	2.752335000	1.480266000
C	-4.346850000	2.537496000	-2.094233000
H	-3.609765000	0.526171000	-2.127122000
C	-4.478435000	3.709924000	-1.357924000
H	-4.051202000	4.691290000	0.505643000
H	-4.747829000	2.477801000	-3.100071000
H	-4.979388000	4.570001000	-1.788278000
C	3.246175000	-1.459613000	-0.327835000
C	4.609339000	-1.571455000	-0.040083000
C	2.646969000	-2.401594000	-1.161024000
C	5.354645000	-2.615380000	-0.569359000
H	5.094239000	-0.832972000	0.590786000
C	3.395730000	-3.445091000	-1.696840000
H	1.590152000	-2.318885000	-1.387701000

C	4.747842000	-3.553882000	-1.400137000
H	6.411807000	-2.695419000	-0.341040000
H	2.919942000	-4.170452000	-2.347453000
H	5.331967000	-4.366853000	-1.817366000
C	3.257334000	1.368583000	-0.067203000
C	3.739247000	2.275430000	0.874274000
C	3.470564000	1.623709000	-1.424738000
C	4.432300000	3.412434000	0.468583000
H	3.577581000	2.110652000	1.933575000
C	4.165842000	2.754133000	-1.828235000
H	3.091729000	0.932710000	-2.171831000
C	4.648753000	3.652790000	-0.881338000
H	4.799935000	4.111398000	1.211975000
H	4.326928000	2.937757000	-2.884725000
H	5.186877000	4.539668000	-1.197224000
H	-1.146907000	0.503333000	3.932408000
H	-1.078111000	1.768727000	2.694866000
H	1.386866000	1.520596000	2.769729000
H	1.233977000	0.194124000	3.935920000
H	-0.097497000	-1.002466000	2.433874000
H	-0.035078000	-1.692586000	0.465604000
C	-0.210474000	-2.813986000	2.517032000
C	-0.095025000	-2.877150000	1.112290000
H	0.839504000	-3.265870000	0.708826000
H	0.657369000	-2.989209000	3.145419000
H	-0.956078000	-3.246100000	0.556963000
H	-1.181032000	-2.930027000	2.989279000

TS2_CH₃

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.026983000	0.062148000	0.114373000
P	2.270309000	-0.021625000	0.385745000
O	0.054872000	-0.431028000	-2.777888000
C	0.037258000	-0.248115000	-1.634373000
N	0.016759000	0.065798000	2.210631000
C	1.258837000	0.520715000	2.860405000
C	-1.175056000	0.658922000	2.839990000
C	-2.415279000	0.025906000	2.221112000
C	2.447054000	-0.181571000	2.212952000
H	-3.335239000	0.481051000	2.592212000
H	2.397575000	-1.253462000	2.424836000
H	-2.437115000	-1.036858000	2.481263000
P	-2.230073000	0.093968000	0.390508000
C	0.066365000	1.825399000	-0.115836000
O	0.103320000	2.967557000	-0.272269000
H	3.401612000	0.186187000	2.594555000
C	-3.390692000	-1.180902000	-0.234354000
C	-4.557914000	-1.503068000	0.460967000
C	-3.125373000	-1.817639000	-1.445594000
C	-5.435735000	-2.455065000	-0.040938000
H	-4.788509000	-1.011963000	1.400255000
C	-4.010725000	-2.760454000	-1.955329000
H	-2.214505000	-1.591551000	-1.986828000
C	-5.164183000	-3.084135000	-1.251567000
H	-6.335522000	-2.703318000	0.511326000
H	-3.791968000	-3.249531000	-2.898095000
H	-5.851439000	-3.825922000	-1.643465000
C	-3.089010000	1.629383000	-0.142582000
C	-3.493975000	2.621615000	0.747578000
C	-3.264539000	1.837959000	-1.512933000
C	-4.075632000	3.795994000	0.278442000
H	-3.356103000	2.496993000	1.815471000
C	-3.847996000	3.006547000	-1.980058000
H	-2.941609000	1.082826000	-2.222814000
C	-4.256786000	3.989789000	-1.083920000
H	-4.385424000	4.559601000	0.983558000
H	-3.980732000	3.153033000	-3.046250000
H	-4.709489000	4.904835000	-1.449403000
C	3.322181000	-1.364320000	-0.287063000
C	4.685780000	-1.421908000	0.014074000
C	2.763964000	-2.342616000	-1.106943000
C	5.472507000	-2.448521000	-0.488488000

H	5.138155000	-0.654754000	0.634825000
C	3.553920000	-3.368930000	-1.615578000
H	1.706006000	-2.305244000	-1.340514000
C	4.906509000	-3.423561000	-1.305865000
H	6.529745000	-2.486248000	-0.249837000
H	3.109510000	-4.123924000	-2.254553000
H	5.523087000	-4.223171000	-1.701757000
C	3.235638000	1.464195000	-0.089242000
C	3.685205000	2.406622000	0.832893000
C	3.447427000	1.694084000	-1.451515000
C	4.345392000	3.554483000	0.403744000
H	3.523227000	2.261108000	1.894945000
C	4.108918000	2.836063000	-1.878378000
H	3.093768000	0.974691000	-2.183925000
C	4.560230000	3.770300000	-0.950483000
H	4.689107000	4.280545000	1.132370000
H	4.268901000	3.000699000	-2.938162000
H	5.072693000	4.665502000	-1.284971000
H	-1.164853000	0.474574000	3.922514000
H	-1.158637000	1.742105000	2.682157000
H	1.335691000	1.606972000	2.748072000
H	1.228627000	0.294333000	3.934505000
H	-0.051027000	-0.977172000	2.433043000
H	0.033215000	-1.681381000	0.504573000
C	-0.093111000	-2.793684000	2.543451000
C	0.142098000	-2.868822000	1.153339000
H	1.186947000	-3.032307000	0.887559000
H	0.735208000	-2.848032000	3.243552000
H	-1.075825000	-3.039896000	2.938702000
C	-0.798893000	-3.679830000	0.280724000
H	-1.842950000	-3.468717000	0.525445000
H	-0.654409000	-3.464861000	-0.782722000
H	-0.624977000	-4.747415000	0.449468000

TS1_CH3

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.055148000	0.142021000	0.047192000
P	2.282292000	-0.154368000	0.320899000
O	0.009946000	0.034560000	-2.886014000
C	0.033654000	0.060957000	-1.729287000
N	-0.001626000	-0.107183000	2.112081000
C	1.269682000	0.097547000	2.832325000
C	-1.105825000	0.591947000	2.793707000
C	-2.429321000	0.229482000	2.130600000
C	2.391904000	-0.624071000	2.096850000
H	-3.235927000	0.891485000	2.451493000
H	2.217823000	-1.703109000	2.131532000
H	-2.705263000	-0.791206000	2.401357000
P	-2.192392000	0.243107000	0.293446000
C	0.215378000	1.908560000	0.033168000
O	0.337829000	3.056429000	0.018643000
H	3.369690000	-0.437360000	2.545298000
C	-3.303226000	-1.089815000	-0.295745000
C	-4.591014000	-1.233369000	0.227495000
C	-2.861531000	-1.981784000	-1.269637000
C	-5.414462000	-2.262675000	-0.205819000
H	-4.953392000	-0.538011000	0.977961000
C	-3.690643000	-3.008360000	-1.712093000
H	-1.862009000	-1.879416000	-1.676230000
C	-4.963651000	-3.153130000	-1.176750000
H	-6.408679000	-2.371995000	0.213232000
H	-3.336012000	-3.699173000	-2.468952000
H	-5.607379000	-3.958040000	-1.514314000
C	-3.060615000	1.746795000	-0.295443000
C	-3.040379000	2.917580000	0.463249000
C	-3.661325000	1.765727000	-1.555047000
C	-3.624099000	4.081956000	-0.020715000
H	-2.559775000	2.932813000	1.435969000
C	-4.242179000	2.931191000	-2.039329000
H	-3.682370000	0.865902000	-2.161037000
C	-4.227503000	4.091040000	-1.272742000
H	-3.601585000	4.984922000	0.579517000

H	-4.708579000	2.931470000	-3.018346000
H	-4.681193000	4.999874000	-1.652305000
C	3.240616000	-1.452588000	-0.549784000
C	4.601904000	-1.636559000	-0.292833000
C	2.604712000	-2.278623000	-1.473815000
C	5.309052000	-2.638531000	-0.942713000
H	5.114898000	-0.985944000	0.408665000
C	3.314559000	-3.279909000	-2.128967000
H	1.548835000	-2.140454000	-1.676073000
C	4.665221000	-3.461858000	-1.862693000
H	6.365198000	-2.774961000	-0.737601000
H	2.809429000	-3.915835000	-2.847474000
H	5.219274000	-4.242460000	-2.372599000
C	3.364824000	1.310831000	0.111141000
C	3.954582000	1.989921000	1.174891000
C	3.532859000	1.805166000	-1.185492000
C	4.708469000	3.137948000	0.946820000
H	3.830057000	1.637687000	2.192483000
C	4.289337000	2.944995000	-1.412991000
H	3.063292000	1.297310000	-2.022734000
C	4.879641000	3.615450000	-0.345166000
H	5.160664000	3.657837000	1.784431000
H	4.412215000	3.317467000	-2.423932000
H	5.463910000	4.511735000	-0.521929000
H	-1.136467000	0.311996000	3.855322000
H	-0.922475000	1.669645000	2.740036000
H	1.470160000	1.172491000	2.893495000
H	1.185261000	-0.287649000	3.857337000
H	-0.213572000	-1.172560000	2.225612000
H	-0.068396000	-1.667489000	0.212382000
C	-0.415939000	-2.913993000	2.119380000
C	-0.083926000	-2.861035000	0.737507000
H	0.930163000	-3.154973000	0.467049000
H	0.383532000	-3.182219000	2.808266000
H	-0.809351000	-3.281893000	0.037254000
C	-1.816423000	-3.293960000	2.545146000
H	-2.109006000	-2.846312000	3.503703000
H	-2.553612000	-2.970633000	1.800840000
H	-1.953387000	-4.381194000	2.658414000

TS2_Ph

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.316759000	0.426710000	0.130407000
P	2.513510000	-0.059231000	0.408657000
O	0.264645000	-0.173373000	-2.741540000
C	0.271029000	0.049152000	-1.605460000
N	0.337544000	0.528266000	2.217338000
C	1.630943000	0.887020000	2.826503000
C	-0.772497000	1.262280000	2.849469000
C	-2.084914000	0.801944000	2.227426000
C	2.729514000	0.005929000	2.241906000
H	-2.941020000	1.352027000	2.622433000
H	2.602317000	-1.018746000	2.600469000
H	-2.237628000	-0.259149000	2.447717000
P	-1.893892000	0.911199000	0.402408000
C	0.699975000	2.134119000	-0.184217000
O	0.952707000	3.239459000	-0.395063000
H	3.723369000	0.343354000	2.542767000
C	-3.312133000	-0.018303000	-0.288769000
C	-4.586700000	0.104927000	0.269746000
C	-3.143856000	-0.781977000	-1.440351000
C	-5.673496000	-0.527889000	-0.316725000
H	-4.738548000	0.706274000	1.160188000
C	-4.236851000	-1.399307000	-2.038544000
H	-2.157692000	-0.907184000	-1.869084000
C	-5.500690000	-1.273882000	-1.478884000
H	-6.658377000	-0.429344000	0.126824000
H	-4.093082000	-1.989819000	-2.936152000
H	-6.352015000	-1.760514000	-1.942434000
C	-2.396338000	2.622292000	-0.048781000
C	-2.689899000	3.614732000	0.883169000
C	-2.427010000	2.941432000	-1.409182000

C	-3.015716000	4.902007000	0.463743000
H	-2.664959000	3.402643000	1.945914000
C	-2.757370000	4.221748000	-1.827126000
H	-2.186912000	2.183539000	-2.148903000
C	-3.052365000	5.207336000	-0.889678000
H	-3.239958000	5.665658000	1.200565000
H	-2.778949000	4.452641000	-2.886448000
H	-3.304344000	6.210674000	-1.215092000
C	3.255106000	-1.663248000	-0.077210000
C	4.483190000	-2.080842000	0.442384000
C	2.595500000	-2.475748000	-0.996223000
C	5.031760000	-3.295964000	0.056242000
H	5.018970000	-1.452346000	1.146766000
C	3.148417000	-3.689957000	-1.390065000
H	1.639814000	-2.161117000	-1.398490000
C	4.364447000	-4.102488000	-0.861731000
H	5.982463000	-3.614357000	0.469542000
H	2.624374000	-4.314078000	-2.105530000
H	4.795306000	-5.050833000	-1.163451000
C	3.738316000	1.125360000	-0.272252000
C	4.164612000	2.234120000	0.457563000
C	4.172466000	0.974021000	-1.590814000
C	5.022998000	3.167070000	-0.113614000
H	3.823914000	2.386871000	1.475861000
C	5.029997000	1.905884000	-2.160320000
H	3.844910000	0.120984000	-2.176553000
C	5.458915000	3.004144000	-1.422364000
H	5.346407000	4.025165000	0.465350000
H	5.362730000	1.773771000	-3.183986000
H	6.128049000	3.732043000	-1.867724000
H	-0.782904000	1.073276000	3.931089000
H	-0.618426000	2.335391000	2.696331000
H	1.826222000	1.946538000	2.633158000
H	1.586537000	0.748446000	3.915021000
H	0.173830000	-0.495341000	2.496579000
H	-0.056676000	-1.274389000	0.583513000
C	-0.070988000	-2.245309000	2.717521000
C	-0.109682000	-2.434948000	1.317768000
H	0.812509000	-2.831163000	0.896523000
H	0.858830000	-2.431976000	3.244645000
H	-0.973099000	-2.305167000	3.316392000
C	-1.302029000	-3.059587000	0.647146000
C	-2.569013000	-3.084145000	1.228940000
C	-1.136583000	-3.672938000	-0.595532000
C	-3.631292000	-3.721348000	0.599862000
H	-2.731784000	-2.614647000	2.192443000
C	-2.192885000	-4.319482000	-1.225041000
H	-0.159044000	-3.655383000	-1.067324000
C	-3.446488000	-4.350057000	-0.625740000
H	-4.608625000	-3.725194000	1.070264000
H	-2.035669000	-4.800996000	-2.184645000
H	-4.276046000	-4.849958000	-1.113843000

TS1_Ph

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.443635000	0.408320000	0.085624000
P	-2.488808000	-0.473317000	-0.276023000
O	-0.888383000	1.295601000	2.846377000
C	-0.716741000	0.935382000	1.760326000
N	0.003531000	-0.464160000	-1.797790000
C	-1.166136000	-0.731734000	-2.655308000
C	1.089447000	0.208764000	-2.537261000
C	2.308441000	0.357576000	-1.634862000
C	-2.248141000	-1.428091000	-1.837345000
H	3.064711000	1.001554000	-2.087194000
H	-1.899471000	-2.418132000	-1.530032000
H	2.766558000	-0.619844000	-1.468455000
P	1.744107000	0.968824000	0.018109000
C	-0.934917000	1.994314000	-0.559085000
O	-1.267012000	3.024903000	-0.958273000
H	-3.165915000	-1.569608000	-2.411698000
C	2.970723000	0.292582000	1.197023000

C	4.341307000	0.405860000	0.953948000
C	2.534191000	-0.354084000	2.350353000
C	5.257617000	-0.136885000	1.843284000
H	4.695848000	0.915011000	0.063511000
C	3.452717000	-0.891635000	3.246919000
H	1.471057000	-0.451622000	2.537441000
C	4.813960000	-0.788703000	2.991081000
H	6.320082000	-0.050478000	1.643460000
H	3.102030000	-1.394572000	4.141346000
H	5.531257000	-1.211832000	3.685868000
C	2.156049000	2.756728000	0.047275000
C	2.233085000	3.511732000	-1.122235000
C	2.289703000	3.400824000	1.279170000
C	2.456936000	4.883140000	-1.063549000
H	2.111964000	3.038952000	-2.091029000
C	2.513348000	4.769745000	1.337173000
H	2.224777000	2.831462000	2.200974000
C	2.599763000	5.514384000	0.165284000
H	2.515780000	5.457046000	-1.981901000
H	2.620168000	5.256118000	2.300495000
H	2.773837000	6.583725000	0.211840000
C	-3.285082000	-1.665167000	0.867373000
C	-4.456926000	-2.336843000	0.508903000
C	-2.723544000	-1.898781000	2.120616000
C	-5.045504000	-3.237296000	1.385945000
H	-4.918783000	-2.147921000	-0.455127000
C	-3.318001000	-2.794926000	3.003482000
H	-1.811945000	-1.384408000	2.402148000
C	-4.476244000	-3.466649000	2.635900000
H	-5.953448000	-3.756124000	1.098618000
H	-2.872187000	-2.966708000	3.976848000
H	-4.939058000	-4.167438000	3.322105000
C	-3.870553000	0.688984000	-0.599889000
C	-4.361836000	0.961306000	-1.874468000
C	-4.386073000	1.395379000	0.490429000
C	-5.360734000	1.913981000	-2.056307000
H	-3.969935000	0.441882000	-2.741716000
C	-5.383669000	2.341697000	0.309439000
H	-4.002655000	1.205763000	1.488519000
C	-5.874995000	2.602821000	-0.966502000
H	-5.734760000	2.116026000	-3.054100000
H	-5.775987000	2.879936000	1.165115000
H	-6.651557000	3.346224000	-1.108788000
H	1.357578000	-0.365836000	-3.432625000
H	0.715974000	1.184671000	-2.862261000
H	-1.527709000	0.225098000	-3.045056000
H	-0.877705000	-1.355148000	-3.511475000
H	0.363279000	-1.389110000	-1.508484000
H	0.027669000	-1.210830000	0.598531000
C	0.354324000	-2.638781000	0.592001000
C	0.771470000	-3.172766000	-0.625645000
H	0.021594000	-3.591602000	-1.292357000
H	-0.621824000	-2.941946000	0.957289000
H	1.083883000	-2.517793000	1.389086000
C	2.136011000	-3.189931000	-1.116389000
C	3.251951000	-2.863326000	-0.320416000
C	2.395663000	-3.518968000	-2.463443000
C	4.535831000	-2.846107000	-0.846785000
H	3.114863000	-2.610844000	0.724822000
C	3.678943000	-3.498800000	-2.986379000
H	1.560425000	-3.783534000	-3.106902000
C	4.765743000	-3.153781000	-2.184512000
H	5.366018000	-2.581568000	-0.199595000
H	3.834998000	-3.749799000	-4.031062000
H	5.769672000	-3.133964000	-2.593626000

TS2_F

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.007996000	0.044656000	0.106918000
P	2.252792000	0.021871000	0.375344000
O	-0.046264000	-0.436336000	-2.788190000
C	-0.019065000	-0.249451000	-1.648515000

N	-0.003118000	0.045464000	2.231050000
C	1.233632000	0.540398000	2.861026000
C	-1.212350000	0.615271000	2.851411000
C	-2.437006000	-0.033614000	2.218480000
C	2.434890000	-0.132328000	2.206202000
H	-3.370081000	0.401486000	2.582043000
H	2.418559000	-1.205127000	2.421219000
H	-2.452577000	-1.099691000	2.465114000
P	-2.248976000	0.049773000	0.385547000
C	0.014637000	1.814859000	-0.103745000
O	0.038732000	2.957965000	-0.253998000
H	3.379824000	0.260907000	2.586261000
C	-3.401649000	-1.229327000	-0.235248000
C	-4.776077000	-1.131295000	0.003535000
C	-2.907065000	-2.313804000	-0.953018000
C	-5.638664000	-2.112934000	-0.461245000
H	-5.175822000	-0.277239000	0.541300000
C	-3.774103000	-3.297513000	-1.420818000
H	-1.842515000	-2.399410000	-1.130845000
C	-5.136731000	-3.198803000	-1.175478000
H	-6.703540000	-2.029210000	-0.273455000
H	-3.378084000	-4.141319000	-1.974701000
H	-5.812488000	-3.964457000	-1.541090000
C	-3.113250000	1.583898000	-0.133603000
C	-3.509554000	2.578455000	0.757536000
C	-3.303410000	1.787305000	-1.503251000
C	-4.095508000	3.751894000	0.290764000
H	-3.363229000	2.455236000	1.824594000
C	-3.890359000	2.954938000	-1.967888000
H	-2.991737000	1.026221000	-2.212053000
C	-4.289160000	3.941493000	-1.070420000
H	-4.399273000	4.517458000	0.996367000
H	-4.034488000	3.098079000	-3.033034000
H	-4.744818000	4.855711000	-1.434337000
C	3.341931000	-1.294351000	-0.290513000
C	4.698601000	-1.333366000	0.044201000
C	2.822101000	-2.263763000	-1.145539000
C	5.517107000	-2.333479000	-0.460484000
H	5.120260000	-0.572331000	0.693496000
C	3.644849000	-3.263472000	-1.656102000
H	1.769185000	-2.244951000	-1.403284000
C	4.990042000	-3.299619000	-1.313876000
H	6.568535000	-2.357024000	-0.195848000
H	3.230213000	-4.012604000	-2.321260000
H	5.631582000	-4.078404000	-1.711584000
C	3.185167000	1.528790000	-0.098466000
C	3.622006000	2.478948000	0.821567000
C	3.385633000	1.762236000	-1.461837000
C	4.259576000	3.638337000	0.389021000
H	3.467546000	2.331222000	1.884457000
C	4.024765000	2.915540000	-1.891995000
H	3.040316000	1.036933000	-2.192513000
C	4.464255000	3.857479000	-0.966201000
H	4.594091000	4.370453000	1.115825000
H	4.176790000	3.082724000	-2.952517000
H	4.959609000	4.761258000	-1.303296000
H	-1.207190000	0.437921000	3.934741000
H	-1.207132000	1.697247000	2.686956000
H	1.273727000	1.625913000	2.727718000
H	1.224990000	0.334130000	3.939185000
H	-0.043184000	-0.976363000	2.421063000
H	0.089575000	-1.671156000	0.429182000
C	-0.106295000	-2.988652000	2.450210000
C	0.322054000	-2.927665000	1.148660000
H	1.387811000	-2.973479000	0.945500000
H	0.624509000	-2.977142000	3.249475000
H	-1.145579000	-3.179676000	2.690660000
F	-0.374048000	-3.654898000	0.185809000

TS1_F

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.038385000	0.099767000	0.058672000

P	2.273298000	-0.063285000	0.348391000
O	0.055075000	-0.082098000	-2.869490000
C	0.048008000	-0.021127000	-1.713688000
N	0.001918000	-0.092521000	2.148846000
C	1.239693000	0.302205000	2.846219000
C	-1.195627000	0.461921000	2.808968000
C	-2.441058000	-0.082750000	2.120307000
C	2.425353000	-0.366567000	2.160783000
H	-3.353442000	0.386889000	2.492837000
H	2.354306000	-1.451013000	2.291287000
H	-2.520883000	-1.156556000	2.306698000
P	-2.210788000	0.104448000	0.299841000
C	0.102913000	1.876212000	-0.001496000
O	0.147979000	3.027577000	-0.060787000
H	3.380558000	-0.045683000	2.581004000
C	-3.299460000	-1.179647000	-0.421967000
C	-4.650015000	-1.250074000	-0.070438000
C	-2.783820000	-2.098559000	-1.332388000
C	-5.465935000	-2.232039000	-0.612980000
H	-5.068047000	-0.530050000	0.626185000
C	-3.603913000	-3.079061000	-1.882921000
H	-1.736691000	-2.046584000	-1.608204000
C	-4.942821000	-3.148196000	-1.521843000
H	-6.512161000	-2.282435000	-0.332037000
H	-3.194234000	-3.788630000	-2.593361000
H	-5.582125000	-3.913876000	-1.947627000
C	-3.096874000	1.641698000	-0.166378000
C	-3.436786000	2.624290000	0.761130000
C	-3.347756000	1.873209000	-1.521336000
C	-4.031921000	3.811423000	0.345027000
H	-3.236930000	2.479043000	1.816849000
C	-3.942070000	3.056513000	-1.935621000
H	-3.079345000	1.122781000	-2.258474000
C	-4.287430000	4.029096000	-1.002064000
H	-4.292944000	4.566905000	1.077986000
H	-4.132895000	3.221875000	-2.990211000
H	-4.750178000	4.954608000	-1.326366000
C	3.303164000	-1.377087000	-0.409412000
C	4.651381000	-1.515717000	-0.067711000
C	2.744369000	-2.249103000	-1.341111000
C	5.420816000	-2.518334000	-0.640243000
H	5.105414000	-0.829003000	0.639969000
C	3.517368000	-3.251433000	-1.919708000
H	1.699666000	-2.143897000	-1.611417000
C	4.853750000	-3.388228000	-1.568163000
H	6.466167000	-2.619282000	-0.369760000
H	3.073350000	-3.923207000	-2.645917000
H	5.457055000	-4.168914000	-2.018411000
C	3.279269000	1.428935000	-0.004101000
C	3.717056000	2.305458000	0.986140000
C	3.528669000	1.739552000	-1.343640000
C	4.403667000	3.467403000	0.645093000
H	3.525062000	2.098098000	2.032979000
C	4.216678000	2.895229000	-1.682583000
H	3.183277000	1.071953000	-2.127301000
C	4.656281000	3.763419000	-0.687474000
H	4.737652000	4.142932000	1.425082000
H	4.405278000	3.121641000	-2.726128000
H	5.188818000	4.670228000	-0.952123000
H	-1.205486000	0.188961000	3.872099000
H	-1.149810000	1.553417000	2.741186000
H	1.327943000	1.392409000	2.811122000
H	1.194006000	0.000973000	3.901026000
H	-0.058792000	-1.144004000	2.276458000
H	-0.026316000	-1.671104000	0.238206000
C	-0.208540000	-2.996898000	2.169959000
C	0.012236000	-2.935246000	0.800982000
H	1.022301000	-3.188658000	0.488803000
H	0.498964000	-3.358559000	2.903229000
H	-0.756670000	-3.338119000	0.142930000
F	-1.535320000	-3.213324000	2.585263000

TS2_NH₂

Coordinates (Angstroms)

	X	Y	Z
Mn	0.039547000	0.099465000	0.104093000
P	2.285424000	0.118311000	0.411709000
O	0.204716000	-0.219085000	-2.808202000
C	0.123257000	-0.109442000	-1.658057000
N	0.034677000	0.022066000	2.190438000
C	1.158192000	0.717676000	2.842026000
C	-1.246530000	0.321294000	2.853421000
C	-2.363546000	-0.437632000	2.147155000
C	2.468427000	0.208775000	2.249598000
H	-3.337510000	-0.226359000	2.591273000
H	2.638348000	-0.816363000	2.588680000
H	-2.184052000	-1.515273000	2.218153000
P	-2.227768000	-0.050100000	0.359744000
C	0.000381000	1.870231000	-0.029353000
O	-0.016176000	3.021004000	-0.108453000
H	3.320555000	0.815699000	2.561481000
C	-3.302117000	-1.263926000	-0.498082000
C	-4.385974000	-1.869923000	0.137252000
C	-3.048193000	-1.559962000	-1.836628000
C	-5.194261000	-2.763979000	-0.552930000
H	-4.597894000	-1.659184000	1.179431000
C	-3.862771000	-2.447902000	-2.530406000
H	-2.206838000	-1.103064000	-2.343867000
C	-4.935416000	-3.054393000	-1.888468000
H	-6.029386000	-3.235766000	-0.046611000
H	-3.654962000	-2.666505000	-3.572119000
H	-5.569146000	-3.750728000	-2.426688000
C	-3.198521000	1.489494000	0.086382000
C	-4.048239000	2.053067000	1.036488000
C	-3.068822000	2.112959000	-1.157095000
C	-4.756577000	3.215988000	0.748015000
H	-4.170084000	1.596354000	2.011869000
C	-3.782681000	3.266071000	-1.449315000
H	-2.393145000	1.699453000	-1.899612000
C	-4.628253000	3.822228000	-0.494656000
H	-5.411432000	3.645449000	1.498524000
H	-3.669275000	3.738205000	-2.418818000
H	-5.179524000	4.729106000	-0.717827000
C	3.352969000	-1.287452000	-0.081901000
C	4.618125000	-1.464469000	0.483981000
C	2.914062000	-2.179529000	-1.057543000
C	5.422847000	-2.523207000	0.086932000
H	4.981650000	-0.768751000	1.233510000
C	3.724285000	-3.235812000	-1.462850000
H	1.931968000	-2.051895000	-1.498040000
C	4.976476000	-3.410388000	-0.888694000
H	6.401101000	-2.655412000	0.535880000
H	3.371760000	-3.924382000	-2.222698000
H	5.607038000	-4.236162000	-1.199705000
C	3.228209000	1.542340000	-0.255281000
C	3.322689000	2.739603000	0.453557000
C	3.774213000	1.467683000	-1.538028000
C	3.964803000	3.839287000	-0.103996000
H	2.886116000	2.827585000	1.442809000
C	4.413868000	2.567317000	-2.094751000
H	3.707138000	0.544896000	-2.104914000
C	4.512440000	3.755075000	-1.378328000
H	4.031071000	4.765115000	0.456778000
H	4.837879000	2.494340000	-3.090197000
H	5.010575000	4.614066000	-1.814121000
H	-1.201263000	0.024450000	3.909504000
H	-1.422471000	1.401952000	2.815747000
H	1.042567000	1.795547000	2.691399000
H	1.146242000	0.527842000	3.923633000
H	0.209468000	-1.024770000	2.381718000
H	0.106925000	-1.672791000	0.416593000
C	0.414034000	-2.795510000	2.409534000
C	0.177179000	-2.850194000	1.012766000
H	1.028567000	-3.199265000	0.421183000
H	1.413708000	-2.997299000	2.781762000
H	-0.412697000	-3.006436000	3.083590000
N	-1.119332000	-3.367857000	0.625446000
H	-1.279799000	-3.282353000	-0.372364000
H	-1.189774000	-4.344115000	0.887549000

TS1_NH₂

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.035987000	0.085489000	0.052462000
P	2.273415000	-0.057234000	0.341800000
O	0.062633000	-0.086567000	-2.876847000
C	0.051011000	-0.032524000	-1.720273000
N	0.003033000	-0.134995000	2.129384000
C	1.228514000	0.276698000	2.837744000
C	-1.205940000	0.377128000	2.802330000
C	-2.442389000	-0.168402000	2.097048000
C	2.431723000	-0.360658000	2.152454000
H	-3.364472000	0.270614000	2.483638000
H	2.384316000	-1.446431000	2.278752000
H	-2.490084000	-1.253535000	2.240324000
P	-2.214135000	0.079864000	0.287723000
C	0.090205000	1.859708000	-0.001884000
O	0.126088000	3.012129000	-0.053854000
H	3.379014000	-0.017893000	2.573521000
C	-3.304609000	-1.177990000	-0.477984000
C	-4.662195000	-1.236851000	-0.152563000
C	-2.783809000	-2.089700000	-1.392577000
C	-5.480311000	-2.199682000	-0.725459000
H	-5.083925000	-0.521638000	0.546769000
C	-3.605502000	-3.051487000	-1.973016000
H	-1.731109000	-2.047881000	-1.647696000
C	-4.951901000	-3.108848000	-1.638380000
H	-6.532570000	-2.239875000	-0.465887000
H	-3.191148000	-3.755150000	-2.686680000
H	-5.592908000	-3.858976000	-2.088783000
C	-3.100266000	1.630380000	-0.132929000
C	-3.452402000	2.580396000	0.823484000
C	-3.343300000	1.904474000	-1.481403000
C	-4.050933000	3.777485000	0.441510000
H	-3.259836000	2.401373000	1.875503000
C	-3.942268000	3.096784000	-1.861604000
H	-3.065066000	1.179213000	-2.239856000
C	-4.299140000	4.037047000	-0.899608000
H	-4.320973000	4.508025000	1.196243000
H	-4.127707000	3.294154000	-2.911677000
H	-4.765321000	4.970023000	-1.196593000
C	3.323232000	-1.351601000	-0.421668000
C	4.673971000	-1.470049000	-0.082386000
C	2.776589000	-2.228683000	-1.355562000
C	5.458431000	-2.457911000	-0.660008000
H	5.117734000	-0.779013000	0.627631000
C	3.564633000	-3.216175000	-1.939464000
H	1.730006000	-2.138348000	-1.623812000
C	4.903641000	-3.332958000	-1.590615000
H	6.505695000	-2.543448000	-0.391441000
H	3.130260000	-3.892182000	-2.667635000
H	5.518788000	-4.102005000	-2.044995000
C	3.255680000	1.452000000	-0.007962000
C	3.664602000	2.340130000	0.984422000
C	3.513926000	1.764030000	-1.345461000
C	4.332412000	3.514197000	0.647779000
H	3.463733000	2.132445000	2.029617000
C	4.182567000	2.932368000	-1.680158000
H	3.190431000	1.087657000	-2.130893000
C	4.594147000	3.811605000	-0.682766000
H	4.644423000	4.198195000	1.429517000
H	4.377865000	3.159823000	-2.722277000
H	5.112038000	4.727882000	-0.943951000
H	-1.210814000	0.070527000	3.857304000
H	-1.180410000	1.471482000	2.774348000
H	1.296636000	1.369089000	2.821307000
H	1.183925000	-0.042232000	3.888023000
H	-0.028131000	-1.205222000	2.250419000
H	-0.035275000	-1.707724000	0.249512000
C	-0.109838000	-2.996116000	2.189024000
C	-0.018975000	-2.925864000	0.779708000
H	0.923881000	-3.253741000	0.345155000
H	0.778428000	-3.309025000	2.739857000

H	-0.877788000	-3.295595000	0.216808000
N	-1.406575000	-3.262632000	2.776504000
H	-1.654092000	-4.248405000	2.751615000
H	-1.448401000	-2.973579000	3.745671000

TS2_SH

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.067780000	0.240306000	0.125064000
P	2.311951000	0.076135000	0.387106000
O	0.085801000	-0.153349000	-2.783771000
C	0.071421000	-0.005802000	-1.636076000
N	0.063859000	0.198010000	2.227924000
C	1.315942000	0.635763000	2.871344000
C	-1.128069000	0.797706000	2.851990000
C	-2.362844000	0.151542000	2.237462000
C	2.488971000	-0.085796000	2.216461000
H	-3.279938000	0.589302000	2.632784000
H	2.424282000	-1.156869000	2.429563000
H	-2.358215000	-0.913456000	2.488107000
P	-2.199356000	0.266972000	0.404755000
C	0.190042000	2.010353000	-0.000227000
O	0.301907000	3.157291000	-0.061373000
H	3.450453000	0.265956000	2.595240000
C	-3.294352000	-1.041705000	-0.267956000
C	-4.181160000	-1.778694000	0.513755000
C	-3.234092000	-1.288991000	-1.641195000
C	-4.980549000	-2.759263000	-0.064135000
H	-4.253551000	-1.607421000	1.581568000
C	-4.035740000	-2.263460000	-2.218581000
H	-2.552935000	-0.721566000	-2.266350000
C	-4.906562000	-3.007098000	-1.428446000
H	-5.655918000	-3.336234000	0.557917000
H	-3.973272000	-2.448085000	-3.285359000
H	-5.525676000	-3.776648000	-1.876145000
C	-3.170049000	1.753377000	-0.086870000
C	-4.354394000	2.106507000	0.563212000
C	-2.760518000	2.498751000	-1.191927000
C	-5.098365000	3.197095000	0.133539000
H	-4.716046000	1.525288000	1.404376000
C	-3.510382000	3.584978000	-1.629888000
H	-1.849171000	2.232602000	-1.715312000
C	-4.676548000	3.940009000	-0.964300000
H	-6.013674000	3.462278000	0.651390000
H	-3.177108000	4.155271000	-2.489791000
H	-5.258185000	4.791113000	-1.301114000
C	3.311848000	-1.305971000	-0.283744000
C	4.656026000	-1.448951000	0.071891000
C	2.735379000	-2.229776000	-1.152642000
C	5.403316000	-2.507681000	-0.423660000
H	5.124019000	-0.725566000	0.732372000
C	3.485759000	-3.289351000	-1.652643000
H	1.691899000	-2.129626000	-1.429257000
C	4.817874000	-3.430042000	-1.287347000
H	6.445025000	-2.613300000	-0.141217000
H	3.023872000	-4.004647000	-2.323766000
H	5.402649000	-4.257323000	-1.674327000
C	3.328807000	1.523996000	-0.094827000
C	3.801103000	2.460094000	0.822176000
C	3.558869000	1.732700000	-1.457390000
C	4.503416000	3.580457000	0.387634000
H	3.624252000	2.331305000	1.884126000
C	4.261304000	2.848004000	-1.889509000
H	3.190464000	1.016962000	-2.186007000
C	4.736061000	3.775629000	-0.966785000
H	4.864858000	4.302027000	1.112083000
H	4.435765000	2.996531000	-2.949393000
H	5.281250000	4.649691000	-1.305361000
H	-1.118659000	0.626987000	3.936320000
H	-1.115695000	1.878220000	2.679804000
H	1.405286000	1.720170000	2.754892000
H	1.288860000	0.413824000	3.945991000
H	-0.011389000	-0.831454000	2.425876000

H	0.014851000	-1.513898000	0.455479000
C	-0.079835000	-2.749098000	2.484946000
C	0.189222000	-2.718601000	1.114542000
H	1.236182000	-2.839039000	0.848954000
H	0.737339000	-2.768799000	3.198785000
H	-1.077022000	-2.959663000	2.856438000
S	-0.883362000	-3.757339000	0.082662000
H	-0.994563000	-2.928448000	-0.974920000

TS1_SH

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.104629000	0.289955000	0.024925000
P	2.316300000	-0.083538000	0.305358000
O	0.269029000	0.652768000	-2.881234000
C	0.192515000	0.502315000	-1.735751000
N	0.019433000	-0.254074000	2.070567000
C	1.269835000	-0.048876000	2.824800000
C	-1.153323000	0.289037000	2.778783000
C	-2.421243000	-0.063233000	2.011680000
C	2.421785000	-0.675301000	2.048678000
H	-3.286358000	0.444007000	2.441047000
H	2.283889000	-1.759215000	2.005094000
H	-2.594202000	-1.140075000	2.076238000
P	-2.154567000	0.324830000	0.223249000
C	0.299039000	2.032735000	0.340433000
O	0.438510000	3.159966000	0.547046000
H	3.388250000	-0.485466000	2.519231000
C	-3.191673000	-0.905210000	-0.664649000
C	-4.287415000	-1.534473000	-0.073398000
C	-2.880472000	-1.196763000	-1.993240000
C	-5.053710000	-2.441335000	-0.796061000
H	-4.547791000	-1.333387000	0.959696000
C	-3.651412000	-2.096589000	-2.718452000
H	-2.025512000	-0.726547000	-2.464546000
C	-4.738854000	-2.722779000	-2.119997000
H	-5.896818000	-2.930672000	-0.320982000
H	-3.398167000	-2.312154000	-3.750622000
H	-5.337174000	-3.430558000	-2.683125000
C	-3.111277000	1.862752000	-0.103190000
C	-4.358470000	2.098828000	0.479868000
C	-2.609191000	2.787118000	-1.017983000
C	-5.077930000	3.244747000	0.169188000
H	-4.784498000	1.383048000	1.174947000
C	-3.332802000	3.931268000	-1.336589000
H	-1.646999000	2.615840000	-1.486201000
C	-4.565079000	4.164405000	-0.740338000
H	-6.043016000	3.417011000	0.633005000
H	-2.928562000	4.641560000	-2.049210000
H	-5.126994000	5.059410000	-0.984173000
C	3.259226000	-1.333270000	-0.646472000
C	4.572477000	-1.657805000	-0.294639000
C	2.670648000	-1.965144000	-1.739246000
C	5.277703000	-2.609153000	-1.017686000
H	5.050423000	-1.158623000	0.542617000
C	3.380142000	-2.915102000	-2.468248000
H	1.653258000	-1.716184000	-2.018178000
C	4.681102000	-3.239004000	-2.107095000
H	6.296210000	-2.855023000	-0.737904000
H	2.913406000	-3.399405000	-3.318740000
H	5.234342000	-3.979450000	-2.674456000
C	3.428839000	1.371872000	0.201857000
C	3.917650000	2.037344000	1.323968000
C	3.709822000	1.886081000	-1.067046000
C	4.684357000	3.190340000	1.181638000
H	3.703104000	1.672104000	2.322077000
C	4.475697000	3.033967000	-1.208355000
H	3.326768000	1.386376000	-1.951556000
C	4.965518000	3.689791000	-0.082623000
H	5.058282000	3.698461000	2.063808000
H	4.685569000	3.422226000	-2.198847000
H	5.558644000	4.590872000	-0.192639000
H	-1.210200000	-0.116760000	3.797649000

H	-1.032241000	1.373198000	2.859065000
H	1.419810000	1.026978000	2.956161000
H	1.192793000	-0.502884000	3.821108000
H	-0.099436000	-1.285913000	2.004083000
H	-0.104854000	-1.430846000	-0.113044000
C	-0.155571000	-3.223458000	1.514076000
C	-0.247293000	-2.833071000	0.177207000
H	0.588158000	-3.098020000	-0.465980000
H	0.796126000	-3.556985000	1.912859000
H	-1.213564000	-2.908729000	-0.317268000
S	-1.581090000	-3.712885000	2.445717000
H	-1.637104000	-2.761833000	3.407922000

TS2_OH

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.005990000	-0.001068000	0.089955000
P	2.249258000	0.028081000	0.365259000
O	-0.123729000	-0.512152000	-2.798712000
C	-0.061708000	-0.305364000	-1.663004000
N	-0.022431000	-0.046050000	2.196778000
C	1.199666000	0.453380000	2.852245000
C	-1.232060000	0.497779000	2.841225000
C	-2.456834000	-0.135263000	2.197899000
C	2.425496000	-0.163790000	2.191074000
H	-3.393765000	0.275695000	2.579099000
H	2.444630000	-1.240175000	2.384174000
H	-2.458734000	-1.210151000	2.404489000
P	-2.285958000	0.010658000	0.371279000
C	-0.014123000	1.769282000	-0.108026000
O	0.013815000	2.913756000	-0.238819000
H	3.352682000	0.255373000	2.586188000
C	-3.490920000	-1.222517000	-0.253922000
C	-4.832761000	-0.906527000	-0.480930000
C	-3.056700000	-2.532760000	-0.448378000
C	-5.721976000	-1.888045000	-0.900714000
H	-5.188557000	0.107805000	-0.337782000
C	-3.949942000	-3.514373000	-0.862581000
H	-2.021577000	-2.798781000	-0.265548000
C	-5.282175000	-3.193696000	-1.093318000
H	-6.761043000	-1.632429000	-1.077763000
H	-3.597631000	-4.530022000	-1.006177000
H	-5.978027000	-3.957631000	-1.422844000
C	-3.081762000	1.594653000	-0.095751000
C	-3.557553000	2.518855000	0.830860000
C	-3.145614000	1.905686000	-1.457312000
C	-4.096733000	3.730045000	0.405035000
H	-3.511404000	2.310209000	1.893566000
C	-3.692122000	3.107266000	-1.881666000
H	-2.767078000	1.201048000	-2.191422000
C	-4.168889000	4.024460000	-0.949327000
H	-4.460114000	4.442791000	1.137280000
H	-3.740948000	3.331716000	-2.941387000
H	-4.590675000	4.967051000	-1.280251000
C	3.377838000	-1.246488000	-0.318601000
C	4.685286000	-1.365123000	0.159546000
C	2.942679000	-2.103652000	-1.326379000
C	5.534582000	-2.336174000	-0.351703000
H	5.045595000	-0.690928000	0.930095000
C	3.795609000	-3.072985000	-1.844734000
H	1.932497000	-2.012624000	-1.708545000
C	5.089388000	-3.192953000	-1.354658000
H	6.545496000	-2.424913000	0.030577000
H	3.445649000	-3.736055000	-2.628032000
H	5.754014000	-3.951186000	-1.753815000
C	3.146759000	1.565520000	-0.075385000
C	3.562122000	2.503842000	0.866300000
C	3.347907000	1.830333000	-1.432731000
C	4.180575000	3.682829000	0.459997000
H	3.405118000	2.331214000	1.924997000
C	3.968523000	3.003087000	-1.836598000
H	3.017283000	1.114611000	-2.179548000
C	4.387339000	3.933150000	-0.889599000

H	4.498949000	4.405995000	1.202765000
H	4.122400000	3.194195000	-2.892805000
H	4.868892000	4.851913000	-1.205481000
H	-1.217792000	0.281716000	3.917410000
H	-1.236045000	1.585435000	2.715975000
H	1.217137000	1.544312000	2.761447000
H	1.186306000	0.206149000	3.921657000
H	-0.053714000	-1.092182000	2.378110000
H	0.165277000	-1.747583000	0.416485000
C	-0.036966000	-2.999945000	2.331121000
C	0.447489000	-2.912105000	1.017286000
H	1.535737000	-2.864330000	0.936823000
H	0.676553000	-3.120266000	3.139301000
H	-1.047658000	-3.360186000	2.499517000
O	-0.110434000	-3.774684000	0.051380000
H	0.156055000	-3.455608000	-0.817378000

TS1_OH

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.033726000	0.088609000	0.054477000
P	2.270957000	-0.045485000	0.341458000
O	0.058613000	-0.110466000	-2.872836000
C	0.048176000	-0.044593000	-1.716882000
N	0.004437000	-0.123007000	2.134228000
C	1.228132000	0.304438000	2.837008000
C	-1.208858000	0.380227000	2.805069000
C	-2.441051000	-0.174145000	2.098715000
C	2.432812000	-0.333459000	2.155121000
H	-3.366253000	0.259068000	2.484035000
H	2.391163000	-1.418543000	2.290995000
H	-2.492693000	-1.257520000	2.238319000
P	-2.212753000	0.074859000	0.286684000
C	0.082103000	1.863169000	-0.010146000
O	0.112411000	3.015468000	-0.070439000
H	3.379057000	0.016343000	2.572462000
C	-3.298817000	-1.188755000	-0.475025000
C	-4.661855000	-1.236368000	-0.170474000
C	-2.767206000	-2.117170000	-1.366366000
C	-5.474596000	-2.205197000	-0.740738000
H	-5.092121000	-0.507307000	0.509141000
C	-3.583691000	-3.084810000	-1.944152000
H	-1.710645000	-2.082689000	-1.606088000
C	-4.935373000	-3.131087000	-1.630211000
H	-6.531047000	-2.236973000	-0.497683000
H	-3.161187000	-3.801671000	-2.639540000
H	-5.572143000	-3.886187000	-2.078164000
C	-3.108901000	1.621197000	-0.127705000
C	-3.472642000	2.564801000	0.830633000
C	-3.347150000	1.898745000	-1.476358000
C	-4.077810000	3.759087000	0.450270000
H	-3.284508000	2.383681000	1.883131000
C	-3.952863000	3.088091000	-1.854848000
H	-3.059824000	1.178476000	-2.236181000
C	-4.321250000	4.021996000	-0.891019000
H	-4.356878000	4.484765000	1.206374000
H	-4.134648000	3.288098000	-2.905026000
H	-4.792548000	4.952781000	-1.186696000
C	3.323404000	-1.345108000	-0.409805000
C	4.672842000	-1.461522000	-0.064642000
C	2.779943000	-2.228577000	-1.339585000
C	5.459024000	-2.453869000	-0.632099000
H	5.114291000	-0.765740000	0.642182000
C	3.569774000	-3.220554000	-1.913355000
H	1.734212000	-2.140183000	-1.612026000
C	4.907352000	-3.335369000	-1.558447000
H	6.505175000	-2.538005000	-0.358857000
H	3.137823000	-3.901837000	-2.637996000
H	5.523789000	-4.108143000	-2.004618000
C	3.251267000	1.461856000	-0.021755000
C	3.663571000	2.356917000	0.962904000
C	3.505067000	1.764348000	-1.362260000
C	4.330546000	3.528405000	0.615848000

H	3.466326000	2.156401000	2.010185000
C	4.172878000	2.930125000	-1.707339000
H	3.179069000	1.082558000	-2.141921000
C	4.588014000	3.816268000	-0.717603000
H	4.645443000	4.217737000	1.391691000
H	4.364950000	3.150147000	-2.751636000
H	5.105482000	4.730374000	-0.987023000
H	-1.211571000	0.079443000	3.862008000
H	-1.194378000	1.474335000	2.772360000
H	1.289029000	1.396792000	2.807597000
H	1.187573000	-0.002836000	3.890983000
H	-0.014908000	-1.189743000	2.261046000
H	-0.034198000	-1.699184000	0.259298000
C	-0.110448000	-2.996150000	2.202812000
C	0.021502000	-2.934873000	0.808059000
H	0.995584000	-3.216222000	0.415276000
H	0.716582000	-3.370054000	2.803183000
H	-0.802033000	-3.339668000	0.218833000
O	-1.398889000	-3.334540000	2.695475000
H	-1.491678000	-2.955365000	3.569350000

TS2_CHO

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.031503000	0.157206000	0.126416000
P	2.280805000	0.052046000	0.389924000
O	0.052947000	-0.307264000	-2.772784000
C	0.037765000	-0.141660000	-1.629186000
N	0.022771000	0.177815000	2.220303000
C	1.272840000	0.628986000	2.861078000
C	-1.160851000	0.798301000	2.843482000
C	-2.414575000	0.187045000	2.230043000
C	2.454077000	-0.090137000	2.219587000
H	-3.324213000	0.672576000	2.587942000
H	2.397645000	-1.159494000	2.443116000
H	-2.471074000	-0.869834000	2.507919000
P	-2.225236000	0.219383000	0.396911000
C	0.090639000	1.918030000	-0.114258000
O	0.135721000	3.058288000	-0.275936000
H	3.411497000	0.273712000	2.597741000
C	-3.372901000	-1.077079000	-0.199780000
C	-4.637320000	-1.237858000	0.373840000
C	-2.993165000	-1.906017000	-1.252589000
C	-5.497440000	-2.222840000	-0.090320000
H	-4.955837000	-0.589584000	1.183882000
C	-3.859531000	-2.886860000	-1.725053000
H	-2.010946000	-1.801133000	-1.697259000
C	-5.108818000	-3.048954000	-1.142035000
H	-6.473445000	-2.345870000	0.366144000
H	-3.546509000	-3.532258000	-2.537716000
H	-5.782130000	-3.818475000	-1.503351000
C	-3.074889000	1.742580000	-0.173180000
C	-3.434533000	2.778895000	0.685681000
C	-3.284097000	1.896014000	-1.546093000
C	-4.005688000	3.944232000	0.182688000
H	-3.269298000	2.696018000	1.753966000
C	-3.855243000	3.056909000	-2.046410000
H	-2.998870000	1.103066000	-2.230549000
C	-4.218948000	4.084990000	-1.181714000
H	-4.281489000	4.742907000	0.862608000
H	-4.013689000	3.162217000	-3.113907000
H	-4.662609000	4.993609000	-1.573301000
C	3.314168000	-1.308549000	-0.270151000
C	4.679001000	-1.374923000	0.025575000
C	2.739728000	-2.296292000	-1.067133000
C	5.450091000	-2.421643000	-0.458720000
H	5.143910000	-0.599897000	0.627048000
C	3.513845000	-3.345117000	-1.553883000
H	1.681501000	-2.256798000	-1.298176000
C	4.866888000	-3.409003000	-1.249463000
H	6.508147000	-2.467130000	-0.225030000
H	3.052239000	-4.111190000	-2.166437000
H	5.470713000	-4.226665000	-1.627726000

C	3.251802000	1.527556000	-0.100616000
C	3.709646000	2.475410000	0.811827000
C	3.461583000	1.742377000	-1.465575000
C	4.376104000	3.614697000	0.369899000
H	3.550105000	2.340522000	1.875689000
C	4.128961000	2.876159000	-1.904849000
H	3.103060000	1.017606000	-2.190221000
C	4.588423000	3.816196000	-0.986916000
H	4.726903000	4.345124000	1.090710000
H	4.287664000	3.029553000	-2.966456000
H	5.105771000	4.704791000	-1.331262000
H	-1.153225000	0.625447000	3.927660000
H	-1.121072000	1.878865000	2.674090000
H	1.356795000	1.712808000	2.733612000
H	1.242986000	0.417537000	3.937959000
H	-0.055984000	-0.855710000	2.464988000
H	0.002711000	-1.612121000	0.507130000
C	-0.123462000	-2.679139000	2.602061000
C	0.135404000	-2.757746000	1.212304000
H	1.162467000	-2.969760000	0.920614000
H	0.690733000	-2.773363000	3.311568000
H	-1.122702000	-2.883290000	2.977286000
C	-0.830397000	-3.586993000	0.435968000
H	-1.876732000	-3.542718000	0.800082000
O	-0.532439000	-4.292619000	-0.497787000

TS1_CHO

Coordinates (Angstroms)			
	X	Y	Z
Mn	-0.072735000	0.278260000	0.018575000
P	2.162945000	0.259068000	0.250101000
O	-0.103377000	0.468775000	-2.904862000
C	-0.095688000	0.395589000	-1.749816000
N	-0.023958000	-0.075570000	2.161863000
C	1.162165000	0.514697000	2.801488000
C	-1.277529000	0.294885000	2.838058000
C	-2.435703000	-0.392093000	2.123347000
C	2.413395000	0.037429000	2.072783000
H	-3.402045000	-0.108328000	2.544735000
H	2.546971000	-1.035052000	2.239425000
H	-2.336727000	-1.476605000	2.232793000
P	-2.284992000	-0.028611000	0.317180000
C	-0.197340000	2.054837000	0.184705000
O	-0.280306000	3.204945000	0.247233000
H	3.308787000	0.541944000	2.441341000
C	-3.213765000	-1.388936000	-0.488742000
C	-4.517711000	-1.706115000	-0.097750000
C	-2.620187000	-2.107892000	-1.523048000
C	-5.206935000	-2.735363000	-0.723723000
H	-5.000610000	-1.141230000	0.693686000
C	-3.313860000	-3.134277000	-2.156913000
H	-1.608600000	-1.863932000	-1.825622000
C	-4.605271000	-3.450303000	-1.756225000
H	-6.217600000	-2.975951000	-0.412480000
H	-2.843551000	-3.684128000	-2.964726000
H	-5.146110000	-4.251799000	-2.247552000
C	-3.396156000	1.398410000	0.004881000
C	-3.843682000	2.247361000	1.015019000
C	-3.709675000	1.702001000	-1.322551000
C	-4.600697000	3.373769000	0.705826000
H	-3.604237000	2.046827000	2.053435000
C	-4.466617000	2.823188000	-1.630222000
H	-3.360415000	1.056052000	-2.122307000
C	-4.914263000	3.663519000	-0.615238000
H	-4.940757000	4.027543000	1.501649000
H	-4.702142000	3.044413000	-2.665358000
H	-5.500350000	4.543693000	-0.855694000
C	3.202299000	-1.054885000	-0.495779000
C	4.469127000	-1.347553000	0.014055000
C	2.730624000	-1.772096000	-1.592720000
C	5.240420000	-2.353896000	-0.552043000
H	4.860030000	-0.788734000	0.858389000
C	3.507743000	-2.771509000	-2.169208000

H	1.744098000	-1.559510000	-1.987217000
C	4.760073000	-3.068119000	-1.645759000
H	6.219035000	-2.578165000	-0.141988000
H	3.129962000	-3.321409000	-3.024219000
H	5.363410000	-3.852676000	-2.089337000
C	3.120900000	1.766306000	-0.181030000
C	3.276830000	2.810186000	0.730927000
C	3.615423000	1.922283000	-1.477397000
C	3.930593000	3.979916000	0.360858000
H	2.883972000	2.723762000	1.738357000
C	4.267091000	3.091866000	-1.847207000
H	3.498256000	1.124685000	-2.204045000
C	4.428938000	4.122935000	-0.928014000
H	4.045869000	4.781397000	1.082386000
H	4.650284000	3.197621000	-2.856258000
H	4.937984000	5.035795000	-1.217001000
H	-1.250997000	-0.002677000	3.893646000
H	-1.381088000	1.383444000	2.794467000
H	1.066387000	1.603103000	2.744255000
H	1.213856000	0.233837000	3.860850000
H	0.061791000	-1.088395000	2.275988000
H	0.077124000	-1.376290000	-0.096504000
C	1.218423000	-3.493272000	1.020394000
C	1.242060000	-3.439552000	2.452013000
O	0.423817000	-2.853614000	3.163774000
C	0.121762000	-3.089577000	0.309840000
H	-0.824827000	-2.942325000	0.816746000
H	0.061454000	-3.280207000	-0.754222000
H	2.081085000	-3.974251000	2.937939000
H	2.108684000	-3.850088000	0.513793000

TS2_CH=CH₂

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.031173000	0.158374000	0.134580000
P	2.275231000	0.074357000	0.398443000
O	0.042530000	-0.377731000	-2.751423000
C	0.032852000	-0.181897000	-1.611061000
N	0.023008000	0.207783000	2.223160000
C	1.266638000	0.677067000	2.860993000
C	-1.166403000	0.815224000	2.845206000
C	-2.412401000	0.179942000	2.239511000
C	2.455625000	-0.038366000	2.228815000
H	-3.328769000	0.653650000	2.596247000
H	2.409601000	-1.104696000	2.467925000
H	-2.448692000	-0.876010000	2.524400000
P	-2.225152000	0.202060000	0.407306000
C	0.074996000	1.915114000	-0.134063000
O	0.115904000	3.053840000	-0.311707000
H	3.409735000	0.341477000	2.599667000
C	-3.384518000	-1.087110000	-0.187605000
C	-4.636956000	-1.259030000	0.407940000
C	-3.032018000	-1.887888000	-1.271434000
C	-5.514017000	-2.224775000	-0.065817000
H	-4.935047000	-0.633957000	1.243539000
C	-3.916788000	-2.846111000	-1.755593000
H	-2.055977000	-1.781178000	-1.728072000
C	-5.155019000	-3.018950000	-1.151547000
H	-6.480517000	-2.355450000	0.408375000
H	-3.629188000	-3.464291000	-2.598833000
H	-5.842477000	-3.770887000	-1.523386000
C	-3.079353000	1.722858000	-0.167899000
C	-3.452231000	2.756721000	0.688220000
C	-3.280746000	1.875856000	-1.542079000
C	-4.027807000	3.918442000	0.181610000
H	-3.293655000	2.674856000	1.757545000
C	-3.856539000	3.032701000	-2.046290000
H	-2.984721000	1.085328000	-2.224771000
C	-4.233181000	4.058247000	-1.184056000
H	-4.313268000	4.715114000	0.859959000
H	-4.008506000	3.137087000	-3.114865000
H	-4.680272000	4.964003000	-1.578448000
C	3.314699000	-1.292073000	-0.244122000

C	4.673870000	-1.365047000	0.073374000
C	2.751736000	-2.271731000	-1.059260000
C	5.451756000	-2.408422000	-0.407954000
H	5.129786000	-0.597448000	0.691005000
C	3.533795000	-3.313793000	-1.547966000
H	1.696313000	-2.226325000	-1.303461000
C	4.881712000	-3.384230000	-1.221631000
H	6.505320000	-2.458786000	-0.155857000
H	3.086983000	-4.068887000	-2.185381000
H	5.491363000	-4.196752000	-1.601583000
C	3.243612000	1.542394000	-0.121154000
C	3.699735000	2.508737000	0.772561000
C	3.450019000	1.733123000	-1.490213000
C	4.361648000	3.641827000	0.308367000
H	3.541131000	2.393456000	1.838880000
C	4.112711000	2.860723000	-1.951904000
H	3.090952000	0.994653000	-2.200655000
C	4.571051000	3.818961000	-1.052310000
H	4.710857000	4.386672000	1.015085000
H	4.268143000	2.995709000	-3.016525000
H	5.084356000	4.702964000	-1.414145000
H	-1.153936000	0.647094000	3.930378000
H	-1.145442000	1.895957000	2.671535000
H	1.343209000	1.760844000	2.725960000
H	1.237696000	0.473370000	3.939692000
H	-0.044191000	-0.834503000	2.480259000
H	0.043169000	-1.590209000	0.558606000
C	-0.073756000	-2.608869000	2.647375000
C	0.164239000	-2.747807000	1.255786000
H	1.203364000	-2.934437000	0.984220000
H	0.758929000	-2.679086000	3.340188000
H	-1.051009000	-2.865553000	3.048054000
C	-0.777841000	-3.577590000	0.458571000
H	-1.831500000	-3.464683000	0.704681000
C	-0.412811000	-4.427083000	-0.496636000
H	0.631901000	-4.568755000	-0.760876000
H	-1.144509000	-5.022266000	-1.033553000

TS1_CH=CH₂

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.109414000	0.223953000	-0.012226000
P	2.306290000	-0.194285000	0.287656000
O	0.128810000	0.419657000	-2.938706000
C	0.127555000	0.335445000	-1.784825000
N	-0.008195000	-0.199598000	2.069010000
C	1.266292000	-0.105534000	2.804617000
C	-1.102019000	0.509128000	2.758382000
C	-2.415389000	0.234142000	2.036903000
C	2.354234000	-0.827530000	2.019083000
H	-3.209459000	0.895482000	2.388685000
H	2.120106000	-1.894476000	1.955218000
H	-2.723908000	-0.795500000	2.234436000
P	-2.136815000	0.375133000	0.209142000
C	0.330696000	1.982416000	0.168569000
O	0.498156000	3.120476000	0.265415000
H	3.332684000	-0.736367000	2.494338000
C	-3.276694000	-0.873737000	-0.496505000
C	-4.553376000	-1.063436000	0.037738000
C	-2.870084000	-1.650509000	-1.578833000
C	-5.400369000	-2.026971000	-0.491128000
H	-4.889237000	-0.459410000	0.874389000
C	-3.723165000	-2.609453000	-2.117038000
H	-1.878306000	-1.512643000	-1.994525000
C	-4.985077000	-2.802745000	-1.569953000
H	-6.385272000	-2.173772000	-0.061833000
H	-3.396119000	-3.210169000	-2.958545000
H	-5.647000000	-3.556740000	-1.981633000
C	-2.948505000	1.945701000	-0.280769000
C	-2.923603000	3.053736000	0.567056000
C	-3.509927000	2.078387000	-1.551550000
C	-3.466856000	4.266076000	0.159612000
H	-2.471381000	2.982259000	1.550836000

C	-4.049608000	3.291925000	-1.959367000
H	-3.533171000	1.230423000	-2.228059000
C	-4.032831000	4.387766000	-1.103895000
H	-3.443026000	5.117627000	0.830793000
H	-4.486453000	3.380367000	-2.948000000
H	-4.456391000	5.333808000	-1.422466000
C	3.233411000	-1.453077000	-0.670975000
C	4.564815000	-1.748413000	-0.365436000
C	2.609824000	-2.126741000	-1.718763000
C	5.253857000	-2.711700000	-1.088711000
H	5.070527000	-1.215366000	0.433727000
C	3.302471000	-3.088620000	-2.447777000
H	1.576760000	-1.902414000	-1.958397000
C	4.622451000	-3.382783000	-2.132611000
H	6.287135000	-2.933573000	-0.845477000
H	2.808573000	-3.604610000	-3.263644000
H	5.163111000	-4.131770000	-2.700934000
C	3.470302000	1.223705000	0.242848000
C	4.084563000	1.755122000	1.374327000
C	3.685804000	1.834395000	-0.995840000
C	4.909499000	2.871907000	1.270108000
H	3.927813000	1.309251000	2.349998000
C	4.513634000	2.942165000	-1.100642000
H	3.201066000	1.440792000	-1.884373000
C	5.127259000	3.464912000	0.034228000
H	5.379566000	3.277682000	2.159324000
H	4.673614000	3.404951000	-2.068097000
H	5.769144000	4.335256000	-0.046057000
H	-1.176443000	0.179986000	3.802528000
H	-0.864552000	1.576939000	2.757231000
H	1.509897000	0.954734000	2.924522000
H	1.162518000	-0.542758000	3.805744000
H	-0.264219000	-1.200827000	2.058092000
H	-0.048358000	-1.513404000	-0.068277000
C	-0.562694000	-3.181065000	1.622982000
C	-0.155673000	-2.913223000	0.314488000
H	0.872346000	-3.140195000	0.046880000
H	0.188240000	-3.317454000	2.399499000
H	-0.864240000	-3.125008000	-0.483255000
C	-1.946459000	-3.309976000	1.987737000
H	-2.652844000	-3.234501000	1.158222000
C	-2.458270000	-3.508426000	3.219011000
H	-3.525700000	-3.622901000	3.372180000
H	-1.819276000	-3.589054000	4.095437000

TS2_C≡CH

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.071505000	0.121399000	0.083327000
P	2.316036000	0.124366000	0.396429000
O	0.240762000	-0.230697000	-2.825377000
C	0.157919000	-0.109080000	-1.677669000
N	0.056684000	0.063537000	2.172147000
C	1.186895000	0.752974000	2.821117000
C	-1.221812000	0.383139000	2.832621000
C	-2.350496000	-0.348907000	2.117031000
C	2.495924000	0.234665000	2.235006000
H	-3.324684000	-0.113063000	2.549158000
H	2.670872000	-0.784295000	2.588808000
H	-2.204531000	-1.430494000	2.202592000
P	-2.195901000	0.039941000	0.327654000
C	0.052977000	1.890529000	-0.081360000
O	0.042392000	3.039075000	-0.187582000
H	3.346786000	0.846708000	2.540170000
C	-3.340673000	-1.114360000	-0.518602000
C	-4.588002000	-1.414221000	0.032445000
C	-2.987063000	-1.671629000	-1.744654000
C	-5.459461000	-2.270842000	-0.626263000
H	-4.886735000	-0.977467000	0.979653000
C	-3.866314000	-2.516285000	-2.413456000
H	-2.015199000	-1.464351000	-2.174439000
C	-5.100043000	-2.821863000	-1.853042000
H	-6.422880000	-2.502878000	-0.185584000

H	-3.578896000	-2.945203000	-3.366985000
H	-5.783287000	-3.486079000	-2.371178000
C	-3.102113000	1.622883000	0.087303000
C	-3.755150000	2.305414000	1.111065000
C	-3.101456000	2.172439000	-1.197571000
C	-4.400527000	3.512158000	0.855687000
H	-3.769328000	1.908433000	2.119488000
C	-3.751173000	3.370538000	-1.454304000
H	-2.581767000	1.662822000	-2.003665000
C	-4.402250000	4.045392000	-0.425822000
H	-4.902018000	4.033502000	1.663934000
H	-3.741268000	3.784739000	-2.456376000
H	-4.903783000	4.986336000	-0.623463000
C	3.379371000	-1.291687000	-0.076510000
C	4.643779000	-1.465882000	0.492285000
C	2.935985000	-2.196540000	-1.038611000
C	5.442818000	-2.535114000	0.112244000
H	5.010967000	-0.760200000	1.230703000
C	3.740568000	-3.263785000	-1.426297000
H	1.953926000	-2.072327000	-1.480674000
C	4.991682000	-3.435580000	-0.848953000
H	6.420262000	-2.665416000	0.563526000
H	3.383779000	-3.962751000	-2.174412000
H	5.617558000	-4.269996000	-1.145951000
C	3.271399000	1.537649000	-0.276459000
C	3.361476000	2.742208000	0.420674000
C	3.831707000	1.447851000	-1.551903000
C	4.013348000	3.833998000	-0.140708000
H	2.913430000	2.842427000	1.403677000
C	4.480935000	2.539902000	-2.112748000
H	3.768275000	0.519492000	-2.109987000
C	4.575171000	3.734725000	-1.407784000
H	4.075917000	4.765455000	0.411098000
H	4.915653000	2.455345000	-3.102603000
H	5.080644000	4.587718000	-1.846867000
H	-1.185500000	0.082686000	3.887859000
H	-1.373997000	1.466864000	2.796552000
H	1.076862000	1.829650000	2.660245000
H	1.170560000	0.572563000	3.904169000
H	0.212711000	-0.974314000	2.374435000
H	0.097307000	-1.652737000	0.400951000
C	0.447542000	-2.755105000	2.469923000
C	0.248897000	-2.861214000	1.074970000
H	1.117136000	-3.152720000	0.487358000
H	1.457516000	-2.796971000	2.862918000
H	-0.360760000	-2.999139000	3.150232000
C	-0.960515000	-3.522409000	0.629442000
C	-1.976100000	-4.067048000	0.288873000
H	-2.878673000	-4.535185000	-0.028947000

TS1_C=CH

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.104395000	0.207653000	0.021314000
P	2.304391000	-0.177508000	0.325626000
O	0.106541000	0.283891000	-2.909946000
C	0.113193000	0.248875000	-1.753607000
N	0.002805000	-0.119283000	2.126047000
C	1.279205000	0.050406000	2.843524000
C	-1.107888000	0.594915000	2.781216000
C	-2.413066000	0.252886000	2.073504000
C	2.378348000	-0.694539000	2.095494000
H	-3.228494000	0.897260000	2.407847000
H	2.169117000	-1.768547000	2.103281000
H	-2.688525000	-0.781925000	2.294096000
P	-2.142318000	0.345015000	0.241996000
C	0.312327000	1.975362000	0.130351000
O	0.471894000	3.117796000	0.178070000
H	3.357399000	-0.551809000	2.556764000
C	-3.282488000	-0.923964000	-0.423501000
C	-4.582011000	-1.047898000	0.073243000
C	-2.852993000	-1.785299000	-1.429119000
C	-5.430098000	-2.030113000	-0.416619000

H	-4.934185000	-0.374239000	0.847922000
C	-3.706308000	-2.765329000	-1.927688000
H	-1.844478000	-1.694190000	-1.816476000
C	-4.991240000	-2.892751000	-1.417652000
H	-6.434224000	-2.125398000	-0.017894000
H	-3.361384000	-3.434554000	-2.708155000
H	-5.653821000	-3.662419000	-1.798250000
C	-2.958671000	1.901044000	-0.286124000
C	-2.952664000	3.025784000	0.539588000
C	-3.500552000	2.006376000	-1.568132000
C	-3.493444000	4.227954000	0.099560000
H	-2.516731000	2.975972000	1.531954000
C	-4.038307000	3.209302000	-2.008473000
H	-3.509363000	1.144506000	-2.227384000
C	-4.038912000	4.322450000	-1.175101000
H	-3.483079000	5.093041000	0.753629000
H	-4.459665000	3.276297000	-3.005525000
H	-4.459922000	5.260369000	-1.520036000
C	3.225373000	-1.495285000	-0.557572000
C	4.546182000	-1.799602000	-0.216652000
C	2.607430000	-2.203151000	-1.585839000
C	5.229408000	-2.805782000	-0.885223000
H	5.047795000	-1.241469000	0.567954000
C	3.294484000	-3.207431000	-2.260875000
H	1.581727000	-1.973406000	-1.850245000
C	4.603402000	-3.510584000	-1.910092000
H	6.254002000	-3.035502000	-0.614067000
H	2.804471000	-3.750226000	-3.061547000
H	5.138963000	-4.294353000	-2.434667000
C	3.463992000	1.235944000	0.168563000
C	4.057467000	1.873794000	1.255351000
C	3.691005000	1.735480000	-1.117023000
C	4.875075000	2.983885000	1.060905000
H	3.888669000	1.518467000	2.265640000
C	4.510018000	2.837645000	-1.310975000
H	3.221732000	1.259470000	-1.972915000
C	5.105038000	3.465643000	-0.220333000
H	5.330385000	3.471351000	1.916137000
H	4.678218000	3.213699000	-2.314009000
H	5.740802000	4.331095000	-0.370920000
H	-1.173458000	0.319731000	3.841573000
H	-0.895599000	1.666413000	2.723923000
H	1.498277000	1.121570000	2.892395000
H	1.194148000	-0.323454000	3.871783000
H	-0.224644000	-1.123300000	2.164610000
H	-0.039023000	-1.503192000	0.021546000
C	-0.488352000	-3.183544000	1.811722000
C	-0.099437000	-2.966641000	0.498416000
H	0.940122000	-3.141514000	0.242924000
H	0.258476000	-3.284041000	2.593501000
H	-0.805652000	-3.198256000	-0.291923000
C	-1.845658000	-3.329626000	2.176794000
C	-3.015652000	-3.439687000	2.467096000
H	-4.045385000	-3.569008000	2.703684000

TS2_Ph-NO₂

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.823765000	0.432424000	0.155972000
P	2.755335000	-0.737783000	0.370286000
O	0.362931000	-0.300751000	-2.648394000
C	0.529967000	-0.015763000	-1.539237000
N	1.015020000	0.636683000	2.228931000
C	2.390961000	0.556946000	2.754586000
C	0.267066000	1.745020000	2.848320000
C	-1.162359000	1.737028000	2.319150000
C	3.074925000	-0.681178000	2.186454000
H	-1.744329000	2.575508000	2.705914000
H	2.608973000	-1.578228000	2.602580000
H	-1.658879000	0.813235000	2.632424000
P	-1.071046000	1.663622000	0.484267000
C	1.736054000	1.888638000	-0.308243000
O	2.332425000	2.826186000	-0.613424000

H	4.136959000	-0.714295000	2.437339000
C	-2.764038000	1.240169000	-0.073964000
C	-3.889911000	1.715565000	0.603764000
C	-2.935816000	0.525344000	-1.257069000
C	-5.162724000	1.475493000	0.105344000
H	-3.777736000	2.280634000	1.523188000
C	-4.210874000	0.306439000	-1.768625000
H	-2.075520000	0.130629000	-1.783287000
C	-5.325400000	0.778452000	-1.088559000
H	-6.030969000	1.840894000	0.642712000
H	-4.330896000	-0.244818000	-2.694669000
H	-6.319425000	0.599302000	-1.482732000
C	-0.986985000	3.411745000	-0.081529000
C	-0.858378000	4.499408000	0.778949000
C	-0.996011000	3.637670000	-1.460558000
C	-0.750460000	5.791150000	0.270355000
H	-0.834516000	4.357930000	1.853442000
C	-0.893871000	4.924557000	-1.966732000
H	-1.078982000	2.800589000	-2.147308000
C	-0.770757000	6.006872000	-1.100406000
H	-0.649870000	6.628347000	0.952596000
H	-0.904504000	5.083521000	-3.039309000
H	-0.684867000	7.012932000	-1.495817000
C	2.928130000	-2.511733000	-0.054442000
C	4.038362000	-3.244664000	0.373101000
C	1.953095000	-3.141681000	-0.823771000
C	4.159249000	-4.588350000	0.048604000
H	4.817151000	-2.761511000	0.954690000
C	2.076418000	-4.487557000	-1.154984000
H	1.092025000	-2.577221000	-1.161825000
C	3.176674000	-5.212026000	-0.716023000
H	5.023002000	-5.149731000	0.387274000
H	1.311753000	-4.968158000	-1.755324000
H	3.273528000	-6.261969000	-0.969427000
C	4.246770000	-0.026015000	-0.424145000
C	5.126276000	0.811200000	0.259401000
C	4.443064000	-0.247441000	-1.789459000
C	6.193422000	1.406390000	-0.405588000
H	4.985054000	1.016683000	1.314642000
C	5.508520000	0.345993000	-2.451780000
H	3.762313000	-0.889479000	-2.339964000
C	6.387652000	1.174066000	-1.760564000
H	6.869729000	2.056097000	0.138968000
H	5.651822000	0.164041000	-3.511118000
H	7.218596000	1.639679000	-2.278765000
H	0.262962000	1.633439000	3.940506000
H	0.769931000	2.686994000	2.607640000
H	2.926225000	1.469021000	2.472979000
H	2.373968000	0.501662000	3.851023000
H	0.534329000	-0.247227000	2.590084000
H	-0.052281000	-1.019977000	0.759847000
C	-0.284085000	-1.811823000	2.957616000
C	-0.463819000	-2.038339000	1.576024000
H	0.224427000	-2.765114000	1.147458000
H	0.550117000	-2.285360000	3.463198000
H	-1.101026000	-1.489515000	3.593049000
C	-1.835624000	-2.196760000	0.988399000
C	-2.982330000	-1.726586000	1.628629000
C	-1.977353000	-2.840694000	-0.244257000
C	-4.235983000	-1.895656000	1.066457000
H	-2.904127000	-1.222498000	2.583564000
C	-3.220180000	-3.022815000	-0.823311000
H	-1.094251000	-3.207235000	-0.755895000
C	-4.338266000	-2.547147000	-0.152669000
H	-5.124238000	-1.517947000	1.553881000
H	-3.329098000	-3.518417000	-1.778595000
N	-5.656737000	-2.689536000	-0.771111000
O	-5.712897000	-3.122695000	-1.909188000
O	-6.633967000	-2.359259000	-0.123083000

TS1_Ph-NO₂

	Coordinates (Angstroms)		
X	Y	Z	

Mn	-0.962948000	0.454575000	0.091402000
P	-2.741893000	-0.858272000	-0.349829000
O	-1.895148000	1.503638000	2.665856000
C	-1.529761000	1.084867000	1.651519000
N	-0.139166000	-0.494960000	-1.635349000
C	-1.135994000	-1.063172000	-2.560904000
C	0.876711000	0.310098000	-2.339052000
C	1.928658000	0.783055000	-1.344138000
C	-2.155581000	-1.878870000	-1.774230000
H	2.611324000	1.506029000	-1.794166000
H	-1.670874000	-2.756931000	-1.337523000
H	2.528668000	-0.066513000	-1.009968000
P	1.068649000	1.439300000	0.158898000
C	-1.671928000	1.834824000	-0.790634000
O	-2.149420000	2.732469000	-1.335738000
H	-2.965282000	-2.237079000	-2.413219000
C	2.269419000	1.147645000	1.510442000
C	3.615487000	1.487750000	1.359474000
C	1.843889000	0.557918000	2.698397000
C	4.525584000	1.215374000	2.370908000
H	3.959771000	1.959722000	0.444827000
C	2.753839000	0.295657000	3.718389000
H	0.800375000	0.289067000	2.817432000
C	4.095602000	0.614682000	3.551337000
H	5.571893000	1.467294000	2.237532000
H	2.413409000	-0.164916000	4.639257000
H	4.808254000	0.399716000	4.340007000
C	1.124688000	3.266032000	0.004424000
C	1.227307000	3.903764000	-1.230433000
C	0.945873000	4.038906000	1.154217000
C	1.168172000	5.290985000	-1.314412000
H	1.347293000	3.328149000	-2.141829000
C	0.886150000	5.423049000	1.069619000
H	0.855304000	3.558231000	2.123231000
C	0.999122000	6.052919000	-0.165630000
H	1.252043000	5.774662000	-2.281352000
H	0.749313000	6.010118000	1.971027000
H	0.950020000	7.134117000	-0.232570000
C	-3.407223000	-2.094629000	0.829679000
C	-4.344216000	-3.044621000	0.414144000
C	-2.990983000	-2.085518000	2.159118000
C	-4.842814000	-3.977871000	1.312003000
H	-4.695353000	-3.049287000	-0.613008000
C	-3.497145000	-3.016091000	3.061821000
H	-2.261879000	-1.352989000	2.486220000
C	-4.419692000	-3.963766000	2.638516000
H	-5.567398000	-4.713125000	0.979964000
H	-3.168235000	-2.998067000	4.094918000
H	-4.812337000	-4.690865000	3.340889000
C	-4.285792000	-0.049988000	-0.922514000
C	-4.611085000	0.095632000	-2.269519000
C	-5.112939000	0.533070000	0.040976000
C	-5.749390000	0.801610000	-2.647486000
H	-3.980855000	-0.332304000	-3.041273000
C	-6.249739000	1.233313000	-0.336147000
H	-4.869374000	0.435619000	1.094623000
C	-6.571108000	1.369493000	-1.683365000
H	-5.988841000	0.909957000	-3.699710000
H	-6.884824000	1.676838000	0.422683000
H	-7.457351000	1.920178000	-1.978592000
H	1.350143000	-0.275374000	-3.137157000
H	0.365926000	1.158982000	-2.803049000
H	-1.620526000	-0.231191000	-3.081049000
H	-0.646624000	-1.691042000	-3.316536000
H	0.348777000	-1.289165000	-1.204445000
H	-0.290920000	-0.925810000	0.857683000
C	0.353613000	-2.392605000	1.071014000
C	1.012170000	-2.921028000	-0.019984000
H	0.445708000	-3.528125000	-0.721642000
H	-0.616661000	-2.798922000	1.329614000
H	0.911157000	-2.000302000	1.914780000
C	2.399534000	-2.702715000	-0.347598000
C	3.300283000	-2.035855000	0.511655000
C	2.904814000	-3.146330000	-1.591471000
C	4.607516000	-1.799574000	0.143106000
H	2.968524000	-1.682816000	1.479697000
C	4.208834000	-2.913136000	-1.972107000

H	2.242392000	-3.675337000	-2.269259000
C	5.056293000	-2.227490000	-1.103613000
H	5.281144000	-1.277882000	0.809537000
H	4.579907000	-3.248644000	-2.931819000
N	6.424405000	-1.955999000	-1.502574000
O	6.804189000	-2.370157000	-2.587954000
O	7.135711000	-1.319620000	-0.739227000

TS2_Ph-OCH₃

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.738383000	0.456422000	0.139146000
P	2.612662000	-0.791703000	0.391237000
O	0.341079000	-0.195821000	-2.694347000
C	0.481243000	0.054440000	-1.572683000
N	0.877511000	0.621506000	2.218583000
C	2.233225000	0.489866000	2.782239000
C	0.144509000	1.739061000	2.838203000
C	-1.268601000	1.777727000	2.268928000
C	2.895480000	-0.760962000	2.215041000
H	-1.842196000	2.623784000	2.651823000
H	2.397187000	-1.648496000	2.613165000
H	-1.797032000	0.861293000	2.549825000
P	-1.127644000	1.729206000	0.436507000
C	1.707239000	1.889727000	-0.273080000
O	2.337240000	2.815092000	-0.549998000
H	3.951045000	-0.823648000	2.487003000
C	-2.812383000	1.342103000	-0.165469000
C	-3.934998000	1.931819000	0.420607000
C	-2.978658000	0.513633000	-1.272033000
C	-5.201956000	1.690329000	-0.092066000
H	-3.823375000	2.591977000	1.274834000
C	-4.246290000	0.287264000	-1.796023000
H	-2.120221000	0.029427000	-1.719917000
C	-5.358497000	0.871618000	-1.206460000
H	-6.068576000	2.147076000	0.373666000
H	-4.364479000	-0.366860000	-2.652125000
H	-6.347619000	0.681750000	-1.607890000
C	-0.992420000	3.483169000	-0.099524000
C	-0.852790000	4.553832000	0.780318000
C	-0.970125000	3.730822000	-1.474761000
C	-0.702610000	5.850345000	0.294877000
H	-0.853722000	4.394242000	1.852554000
C	-0.825395000	5.022445000	-1.958160000
H	-1.063135000	2.906608000	-2.175771000
C	-0.690904000	6.087709000	-1.072430000
H	-0.593611000	6.673964000	0.992272000
H	-0.810904000	5.198160000	-3.028140000
H	-0.571931000	7.097301000	-1.450058000
C	2.711575000	-2.568931000	-0.046414000
C	3.732574000	-3.380200000	0.454970000
C	1.765682000	-3.121490000	-0.906640000
C	3.795547000	-4.723032000	0.109787000
H	4.485735000	-2.962005000	1.115325000
C	1.833302000	-4.465342000	-1.260526000
H	0.966841000	-2.499397000	-1.292901000
C	2.845736000	-5.267254000	-0.750671000
H	4.588632000	-5.346413000	0.507865000
H	1.092203000	-4.883350000	-1.932957000
H	2.897916000	-6.316279000	-1.020696000
C	4.155630000	-0.145544000	-0.361447000
C	5.029372000	0.681927000	0.341605000
C	4.402285000	-0.400415000	-1.712500000
C	6.139604000	1.233527000	-0.289073000
H	4.849660000	0.912936000	1.385699000
C	5.510302000	0.150712000	-2.341238000
H	3.727457000	-1.034840000	-2.278751000
C	6.383120000	0.968345000	-1.630149000
H	6.810668000	1.875637000	0.270813000
H	5.690804000	-0.055648000	-3.390417000
H	7.247150000	1.400932000	-2.122254000
H	0.105784000	1.606738000	3.927605000
H	0.678695000	2.671986000	2.630507000

H	2.805662000	1.388930000	2.532612000
H	2.181696000	0.417133000	3.876817000
H	0.355190000	-0.256114000	2.550018000
H	-0.215254000	-0.968313000	0.686434000
C	-0.505006000	-1.781899000	2.864894000
C	-0.658562000	-2.002038000	1.477074000
H	0.043882000	-2.722416000	1.061032000
H	0.309218000	-2.274137000	3.386431000
H	-1.345701000	-1.483893000	3.481943000
C	-2.019168000	-2.178930000	0.862915000
C	-3.185313000	-1.704491000	1.460752000
C	-2.137664000	-2.867959000	-0.344627000
C	-4.430625000	-1.930888000	0.889455000
H	-3.131764000	-1.159014000	2.396056000
C	-3.376378000	-3.103999000	-0.925244000
H	-1.241111000	-3.232303000	-0.836481000
C	-4.527825000	-2.638352000	-0.301235000
H	-5.333899000	-1.552265000	1.354286000
H	-3.454912000	-3.637849000	-1.866500000
O	-5.761269000	-2.828260000	-0.876492000
C	-6.279425000	-4.138640000	-0.711852000
H	-6.434265000	-4.367096000	0.349677000
H	-7.238299000	-4.168528000	-1.230772000
H	-5.612235000	-4.893054000	-1.144995000

TS1_Ph_OCH₃

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.834020000	0.421387000	0.099223000
P	-2.655111000	-0.841107000	-0.327511000
O	-1.666056000	1.399074000	2.736745000
C	-1.338189000	1.005027000	1.699387000
N	-0.078227000	-0.494283000	-1.659767000
C	-1.102828000	-1.032468000	-2.574239000
C	0.934940000	0.301356000	-2.380661000
C	2.022576000	0.748595000	-1.412160000
C	-2.120682000	-1.844804000	-1.781267000
H	2.693668000	1.476939000	-1.870551000
H	-1.641488000	-2.737350000	-1.369324000
H	2.628051000	-0.110060000	-1.114728000
P	1.215267000	1.379814000	0.127110000
C	-1.544998000	1.839084000	-0.710760000
O	-2.020868000	2.761080000	-1.215569000
H	-2.950224000	-2.178358000	-2.408044000
C	2.443008000	1.055483000	1.445812000
C	3.785742000	1.399656000	1.276972000
C	2.039910000	0.439169000	2.627901000
C	4.712931000	1.110865000	2.267819000
H	4.112743000	1.887318000	0.364322000
C	2.967540000	0.158339000	3.626417000
H	0.999511000	0.164777000	2.760016000
C	4.304901000	0.486331000	3.443601000
H	5.756155000	1.369026000	2.122174000
H	2.644330000	-0.323437000	4.542620000
H	5.030914000	0.258822000	4.216513000
C	1.275617000	3.209569000	0.006744000
C	1.361783000	3.869261000	-1.217792000
C	1.116263000	3.962832000	1.172363000
C	1.305385000	5.257948000	-1.276562000
H	1.465692000	3.309395000	-2.140768000
C	1.059947000	5.348469000	1.113112000
H	1.037798000	3.465448000	2.133978000
C	1.156236000	6.000045000	-0.112311000
H	1.375462000	5.757963000	-2.236319000
H	0.938130000	5.919704000	2.026820000
H	1.109260000	7.082456000	-0.159189000
C	-3.331688000	-2.080708000	0.842285000
C	-4.328636000	-2.973428000	0.439310000
C	-2.856534000	-2.136162000	2.150570000
C	-4.827931000	-3.915022000	1.328006000
H	-4.726233000	-2.925343000	-0.569616000
C	-3.362181000	-3.075563000	3.044169000
H	-2.082923000	-1.446473000	2.468522000

C	-4.344020000	-3.967196000	2.632657000
H	-5.598432000	-4.606736000	1.005757000
H	-2.984599000	-3.110071000	4.060053000
H	-4.735929000	-4.701812000	3.327628000
C	-4.185288000	0.024522000	-0.850928000
C	-4.561868000	0.166838000	-2.184551000
C	-4.947605000	0.650269000	0.139166000
C	-5.688106000	0.911465000	-2.523341000
H	-3.982450000	-0.294455000	-2.976501000
C	-6.071944000	1.389185000	-0.198584000
H	-4.661738000	0.556914000	1.182549000
C	-6.445280000	1.521894000	-1.532833000
H	-5.968424000	1.016453000	-3.565800000
H	-6.655137000	1.867304000	0.580634000
H	-7.321645000	2.103077000	-1.797767000
H	1.379207000	-0.288374000	-3.191970000
H	0.428028000	1.162086000	-2.827409000
H	-1.584411000	-0.187470000	-3.076143000
H	-0.635957000	-1.658950000	-3.345201000
H	0.409988000	-1.315442000	-1.261469000
H	-0.133845000	-1.051456000	0.784755000
C	0.430267000	-2.371187000	0.928693000
C	1.062623000	-2.900945000	-0.198071000
H	0.474650000	-3.501765000	-0.887607000
H	-0.503431000	-2.836303000	1.229639000
H	1.037845000	-2.072000000	1.779940000
C	2.448889000	-2.678086000	-0.565790000
C	3.399593000	-2.112091000	0.305514000
C	2.897317000	-2.992791000	-1.864884000
C	4.699889000	-1.852371000	-0.103164000
H	3.118681000	-1.850202000	1.318965000
C	4.195953000	-2.736293000	-2.276858000
H	2.195120000	-3.429925000	-2.569897000
C	5.103926000	-2.153070000	-1.398523000
H	5.404309000	-1.394844000	0.583771000
H	4.513245000	-2.970667000	-3.288007000
O	6.377877000	-1.849136000	-1.825147000
C	7.342869000	-2.833798000	-1.495160000
H	7.100006000	-3.797259000	-1.960220000
H	8.301476000	-2.481088000	-1.879067000
H	7.418762000	-2.972598000	-0.409846000

A3_H

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.001761000	0.155148000	0.230824000
P	-2.260281000	0.136561000	0.534178000
O	0.047723000	0.619333000	-2.673596000
C	0.022235000	0.468310000	-1.527858000
N	-0.002110000	-0.097973000	2.308703000
C	-1.184023000	-0.709101000	2.870902000
C	1.184287000	-0.697086000	2.875003000
C	2.425883000	0.029885000	2.363794000
C	-2.431043000	0.008141000	2.359528000
H	3.363634000	-0.435207000	2.677373000
H	-2.432086000	1.037401000	2.730622000
H	2.418438000	1.060662000	2.730763000
P	2.255872000	0.151545000	0.538022000
C	0.005268000	-1.613344000	-0.045516000
O	0.006038000	-2.750469000	-0.200214000
H	-3.362973000	-0.468329000	2.673039000
C	3.316877000	1.569942000	0.063420000
C	2.770703000	2.663311000	-0.604782000
C	4.679648000	1.574220000	0.375797000
C	3.568996000	3.749977000	-0.950794000
H	1.718090000	2.666116000	-0.863311000
C	5.475164000	2.658370000	0.033960000
H	5.122915000	0.720517000	0.878795000
C	4.919765000	3.749253000	-0.629951000
H	3.132854000	4.594526000	-1.472734000
H	6.531503000	2.651618000	0.279354000
H	5.543246000	4.594561000	-0.900163000
C	3.177970000	-1.258560000	-0.181454000

C	3.553139000	-2.372300000	0.566870000
C	3.430787000	-1.246566000	-1.555940000
C	4.182198000	-3.451668000	-0.046545000
H	3.350129000	-2.415060000	1.630793000
C	4.061184000	-2.321467000	-2.165445000
H	3.136655000	-0.389524000	-2.154060000
C	4.438850000	-3.428262000	-1.410722000
H	4.467103000	-4.314025000	0.546255000
H	4.253647000	-2.297426000	-3.232387000
H	4.926710000	-4.271316000	-1.887416000
C	-3.316587000	1.559868000	0.062045000
C	-4.605010000	1.695286000	0.586966000
C	-2.846937000	2.515365000	-0.836494000
C	-5.401231000	2.773109000	0.226367000
H	-4.989676000	0.952891000	1.278918000
C	-3.648901000	3.591237000	-1.206570000
H	-1.852495000	2.418344000	-1.257120000
C	-4.923936000	3.722857000	-0.672984000
H	-6.397028000	2.872145000	0.644311000
H	-3.274540000	4.325150000	-1.911685000
H	-5.548667000	4.562453000	-0.957621000
C	-3.184769000	-1.269648000	-0.191569000
C	-3.551439000	-2.389838000	0.551495000
C	-3.446204000	-1.249055000	-1.564132000
C	-4.180823000	-3.466931000	-0.065367000
H	-3.340952000	-2.439665000	1.613700000
C	-4.076859000	-2.321969000	-2.177090000
H	-3.157958000	-0.387669000	-2.158899000
C	-4.446151000	-3.435093000	-1.427785000
H	-4.458895000	-4.334466000	0.523118000
H	-4.275883000	-2.291201000	-3.242667000
H	-4.934137000	-4.276538000	-1.907180000
H	1.169207000	-0.631142000	3.976456000
H	1.274199000	-1.780307000	2.641280000
H	-1.263842000	-1.792690000	2.634921000
H	-1.172268000	-0.645556000	3.972551000
H	0.038744000	1.711507000	1.087110000
H	-0.105098000	1.947394000	0.350924000

A3_Ph-OCH₃

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.842593000	0.373098000	0.108827000
P	-2.635073000	-0.981033000	-0.307728000
O	-1.701253000	1.269356000	2.774114000
C	-1.353469000	0.902439000	1.736973000
N	-0.098311000	-0.459934000	-1.656417000
C	-1.105423000	-1.039624000	-2.567842000
C	0.860344000	0.384606000	-2.398430000
C	1.950871000	0.875692000	-1.454445000
C	-2.062205000	-1.926622000	-1.778623000
H	2.599379000	1.613446000	-1.929901000
H	-1.519735000	-2.790404000	-1.384147000
H	2.580821000	0.036186000	-1.149450000
P	1.146237000	1.499765000	0.080576000
C	-1.667452000	1.759015000	-0.634044000
O	-2.201049000	2.654541000	-1.120458000
H	-2.877404000	-2.304278000	-2.399171000
C	2.405701000	1.313051000	1.391165000
C	3.699419000	1.806318000	1.208501000
C	2.086182000	0.649451000	2.573227000
C	4.662301000	1.622525000	2.189990000
H	3.958451000	2.329501000	0.293628000
C	3.050346000	0.471394000	3.560439000
H	1.087496000	0.253352000	2.717071000
C	4.338555000	0.952774000	3.367050000
H	5.667277000	1.999847000	2.036827000
H	2.794957000	-0.050387000	4.475980000
H	5.093055000	0.807503000	4.132402000
C	1.032182000	3.319824000	-0.094744000
C	1.148931000	3.963931000	-1.324493000
C	0.720147000	4.072208000	1.040618000
C	0.968671000	5.340582000	-1.417093000

H	1.375631000	3.402751000	-2.224026000
C	0.542159000	5.444943000	0.947137000
H	0.619065000	3.583816000	2.004829000
C	0.666498000	6.082808000	-0.283401000
H	1.063951000	5.830517000	-2.379783000
H	0.303085000	6.017451000	1.836513000
H	0.523858000	7.155136000	-0.357872000
C	-3.251225000	-2.253666000	0.854637000
C	-4.255737000	-3.143421000	0.464205000
C	-2.722102000	-2.343012000	2.140223000
C	-4.712139000	-4.114052000	1.344279000
H	-4.692480000	-3.069804000	-0.526731000
C	-3.183353000	-3.313572000	3.024202000
H	-1.943110000	-1.656578000	2.451864000
C	-4.174988000	-4.200289000	2.626002000
H	-5.489860000	-4.802522000	1.032975000
H	-2.763614000	-3.376282000	4.021866000
H	-4.533521000	-4.957658000	3.314375000
C	-4.185056000	-0.138084000	-0.797654000
C	-4.612382000	-0.033418000	-2.119177000
C	-4.919765000	0.496278000	0.207981000
C	-5.763522000	0.684876000	-2.430415000
H	-4.055248000	-0.504676000	-2.920966000
C	-6.068674000	1.208077000	-0.102988000
H	-4.592888000	0.431221000	1.241386000
C	-6.493349000	1.304205000	-1.425020000
H	-6.086168000	0.760872000	-3.462994000
H	-6.630786000	1.693400000	0.687054000
H	-7.389520000	1.863783000	-1.669141000
H	1.312775000	-0.187830000	-3.217175000
H	0.311731000	1.224179000	-2.837665000
H	-1.643534000	-0.221207000	-3.057117000
H	-0.608939000	-1.629468000	-3.348634000
H	0.465970000	-1.300006000	-1.304418000
H	0.109465000	-1.179953000	0.784823000
C	0.546607000	-2.280084000	0.811082000
C	1.202359000	-2.723744000	-0.417425000
H	0.691784000	-3.483099000	-1.004527000
H	-0.327731000	-2.878132000	1.068769000
H	1.188816000	-2.210654000	1.695879000
C	2.607045000	-2.570332000	-0.659944000
C	3.472136000	-1.835068000	0.186301000
C	3.212917000	-3.119044000	-1.821720000
C	4.816887000	-1.647943000	-0.112765000
H	3.084928000	-1.382680000	1.091319000
C	4.550658000	-2.930977000	-2.117554000
H	2.596868000	-3.697580000	-2.505514000
C	5.367066000	-2.184683000	-1.266983000
H	5.444249000	-1.063560000	0.553706000
H	4.977382000	-3.356620000	-3.021255000
O	6.695217000	-1.962833000	-1.581663000
C	7.562457000	-2.981640000	-1.120140000
H	7.326275000	-3.948651000	-1.582309000
H	8.578160000	-2.692734000	-1.397951000
H	7.503706000	-3.089924000	-0.029622000

A3_CH=CH₂

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.104411000	0.178975000	-0.015106000
P	2.327599000	-0.219862000	0.288762000
O	0.137188000	0.431731000	-2.943045000
C	0.127091000	0.311851000	-1.795394000
N	-0.011800000	-0.240085000	2.038209000
C	1.255574000	-0.160875000	2.790923000
C	-1.098795000	0.465373000	2.746258000
C	-2.422689000	0.209062000	2.037453000
C	2.358862000	-0.865842000	2.011698000
H	-3.207078000	0.875063000	2.401746000
H	2.134109000	-1.933764000	1.935757000
H	-2.736116000	-0.819911000	2.231716000
P	-2.161733000	0.359554000	0.213302000
C	0.325497000	1.933136000	0.152985000

O	0.487736000	3.067425000	0.265441000
H	3.331917000	-0.768476000	2.496855000
C	-3.304957000	-0.871484000	-0.508942000
C	-4.574315000	-1.073836000	0.037480000
C	-2.911714000	-1.619743000	-1.615995000
C	-5.429054000	-2.020827000	-0.507808000
H	-4.896764000	-0.496670000	0.897788000
C	-3.772468000	-2.562885000	-2.168761000
H	-1.925309000	-1.474807000	-2.041752000
C	-5.028268000	-2.767403000	-1.612170000
H	-6.407897000	-2.179215000	-0.069263000
H	-3.455768000	-3.143034000	-3.028322000
H	-5.695985000	-3.510012000	-2.034859000
C	-2.930217000	1.949136000	-0.275279000
C	-2.912287000	3.045597000	0.587157000
C	-3.458281000	2.102286000	-1.558142000
C	-3.429787000	4.269488000	0.180122000
H	-2.487770000	2.955870000	1.581591000
C	-3.973144000	3.326833000	-1.964019000
H	-3.477339000	1.261765000	-2.244024000
C	-3.963076000	4.412323000	-1.095091000
H	-3.412949000	5.112533000	0.862022000
H	-4.386549000	3.431795000	-2.961019000
H	-4.368141000	5.366875000	-1.412225000
C	3.273183000	-1.449750000	-0.683211000
C	4.613463000	-1.713094000	-0.387195000
C	2.657584000	-2.135929000	-1.727668000
C	5.320341000	-2.656595000	-1.118909000
H	5.111257000	-1.170779000	0.410623000
C	3.368260000	-3.078419000	-2.464299000
H	1.618380000	-1.938489000	-1.963551000
C	4.697515000	-3.339990000	-2.159978000
H	6.360281000	-2.854323000	-0.883827000
H	2.880807000	-3.604924000	-3.277168000
H	5.252250000	-4.073426000	-2.734813000
C	3.446227000	1.230544000	0.262417000
C	4.033253000	1.767592000	1.405553000
C	3.657793000	1.855332000	-0.969805000
C	4.826335000	2.908451000	1.318973000
H	3.879312000	1.307548000	2.375006000
C	4.453961000	2.987525000	-1.056027000
H	3.195885000	1.453880000	-1.866928000
C	5.038950000	3.518054000	0.090244000
H	5.276093000	3.319619000	2.216026000
H	4.612061000	3.462337000	-2.017862000
H	5.654988000	4.407988000	0.024240000
H	-1.165719000	0.113941000	3.782897000
H	-0.858367000	1.532867000	2.766828000
H	1.498663000	0.895682000	2.943426000
H	1.135386000	-0.624037000	3.777975000
H	-0.281068000	-1.262399000	2.037447000
H	-0.057566000	-1.697672000	-0.046500000
C	-0.562164000	-3.093098000	1.658437000
C	-0.185826000	-2.850221000	0.274759000
H	0.790490000	-3.247541000	-0.009540000
H	0.218830000	-3.348691000	2.372251000
H	-0.931691000	-3.168405000	-0.457601000
C	-1.918736000	-3.269891000	2.041428000
H	-2.638304000	-3.163455000	1.223368000
C	-2.450284000	-3.526865000	3.267470000
H	-3.518219000	-3.666214000	3.394985000
H	-1.824136000	-3.648965000	4.148773000

A3_Ph

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.442180000	0.379156000	0.094601000
P	-2.500631000	-0.541888000	-0.269876000
O	-0.916787000	1.289483000	2.849908000
C	-0.728612000	0.910317000	1.776826000
N	0.009901000	-0.476110000	-1.759512000
C	-1.145931000	-0.773301000	-2.628506000
C	1.085278000	0.197975000	-2.515880000

C	2.306616000	0.381832000	-1.623844000
C	-2.221390000	-1.492058000	-1.821522000
H	3.062261000	1.011435000	-2.097082000
H	-1.848214000	-2.469946000	-1.505062000
H	2.766693000	-0.589089000	-1.421837000
P	1.742463000	1.039413000	0.003189000
C	-0.982396000	1.953872000	-0.522065000
O	-1.333878000	2.971358000	-0.927833000
H	-3.129886000	-1.659580000	-2.403456000
C	2.986196000	0.457883000	1.208451000
C	4.349694000	0.642523000	0.968245000
C	2.579206000	-0.203154000	2.364812000
C	5.289282000	0.157577000	1.865942000
H	4.680017000	1.160453000	0.073664000
C	3.521836000	-0.683488000	3.268472000
H	1.523628000	-0.360803000	2.553566000
C	4.876123000	-0.508187000	3.017054000
H	6.346315000	0.296987000	1.668308000
H	3.195459000	-1.201374000	4.163354000
H	5.611975000	-0.889252000	3.716551000
C	2.047780000	2.844689000	-0.036597000
C	2.145780000	3.552549000	-1.233341000
C	2.088262000	3.543419000	1.172268000
C	2.298678000	4.935208000	-1.222134000
H	2.099743000	3.036255000	-2.186060000
C	2.241784000	4.922790000	1.181663000
H	2.008068000	3.008525000	2.113389000
C	2.349122000	5.622016000	-0.016331000
H	2.377122000	5.473481000	-2.160222000
H	2.278001000	5.452516000	2.127110000
H	2.470472000	6.699546000	-0.008220000
C	-3.286374000	-1.731487000	0.877837000
C	-4.457329000	-2.405452000	0.520589000
C	-2.716963000	-1.969126000	2.126774000
C	-5.037994000	-3.311935000	1.396272000
H	-4.923052000	-2.214740000	-0.441128000
C	-3.303028000	-2.872755000	3.007274000
H	-1.806710000	-1.454388000	2.411360000
C	-4.460835000	-3.546069000	2.641683000
H	-5.945099000	-3.833008000	1.110759000
H	-2.850724000	-3.049573000	3.976582000
H	-4.916730000	-4.253004000	3.326083000
C	-3.869977000	0.625433000	-0.607243000
C	-4.360770000	0.877406000	-1.886168000
C	-4.384863000	1.345844000	0.474112000
C	-5.359253000	1.827764000	-2.080750000
H	-3.970080000	0.343329000	-2.744865000
C	-5.382444000	2.289303000	0.279372000
H	-4.003132000	1.168296000	1.475025000
C	-5.872764000	2.532177000	-1.000535000
H	-5.734255000	2.015135000	-3.080894000
H	-5.775795000	2.838969000	1.127154000
H	-6.649410000	3.273288000	-1.153408000
H	1.358699000	-0.397868000	-3.395111000
H	0.702754000	1.161465000	-2.868139000
H	-1.526747000	0.168443000	-3.037445000
H	-0.829895000	-1.401673000	-3.470624000
H	0.399181000	-1.432207000	-1.487439000
H	0.184993000	-1.378596000	0.624089000
C	0.411452000	-2.538602000	0.581314000
C	0.846463000	-3.046576000	-0.718831000
H	0.123433000	-3.619284000	-1.294413000
H	-0.528693000	-2.973612000	0.921786000
H	1.145597000	-2.625721000	1.388478000
C	2.214915000	-3.193590000	-1.102582000
C	3.309626000	-2.738471000	-0.322721000
C	2.559503000	-3.789733000	-2.347644000
C	4.622264000	-2.855245000	-0.761186000
H	3.129194000	-2.278062000	0.641789000
C	3.868833000	-3.899084000	-2.775354000
H	1.759584000	-4.166248000	-2.980860000
C	4.927357000	-3.427456000	-1.992162000
H	5.419764000	-2.486485000	-0.121941000
H	4.074116000	-4.362394000	-3.736554000
H	5.953631000	-3.515800000	-2.330412000

A3_C≡CH

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.088445000	0.111184000	0.021519000
P	2.333204000	-0.199049000	0.334972000
O	0.097944000	0.187258000	-2.918501000
C	0.096708000	0.134661000	-1.766616000
N	-0.000699000	-0.181734000	2.088206000
C	1.260316000	0.011839000	2.828850000
C	-1.125551000	0.494116000	2.764369000
C	-2.430935000	0.126365000	2.069140000
C	2.392671000	-0.704995000	2.102211000
H	-3.269149000	0.720195000	2.438387000
H	2.207392000	-1.783028000	2.109747000
H	-2.660833000	-0.927957000	2.253350000
P	-2.185171000	0.282930000	0.250876000
C	0.266458000	1.877190000	0.069301000
O	0.391272000	3.019658000	0.111580000
H	3.361643000	-0.536077000	2.575752000
C	-3.341125000	-0.927308000	-0.480668000
C	-4.680504000	-0.956558000	-0.085174000
C	-2.886570000	-1.842271000	-1.425909000
C	-5.546619000	-1.897803000	-0.620626000
H	-5.047399000	-0.242980000	0.645682000
C	-3.757419000	-2.782172000	-1.968226000
H	-1.847206000	-1.828756000	-1.732855000
C	-5.084678000	-2.812812000	-1.563315000
H	-6.583380000	-1.920250000	-0.303574000
H	-3.394118000	-3.494889000	-2.700067000
H	-5.762589000	-3.550560000	-1.978439000
C	-2.916438000	1.887901000	-0.241681000
C	-3.112464000	2.922807000	0.670689000
C	-3.192371000	2.110488000	-1.592950000
C	-3.591017000	4.156778000	0.241968000
H	-2.890821000	2.780238000	1.722538000
C	-3.669454000	3.342003000	-2.019143000
H	-3.041877000	1.315947000	-2.317202000
C	-3.870789000	4.368440000	-1.101416000
H	-3.741149000	4.953225000	0.962491000
H	-3.882454000	3.501373000	-3.070342000
H	-4.243557000	5.330477000	-1.435296000
C	3.308314000	-1.468736000	-0.551741000
C	4.647623000	-1.699327000	-0.225629000
C	2.713834000	-2.218749000	-1.564023000
C	5.373265000	-2.673873000	-0.896019000
H	5.128703000	-1.108298000	0.547556000
C	3.443065000	-3.192119000	-2.239221000
H	1.675374000	-2.048638000	-1.822868000
C	4.770989000	-3.421202000	-1.904767000
H	6.411993000	-2.847450000	-0.637680000
H	2.970666000	-3.769195000	-3.026190000
H	5.340183000	-4.180291000	-2.430037000
C	3.392934000	1.285816000	0.180563000
C	3.957427000	1.941791000	1.271937000
C	3.576447000	1.813508000	-1.100625000
C	4.701152000	3.103672000	1.085430000
H	3.821667000	1.560729000	2.277500000
C	4.322510000	2.967643000	-1.285695000
H	3.129560000	1.320566000	-1.958897000
C	4.886396000	3.616747000	-0.190887000
H	5.134298000	3.606438000	1.943122000
H	4.458112000	3.367424000	-2.284363000
H	5.462123000	4.524299000	-0.334490000
H	-1.172048000	0.188708000	3.816965000
H	-0.948870000	1.574306000	2.734616000
H	1.461603000	1.085587000	2.905222000
H	1.160435000	-0.385152000	3.846858000
H	-0.212710000	-1.235512000	2.164071000
H	-0.071610000	-1.809002000	0.090790000
C	-0.434796000	-3.019444000	1.933864000
C	-0.063850000	-2.897026000	0.508107000
H	0.953646000	-3.233330000	0.300494000
H	0.325138000	-3.406009000	2.607901000
H	-0.747694000	-3.391897000	-0.187122000

C	-1.767462000	-3.308916000	2.262004000
C	-2.948742000	-3.473217000	2.516990000
H	-3.961489000	-3.742645000	2.702057000

A3_Ph-NO₂

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.901691000	0.389877000	0.134035000
P	-2.729191000	-0.926807000	-0.342125000
O	-1.883617000	1.488004000	2.682909000
C	-1.489926000	1.039392000	1.699446000
N	-0.095023000	-0.529843000	-1.590916000
C	-1.091135000	-1.091281000	-2.527953000
C	0.914439000	0.281354000	-2.306666000
C	1.976788000	0.767230000	-1.330368000
C	-2.118422000	-1.920832000	-1.766039000
H	2.664135000	1.471464000	-1.802175000
H	-1.638281000	-2.803275000	-1.334602000
H	2.571161000	-0.079154000	-0.975640000
P	1.139411000	1.462781000	0.156500000
C	-1.641344000	1.774148000	-0.706121000
O	-2.118361000	2.666366000	-1.247118000
H	-2.917295000	-2.271767000	-2.422208000
C	2.335890000	1.258229000	1.518019000
C	3.674126000	1.616823000	1.342718000
C	1.925876000	0.706811000	2.729962000
C	4.592221000	1.405470000	2.360577000
H	4.007396000	2.048532000	0.404684000
C	2.845457000	0.505130000	3.754170000
H	0.890831000	0.418053000	2.873410000
C	4.178499000	0.846452000	3.566712000
H	5.633628000	1.665723000	2.209210000
H	2.520272000	0.069889000	4.692409000
H	4.899643000	0.675370000	4.358144000
C	1.071269000	3.276018000	-0.071497000
C	1.224221000	3.878577000	-1.318228000
C	0.758411000	4.067164000	1.036588000
C	1.077347000	5.255248000	-1.454449000
H	1.456461000	3.285356000	-2.195538000
C	0.613160000	5.439930000	0.898548000
H	0.634334000	3.610809000	2.013778000
C	0.772097000	6.036877000	-0.348271000
H	1.201655000	5.714799000	-2.428590000
H	0.373925000	6.044841000	1.766033000
H	0.655312000	7.109295000	-0.456790000
C	-3.442431000	-2.146254000	0.817130000
C	-4.343013000	-3.112700000	0.361403000
C	-3.109745000	-2.105187000	2.169457000
C	-4.890428000	-4.030100000	1.246600000
H	-4.622816000	-3.146229000	-0.686737000
C	-3.664791000	-3.020805000	3.057638000
H	-2.408711000	-1.362715000	2.532980000
C	-4.552534000	-3.983754000	2.596410000
H	-5.586424000	-4.779016000	0.885757000
H	-3.401243000	-2.979752000	4.108411000
H	-4.982633000	-4.699942000	3.287682000
C	-4.212464000	-0.031545000	-0.930295000
C	-4.540020000	0.089428000	-2.278852000
C	-4.992526000	0.627151000	0.023691000
C	-5.637309000	0.851923000	-2.668055000
H	-3.946646000	-0.401808000	-3.041683000
C	-6.088395000	1.382730000	-0.366083000
H	-4.746766000	0.545442000	1.078040000
C	-6.412258000	1.497915000	-1.714667000
H	-5.881251000	0.942034000	-3.720748000
H	-6.688408000	1.886489000	0.383374000
H	-7.265796000	2.092915000	-2.019694000
H	1.383170000	-0.312022000	-3.099595000
H	0.396010000	1.122230000	-2.777269000
H	-1.573082000	-0.256326000	-3.045900000
H	-0.592207000	-1.710665000	-3.282208000
H	0.411075000	-1.344464000	-1.189757000
H	0.014816000	-1.198262000	1.033095000

C	0.301468000	-2.291756000	1.167525000
C	0.974995000	-2.899152000	-0.007581000
H	0.387878000	-3.565991000	-0.633142000
H	-0.627761000	-2.803909000	1.417033000
H	0.919839000	-2.259252000	2.070414000
C	2.316688000	-2.748893000	-0.307297000
C	3.226980000	-1.975600000	0.501148000
C	2.893038000	-3.331435000	-1.497980000
C	4.523200000	-1.757368000	0.127679000
H	2.877070000	-1.538319000	1.428018000
C	4.183215000	-3.100151000	-1.871029000
H	2.262860000	-3.960437000	-2.120395000
C	5.023481000	-2.287642000	-1.075607000
H	5.177257000	-1.161381000	0.751423000
H	4.583155000	-3.534567000	-2.778855000
N	6.345706000	-2.016364000	-1.477466000
O	6.763676000	-2.501683000	-2.535826000
O	7.055165000	-1.291982000	-0.767524000

A3_CHO

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.041606000	0.085006000	0.013833000
P	2.245223000	0.139556000	0.282247000
O	-0.093014000	0.274519000	-2.922748000
C	-0.069737000	0.175821000	-1.775916000
N	-0.009396000	-0.157491000	2.134333000
C	1.180711000	0.429171000	2.776328000
C	-1.245408000	0.273280000	2.810173000
C	-2.435414000	-0.403274000	2.140095000
C	2.433506000	-0.107039000	2.094458000
H	-3.386973000	-0.093535000	2.576337000
H	2.492830000	-1.189119000	2.244324000
H	-2.344513000	-1.486825000	2.264855000
P	-2.318211000	-0.075509000	0.334602000
C	-0.124300000	1.862976000	0.078917000
O	-0.170528000	3.009745000	0.107504000
H	3.342652000	0.342511000	2.498128000
C	-3.372326000	-1.341107000	-0.456322000
C	-4.667611000	-1.576064000	0.012068000
C	-2.900234000	-2.061379000	-1.550948000
C	-5.471935000	-2.524630000	-0.602339000
H	-5.053287000	-1.012152000	0.855342000
C	-3.709786000	-3.007836000	-2.170997000
H	-1.896002000	-1.888382000	-1.920352000
C	-4.993523000	-3.241011000	-1.696101000
H	-6.474525000	-2.703659000	-0.230268000
H	-3.333538000	-3.563009000	-3.022835000
H	-5.624251000	-3.980730000	-2.176683000
C	-3.266071000	1.460091000	0.019718000
C	-3.671913000	2.324433000	1.034112000
C	-3.519073000	1.804862000	-1.310629000
C	-4.328855000	3.511510000	0.723884000
H	-3.479268000	2.088986000	2.074618000
C	-4.177456000	2.986384000	-1.617797000
H	-3.205365000	1.142985000	-2.112097000
C	-4.583459000	3.843815000	-0.599701000
H	-4.639398000	4.177318000	1.521511000
H	-4.371106000	3.239397000	-2.654174000
H	-5.094031000	4.769947000	-0.839173000
C	3.365255000	-1.081824000	-0.487050000
C	4.649458000	-1.276746000	0.025979000
C	2.952872000	-1.819441000	-1.593975000
C	5.501211000	-2.205834000	-0.553202000
H	4.988175000	-0.703594000	0.882843000
C	3.810509000	-2.744552000	-2.180022000
H	1.956173000	-1.683197000	-1.997578000
C	5.082059000	-2.941449000	-1.657892000
H	6.493005000	-2.357409000	-0.142034000
H	3.479359000	-3.316003000	-3.039914000
H	5.748249000	-3.668640000	-2.108899000
C	3.057024000	1.730946000	-0.121383000
C	3.358115000	2.687609000	0.845878000

C	3.302834000	2.020590000	-1.465823000
C	3.908887000	3.910798000	0.475819000
H	3.165216000	2.494669000	1.895101000
C	3.853954000	3.239750000	-1.832731000
H	3.069873000	1.286764000	-2.231078000
C	4.158654000	4.188397000	-0.861345000
H	4.140751000	4.647126000	1.237296000
H	4.044443000	3.450009000	-2.879241000
H	4.588653000	5.141667000	-1.147870000
H	-1.209589000	-0.002437000	3.870542000
H	-1.324795000	1.363998000	2.747345000
H	1.122220000	1.520254000	2.695876000
H	1.200756000	0.168099000	3.840638000
H	0.055690000	-1.191117000	2.350478000
H	0.392964000	-1.792060000	-0.194951000
C	1.032688000	-3.525919000	0.970357000
C	1.018568000	-3.423431000	2.331375000
O	0.257899000	-2.669596000	3.044761000
C	0.032023000	-2.812609000	0.125327000
H	-0.921922000	-2.702105000	0.644213000
H	-0.156030000	-3.315718000	-0.826759000
H	1.743601000	-4.058109000	2.873999000
H	1.768507000	-4.164427000	0.493554000

TS3_H

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.000000000	0.136414000	0.224108000
P	-2.251934000	0.134333000	0.511236000
O	0.000001000	0.938435000	-2.603362000
C	0.000000000	0.629937000	-1.490519000
N	0.000000000	-0.076834000	2.336248000
C	-1.201374000	-0.645522000	2.902260000
C	1.201374000	-0.645522000	2.902260000
C	2.430810000	0.066617000	2.343956000
C	-2.430809000	0.066618000	2.343956000
H	3.370303000	-0.388684000	2.665515000
H	-2.433932000	1.109193000	2.676503000
H	2.433933000	1.109192000	2.676504000
P	2.251934000	0.134333000	0.511237000
C	0.000000000	-1.609899000	-0.192867000
O	0.000001000	-2.732368000	-0.439612000
H	-3.370303000	-0.388682000	2.665515000
C	3.309487000	1.548725000	0.019802000
C	2.727801000	2.709892000	-0.485123000
C	4.697512000	1.493398000	0.176162000
C	3.519439000	3.802823000	-0.826158000
H	1.652566000	2.759996000	-0.614240000
C	5.486041000	2.584528000	-0.160928000
H	5.165460000	0.590106000	0.554459000
C	4.897273000	3.741594000	-0.663794000
H	3.056944000	4.699303000	-1.224090000
H	6.561896000	2.530954000	-0.035248000
H	5.514685000	4.591935000	-0.932341000
C	3.176852000	-1.292131000	-0.168954000
C	3.570013000	-2.378606000	0.609201000
C	3.406782000	-1.324538000	-1.547322000
C	4.195622000	-3.474582000	0.021880000
H	3.384759000	-2.387494000	1.677305000
C	4.034191000	-2.415265000	-2.130893000
H	3.094739000	-0.490448000	-2.168604000
C	4.430878000	-3.494399000	-1.346141000
H	4.495151000	-4.315173000	0.638279000
H	4.208991000	-2.426650000	-3.201075000
H	4.915881000	-4.350001000	-1.802922000
C	-3.309487000	1.548725000	0.019802000
C	-4.697512000	1.493399000	0.176161000
C	-2.727800000	2.709892000	-0.485124000
C	-5.486040000	2.584528000	-0.160929000
H	-5.165460000	0.590107000	0.554458000
C	-3.519439000	3.802824000	-0.826159000
H	-1.652566000	2.759996000	-0.614240000
C	-4.897273000	3.741595000	-0.663795000

H	-6.561895000	2.530955000	-0.035250000
H	-3.056943000	4.699303000	-1.224090000
H	-5.514684000	4.591936000	-0.932342000
C	-3.176853000	-1.292131000	-0.168954000
C	-3.570015000	-2.378605000	0.609201000
C	-3.406781000	-1.324539000	-1.547321000
C	-4.195624000	-3.474581000	0.021881000
H	-3.384762000	-2.387492000	1.677306000
C	-4.034191000	-2.415265000	-2.130893000
H	-3.094737000	-0.490449000	-2.168604000
C	-4.430880000	-3.494399000	-1.346140000
H	-4.495154000	-4.315171000	0.638280000
H	-4.208991000	-2.426651000	-3.201075000
H	-4.915883000	-4.350001000	-1.802921000
H	1.202327000	-0.546902000	4.000157000
H	1.275570000	-1.729967000	2.686818000
H	-1.275571000	-1.729967000	2.686818000
H	-1.202327000	-0.546902000	4.000156000
H	0.000000000	1.211341000	1.565603000
H	0.000000000	1.754617000	0.816584000

TS3_Ph-OCH₃

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.850864000	0.369554000	0.109268000
P	-2.628716000	-1.008711000	-0.299649000
O	-1.708325000	1.237425000	2.786402000
C	-1.357829000	0.878412000	1.747058000
N	-0.106682000	-0.453100000	-1.625563000
C	-1.083707000	-1.065607000	-2.542919000
C	0.843412000	0.378519000	-2.386248000
C	1.930680000	0.910119000	-1.459627000
C	-2.042569000	-1.957296000	-1.760926000
H	2.554058000	1.662476000	-1.946035000
H	-1.498797000	-2.816161000	-1.358361000
H	2.586344000	0.092274000	-1.152416000
P	1.123197000	1.523603000	0.075741000
C	-1.698173000	1.748243000	-0.612815000
O	-2.240244000	2.636457000	-1.102964000
H	-2.852656000	-2.342396000	-2.383839000
C	2.389980000	1.346963000	1.382025000
C	3.676280000	1.858735000	1.196897000
C	2.086887000	0.668044000	2.559696000
C	4.646848000	1.680114000	2.171769000
H	3.923155000	2.392875000	0.284985000
C	3.058785000	0.494194000	3.540118000
H	1.094576000	0.257503000	2.706672000
C	4.338907000	0.995747000	3.344679000
H	5.645423000	2.073398000	2.016894000
H	2.815145000	-0.038506000	4.452595000
H	5.099130000	0.855283000	4.105284000
C	0.981911000	3.341631000	-0.094036000
C	1.064723000	3.984894000	-1.327096000
C	0.681033000	4.091084000	1.046195000
C	0.863749000	5.358703000	-1.417871000
H	1.279138000	3.424355000	-2.230082000
C	0.482465000	5.461170000	0.954298000
H	0.604284000	3.602582000	2.012570000
C	0.574273000	6.098626000	-0.279283000
H	0.932481000	5.848333000	-2.382961000
H	0.252556000	6.031744000	1.847331000
H	0.416106000	7.168891000	-0.352370000
C	-3.235678000	-2.279087000	0.870650000
C	-4.258093000	-3.155410000	0.496390000
C	-2.677513000	-2.385633000	2.142615000
C	-4.704645000	-4.128593000	1.378713000
H	-4.716091000	-3.068807000	-0.483838000
C	-3.128328000	-3.359218000	3.028779000
H	-1.884857000	-1.709687000	2.442580000
C	-4.138865000	-4.231659000	2.646792000
H	-5.496973000	-4.805883000	1.079838000
H	-2.686742000	-3.434664000	4.016092000
H	-4.490027000	-4.990557000	3.337292000

C	-4.183398000	-0.179528000	-0.796208000
C	-4.599466000	-0.072501000	-2.121212000
C	-4.933039000	0.443050000	0.205723000
C	-5.754403000	0.636534000	-2.439360000
H	-4.029742000	-0.534117000	-2.919650000
C	-6.085804000	1.145476000	-0.112287000
H	-4.614610000	0.375949000	1.241641000
C	-6.499287000	1.243936000	-1.437733000
H	-6.067888000	0.714923000	-3.474582000
H	-6.659723000	1.621737000	0.674784000
H	-7.398378000	1.796389000	-1.687343000
H	1.307336000	-0.215399000	-3.184682000
H	0.299168000	1.203394000	-2.861629000
H	-1.630680000	-0.276328000	-3.072359000
H	-0.559189000	-1.667584000	-3.297720000
H	0.528359000	-1.374225000	-1.258489000
C	0.589381000	-2.291313000	0.760130000
C	1.207867000	-2.592341000	-0.555381000
H	0.766987000	-3.443556000	-1.074570000
H	-0.277800000	-2.919023000	0.969131000
H	1.259035000	-2.346979000	1.626198000
C	2.646554000	-2.488592000	-0.735997000
C	3.495081000	-1.799156000	0.153694000
C	3.267571000	-3.025996000	-1.887550000
C	4.854703000	-1.638853000	-0.096071000
H	3.087648000	-1.356691000	1.054936000
C	4.619880000	-2.870629000	-2.137893000
H	2.656361000	-3.568877000	-2.603983000
C	5.425516000	-2.166708000	-1.243469000
H	5.475414000	-1.085716000	0.602107000
H	5.064840000	-3.287509000	-3.036518000
O	6.767158000	-1.975184000	-1.509628000
C	7.591455000	-3.027665000	-1.043064000
H	7.341454000	-3.978283000	-1.530939000
H	8.622264000	-2.762688000	-1.285665000
H	7.497194000	-3.153931000	0.042872000
H	0.185291000	-1.215120000	0.844559000

TS3_CH=CH₂

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.103253000	0.175712000	-0.015729000
P	2.330253000	-0.226212000	0.283074000
O	0.140167000	0.427254000	-2.946410000
C	0.126525000	0.301894000	-1.799047000
N	-0.014219000	-0.273716000	1.985204000
C	1.232125000	-0.235546000	2.767856000
C	-1.092010000	0.394810000	2.733635000
C	-2.427605000	0.191793000	2.027126000
C	2.357608000	-0.906402000	1.989747000
H	-3.192120000	0.875433000	2.401238000
H	2.152375000	-1.975631000	1.887285000
H	-2.775585000	-0.828454000	2.201372000
P	-2.162687000	0.364462000	0.207737000
C	0.328983000	1.924272000	0.146170000
O	0.490457000	3.056077000	0.280220000
H	3.326325000	-0.802165000	2.482836000
C	-3.305169000	-0.859917000	-0.529492000
C	-4.591209000	-1.031639000	-0.011078000
C	-2.896420000	-1.638396000	-1.609602000
C	-5.446657000	-1.977863000	-0.556216000
H	-4.925844000	-0.427970000	0.826248000
C	-3.757574000	-2.581616000	-2.162355000
H	-1.898744000	-1.516650000	-2.015556000
C	-5.029493000	-2.755558000	-1.633016000
H	-6.438793000	-2.111510000	-0.139717000
H	-3.428725000	-3.185368000	-3.000858000
H	-5.697780000	-3.497496000	-2.056030000
C	-2.924774000	1.959006000	-0.272064000
C	-2.899723000	3.050160000	0.596944000
C	-3.453603000	2.122216000	-1.553429000
C	-3.411562000	4.279020000	0.197687000
H	-2.472902000	2.952064000	1.589598000

C	-3.962941000	3.351687000	-1.951310000
H	-3.476968000	1.285955000	-2.244374000
C	-3.946201000	4.431850000	-1.075826000
H	-3.388956000	5.118124000	0.884241000
H	-4.376971000	3.464731000	-2.947176000
H	-4.346835000	5.390345000	-1.386716000
C	3.283253000	-1.433352000	-0.710663000
C	4.633561000	-1.670851000	-0.439213000
C	2.660438000	-2.137544000	-1.738861000
C	5.343715000	-2.605125000	-1.179658000
H	5.135671000	-1.115588000	0.346875000
C	3.374075000	-3.071042000	-2.484127000
H	1.613676000	-1.960416000	-1.956651000
C	4.713768000	-3.305970000	-2.204718000
H	6.391318000	-2.782835000	-0.963271000
H	2.880970000	-3.610851000	-3.284833000
H	5.271026000	-4.031836000	-2.786706000
C	3.433621000	1.234734000	0.282448000
C	3.976725000	1.782721000	1.442198000
C	3.672642000	1.860826000	-0.944082000
C	4.755031000	2.935079000	1.376885000
H	3.799047000	1.322638000	2.407603000
C	4.453139000	3.005283000	-1.008422000
H	3.243986000	1.450923000	-1.853770000
C	4.995427000	3.546071000	0.153927000
H	5.171582000	3.354382000	2.286114000
H	4.632245000	3.481386000	-1.965955000
H	5.599425000	4.445329000	0.104772000
H	-1.158641000	-0.021104000	3.747730000
H	-0.858457000	1.462067000	2.830916000
H	1.487672000	0.806910000	2.995176000
H	1.086511000	-0.753859000	3.725646000
H	-0.317988000	-1.433980000	1.984946000
C	-0.549882000	-2.919127000	1.744505000
C	-0.183271000	-2.862376000	0.305529000
H	0.782914000	-3.317262000	0.075031000
H	0.204116000	-3.365211000	2.395552000
H	-0.932733000	-3.281400000	-0.371777000
C	-1.915239000	-3.247714000	2.087776000
H	-2.642789000	-3.093077000	1.285042000
C	-2.411670000	-3.668726000	3.269958000
H	-3.473147000	-3.850019000	3.401139000
H	-1.767062000	-3.853524000	4.126650000
H	-0.061874000	-1.787207000	-0.103739000

TS3_Ph

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.452432000	0.382719000	0.088970000
P	-2.500982000	-0.564561000	-0.266327000
O	-0.932963000	1.268340000	2.853184000
C	-0.739832000	0.894686000	1.778527000
N	0.004916000	-0.471499000	-1.725422000
C	-1.126166000	-0.810949000	-2.605526000
C	1.070197000	0.184729000	-2.503790000
C	2.295344000	0.420200000	-1.627663000
C	-2.208269000	-1.527944000	-1.804875000
H	3.023132000	1.075431000	-2.110039000
H	-1.834271000	-2.500759000	-1.474556000
H	2.791263000	-0.531440000	-1.422534000
P	1.724055000	1.066397000	-0.000127000
C	-1.013450000	1.952079000	-0.509843000
O	-1.376390000	2.962012000	-0.924431000
H	-3.113119000	-1.704276000	-2.390188000
C	2.971239000	0.483965000	1.202738000
C	4.333295000	0.684348000	0.966553000
C	2.570138000	-0.198641000	2.348600000
C	5.276868000	0.195733000	1.858107000
H	4.658974000	1.218383000	0.079730000
C	3.516564000	-0.683514000	3.246009000
H	1.516054000	-0.369095000	2.534656000
C	4.869344000	-0.490979000	2.998924000
H	6.332664000	0.348400000	1.663556000

H	3.194404000	-1.217287000	4.133080000
H	5.608246000	-0.874308000	3.694006000
C	2.012745000	2.873959000	-0.024150000
C	2.062357000	3.594072000	-1.216826000
C	2.087345000	3.561085000	1.189518000
C	2.202542000	4.977817000	-1.197018000
H	1.985308000	3.085467000	-2.171794000
C	2.228084000	4.941871000	1.207275000
H	2.043757000	3.016328000	2.127355000
C	2.288228000	5.653400000	0.013331000
H	2.242213000	5.526250000	-2.131678000
H	2.291623000	5.462828000	2.156149000
H	2.399754000	6.731937000	0.028040000
C	-3.272489000	-1.751265000	0.895048000
C	-4.456876000	-2.413334000	0.560196000
C	-2.674009000	-2.006558000	2.126864000
C	-5.023040000	-3.324056000	1.441027000
H	-4.943366000	-2.209761000	-0.388591000
C	-3.244949000	-2.914960000	3.012415000
H	-1.753400000	-1.501167000	2.394471000
C	-4.417076000	-3.575340000	2.669319000
H	-5.941101000	-3.835230000	1.173084000
H	-2.770821000	-3.104596000	3.968836000
H	-4.861608000	-4.285284000	3.358116000
C	-3.880614000	0.586364000	-0.613929000
C	-4.353559000	0.838633000	-1.899569000
C	-4.421083000	1.295392000	0.462460000
C	-5.359882000	1.778068000	-2.105775000
H	-3.941363000	0.313503000	-2.753673000
C	-5.426860000	2.227705000	0.255910000
H	-4.053053000	1.117483000	1.468506000
C	-5.899426000	2.470850000	-1.030651000
H	-5.720259000	1.966374000	-3.111113000
H	-5.840647000	2.768286000	1.099814000
H	-6.682168000	3.203581000	-1.192629000
H	1.353878000	-0.445306000	-3.357283000
H	0.689542000	1.131499000	-2.905714000
H	-1.522406000	0.103357000	-3.063481000
H	-0.781662000	-1.464595000	-3.418922000
H	0.449604000	-1.535601000	-1.444890000
C	0.425323000	-2.569921000	0.510109000
C	0.869328000	-2.902062000	-0.868646000
H	0.207866000	-3.586494000	-1.400183000
H	-0.526755000	-3.036073000	0.768240000
H	1.140965000	-2.803365000	1.305791000
C	2.272716000	-3.117696000	-1.171221000
C	3.327146000	-2.713094000	-0.325434000
C	2.656624000	-3.704290000	-2.400895000
C	4.660302000	-2.870005000	-0.689210000
H	3.106078000	-2.256973000	0.632562000
C	3.984154000	-3.858987000	-2.759000000
H	1.878729000	-4.038203000	-3.083182000
C	5.009207000	-3.438643000	-1.908240000
H	5.433490000	-2.538264000	-0.002413000
H	4.227440000	-4.316730000	-3.713522000
H	6.049458000	-3.561742000	-2.188416000
H	0.237600000	-1.446691000	0.675287000

TS3_C≡CH

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.092691000	0.118274000	0.021724000
P	2.335625000	-0.215541000	0.327248000
O	0.077218000	0.180212000	-2.919837000
C	0.088098000	0.128125000	-1.767530000
N	0.005571000	-0.189389000	2.055901000
C	1.257067000	-0.047632000	2.817064000
C	-1.092446000	0.490859000	2.761929000
C	-2.422599000	0.197505000	2.075611000
C	2.393219000	-0.752227000	2.083775000
H	-3.217724000	0.855768000	2.431436000
H	2.210350000	-1.830250000	2.070704000
H	-2.720385000	-0.834882000	2.277075000

P	-2.176941000	0.308994000	0.252440000
C	0.291982000	1.878053000	0.053361000
O	0.431542000	3.018881000	0.100657000
H	3.362472000	-0.590760000	2.559845000
C	-3.329214000	-0.927451000	-0.443158000
C	-4.660372000	-0.970163000	-0.021498000
C	-2.880878000	-1.850050000	-1.383862000
C	-5.523788000	-1.930659000	-0.526422000
H	-5.022758000	-0.251445000	0.706603000
C	-3.748783000	-2.809959000	-1.895344000
H	-1.848665000	-1.827207000	-1.713263000
C	-5.067394000	-2.853300000	-1.464462000
H	-6.553827000	-1.962472000	-0.188730000
H	-3.389608000	-3.527743000	-2.624325000
H	-5.742904000	-3.605949000	-1.856124000
C	-2.920053000	1.896059000	-0.277475000
C	-2.948487000	2.998076000	0.576869000
C	-3.377144000	2.040417000	-1.588840000
C	-3.441455000	4.219850000	0.133056000
H	-2.578952000	2.914981000	1.593394000
C	-3.868729000	3.261698000	-2.030609000
H	-3.358280000	1.194614000	-2.268570000
C	-3.904346000	4.353779000	-1.169896000
H	-3.459632000	5.068117000	0.808451000
H	-4.226429000	3.360052000	-3.049627000
H	-4.290020000	5.306326000	-1.516072000
C	3.307233000	-1.473673000	-0.581018000
C	4.652407000	-1.696379000	-0.273901000
C	2.703905000	-2.226675000	-1.585880000
C	5.375360000	-2.664968000	-0.955761000
H	5.140105000	-1.103271000	0.493497000
C	3.430187000	-3.194401000	-2.272483000
H	1.661193000	-2.062468000	-1.831025000
C	4.764254000	-3.414984000	-1.957149000
H	6.418773000	-2.831767000	-0.712139000
H	2.950990000	-3.773094000	-3.054172000
H	5.331418000	-4.168946000	-2.491912000
C	3.398750000	1.268922000	0.195247000
C	3.951007000	1.914760000	1.298893000
C	3.594473000	1.809437000	-1.078801000
C	4.695019000	3.079349000	1.131440000
H	3.804692000	1.523695000	2.299087000
C	4.340587000	2.966456000	-1.244694000
H	3.156155000	1.324979000	-1.946301000
C	4.892316000	3.605379000	-0.137791000
H	5.118449000	3.574415000	1.998436000
H	4.485175000	3.376722000	-2.237849000
H	5.467861000	4.515304000	-0.266434000
H	-1.142578000	0.143471000	3.802793000
H	-0.893822000	1.569324000	2.785713000
H	1.485165000	1.016619000	2.953939000
H	1.137286000	-0.489644000	3.816082000
H	-0.250040000	-1.354912000	2.143970000
C	-0.460353000	-2.865124000	1.979951000
C	-0.067674000	-2.890578000	0.532990000
H	0.964342000	-3.213321000	0.383621000
H	0.256045000	-3.351988000	2.642029000
H	-0.716034000	-3.492412000	-0.110264000
C	-1.808013000	-3.209511000	2.264062000
C	-2.983383000	-3.428084000	2.474810000
H	-4.008541000	-3.652787000	2.650338000
H	-0.121359000	-1.862179000	0.038629000

TS3_Ph-NO₂

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.959061000	0.371930000	0.127151000
P	-2.765459000	-0.967594000	-0.325603000
O	-1.861630000	1.269438000	2.781910000
C	-1.493083000	0.897933000	1.754403000
N	-0.182255000	-0.496372000	-1.555303000
C	-1.123077000	-1.122732000	-2.496360000
C	0.809069000	0.289165000	-2.308046000

C	1.878652000	0.838396000	-1.371510000
C	-2.149242000	-1.962833000	-1.743211000
H	2.510828000	1.581712000	-1.860444000
H	-1.663083000	-2.837875000	-1.303758000
H	2.530200000	0.030356000	-1.033815000
P	1.046914000	1.482752000	0.137925000
C	-1.760432000	1.774344000	-0.601145000
O	-2.269673000	2.674624000	-1.101829000
H	-2.947789000	-2.324505000	-2.394681000
C	2.281852000	1.275384000	1.469980000
C	3.591466000	1.728481000	1.294018000
C	1.936143000	0.626168000	2.652851000
C	4.543623000	1.517451000	2.280421000
H	3.872219000	2.240753000	0.379311000
C	2.889657000	0.420940000	3.645605000
H	0.924675000	0.264135000	2.797919000
C	4.193528000	0.860344000	3.457233000
H	5.561373000	1.859592000	2.129894000
H	2.613111000	-0.088754000	4.561834000
H	4.939916000	0.692519000	4.225766000
C	0.947513000	3.300845000	-0.040632000
C	1.060046000	3.935679000	-1.275577000
C	0.648738000	4.060562000	1.093180000
C	0.890377000	5.313086000	-1.374203000
H	1.273823000	3.366410000	-2.173347000
C	0.480752000	5.434110000	0.992799000
H	0.550118000	3.577863000	2.060534000
C	0.602134000	6.063674000	-0.242217000
H	0.982562000	5.797232000	-2.340019000
H	0.252150000	6.013617000	1.880335000
H	0.467696000	7.136654000	-0.321682000
C	-3.453178000	-2.195972000	0.843737000
C	-4.503590000	-3.032972000	0.456519000
C	-2.921466000	-2.317149000	2.125772000
C	-5.002867000	-3.982299000	1.336642000
H	-4.940998000	-2.934516000	-0.531964000
C	-3.424409000	-3.267265000	3.009074000
H	-2.107986000	-1.671750000	2.436853000
C	-4.462295000	-4.101044000	2.614346000
H	-5.816833000	-4.628963000	1.028254000
H	-3.002734000	-3.354206000	4.004094000
H	-4.854195000	-4.842025000	3.302357000
C	-4.267511000	-0.098801000	-0.904606000
C	-4.581387000	0.048107000	-2.254022000
C	-5.074943000	0.518287000	0.054562000
C	-5.691826000	0.793562000	-2.638912000
H	-3.965034000	-0.409303000	-3.019493000
C	-6.184272000	1.256514000	-0.330834000
H	-4.837937000	0.417300000	1.109332000
C	-6.494590000	1.396698000	-1.680332000
H	-5.924263000	0.904285000	-3.692315000
H	-6.805535000	1.727398000	0.422774000
H	-7.358739000	1.978144000	-1.981879000
H	1.288048000	-0.339495000	-3.071253000
H	0.301977000	1.108693000	-2.834267000
H	-1.622556000	-0.346580000	-3.090415000
H	-0.575215000	-1.765791000	-3.200225000
H	0.476044000	-1.499731000	-1.120445000
C	0.402866000	-2.438350000	0.862575000
C	1.048542000	-2.646897000	-0.479905000
H	0.623892000	-3.467530000	-1.059583000
H	-0.534901000	-2.989611000	0.942736000
H	1.022813000	-2.721514000	1.720785000
C	2.476625000	-2.544169000	-0.613012000
C	3.295674000	-1.912150000	0.354857000
C	3.127542000	-3.002900000	-1.789708000
C	4.645608000	-1.717018000	0.151951000
H	2.858370000	-1.549342000	1.276387000
C	4.470958000	-2.812620000	-2.002291000
H	2.537805000	-3.508844000	-2.548073000
C	5.235694000	-2.154707000	-1.031408000
H	5.248309000	-1.221270000	0.901768000
H	4.946217000	-3.163858000	-2.909108000
N	6.642057000	-1.934033000	-1.253657000
O	7.141735000	-2.349752000	-2.292322000
O	7.283639000	-1.334678000	-0.398561000
H	0.145806000	-1.360159000	1.055769000

TS3_CHO

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.020034000	0.172660000	-0.021271000
P	2.286937000	0.119349000	0.278952000
O	0.130624000	0.495896000	-2.945779000
C	0.080724000	0.340960000	-1.803950000
N	0.006463000	-0.355353000	1.947298000
C	1.142196000	0.091764000	2.767070000
C	-1.242292000	-0.185054000	2.703376000
C	-2.426997000	-0.674552000	1.877590000
C	2.461066000	-0.245634000	2.077741000
H	-3.386349000	-0.445094000	2.345760000
H	2.653346000	-1.317627000	2.154252000
H	-2.374153000	-1.760163000	1.760248000
P	-2.253449000	0.010122000	0.183386000
C	-0.024775000	1.933173000	0.156719000
O	-0.063163000	3.072187000	0.309749000
H	3.307379000	0.273991000	2.531199000
C	-3.281469000	-1.083270000	-0.865337000
C	-4.651981000	-1.216384000	-0.625740000
C	-2.698339000	-1.805347000	-1.904263000
C	-5.421101000	-2.064826000	-1.409347000
H	-5.122662000	-0.647596000	0.169889000
C	-3.470812000	-2.651295000	-2.693743000
H	-1.636352000	-1.710724000	-2.097961000
C	-4.830598000	-2.782652000	-2.446118000
H	-6.483374000	-2.164227000	-1.215765000
H	-3.007329000	-3.204528000	-3.502893000
H	-5.434188000	-3.440798000	-3.061335000
C	-3.185062000	1.583862000	0.139777000
C	-3.653343000	2.220802000	1.286666000
C	-3.357562000	2.200002000	-1.102676000
C	-4.296438000	3.451693000	1.191512000
H	-3.520360000	1.769534000	2.263355000
C	-4.003027000	3.423889000	-1.195950000
H	-2.985274000	1.719374000	-2.002515000
C	-4.474150000	4.052830000	-0.047029000
H	-4.657591000	3.939178000	2.090330000
H	-4.134388000	3.891211000	-2.165452000
H	-4.974330000	5.012119000	-0.119676000
C	3.342979000	-1.126310000	-0.544871000
C	4.683563000	-1.275956000	-0.177457000
C	2.812770000	-1.947059000	-1.537452000
C	5.473586000	-2.238414000	-0.788324000
H	5.112788000	-0.632794000	0.584326000
C	3.606585000	-2.910691000	-2.152504000
H	1.775548000	-1.836493000	-1.832045000
C	4.934755000	-3.058384000	-1.776771000
H	6.511889000	-2.350346000	-0.496443000
H	3.184290000	-3.545301000	-2.923612000
H	5.553777000	-3.810559000	-2.253261000
C	3.190513000	1.679662000	-0.030139000
C	3.299662000	2.659009000	0.956642000
C	3.691192000	1.939981000	-1.307521000
C	3.915920000	3.873285000	0.676264000
H	2.897133000	2.488116000	1.949393000
C	4.306457000	3.153266000	-1.585176000
H	3.609210000	1.190130000	-2.087749000
C	4.422535000	4.121407000	-0.593328000
H	3.995308000	4.627100000	1.451612000
H	4.697883000	3.341446000	-2.578755000
H	4.903748000	5.068462000	-0.810834000
H	-1.194520000	-0.756240000	3.641486000
H	-1.374762000	0.871432000	2.974029000
H	1.065888000	1.172594000	2.946899000
H	1.115648000	-0.402372000	3.748060000
H	0.145739000	-1.658088000	1.919859000
C	0.322128000	-3.012163000	1.653024000
C	-0.496019000	-3.694790000	2.609977000
O	-0.162691000	-4.095296000	3.722011000
C	-0.113511000	-2.987426000	0.217548000

H	-1.167034000	-3.260518000	0.100439000
H	-0.023513000	-1.963208000	-0.240062000
H	0.478914000	-3.627813000	-0.441856000
H	-1.564430000	-3.815633000	2.302924000
H	1.390625000	-3.160208000	1.816664000

References

- 1 L. C. Allen, D. A. Egolf, E. T. Knight and C. Liang, Bond Polarity Index, *J. Phys. Chem.*, 1990, **94**, 5602-5607.
- 2 T. Lu and F. Chen, Multiwfn: a multifunctional wavefunction analyzer, *J. Comput. Chem.*, 2012, **33**, 580-592.
- 3 E. D. Glendening and F. Weinhold, Natural Resonance Theory: I. General Formalism, *J. Comput. Chem.*, 1998, **19**, 593-609
- 4 K. H. Hopmann, Quantum chemical studies of asymmetric reactions: Historical aspects and recent examples, *Int. J. Quantum Chem.*, 2015, **115**, 1232-1249.