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Electronic Supplementary Information

For

The Theoretical Design of Manganese Catalysts with Si-N-Si-C-Si-C Six-membered Ring Core-based Bowl-shaped Quadridentate Ligand for the Hydrogenation of C=O/C=N Bonds

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1. The APT charge on the metal center Mn.

Table S1 The calculated Gibbs free energy barriers ($\Delta G1^{\square}_{DFT}$ in kcal/mol) and APT Charges of Mn of Mn(CO)-LYG where -PH_2/-$P(NH_2)_2$ is used as an axial/equatorial ligand.

Ligand	$\Delta G1^{\square}_{DFT}$ (kcal/mol)	APT Charge of Mn
LYG8 (NH_2 axial)	22.4	-1.910
LYG12 (NH_2 equatorial)	20.4	-1.836
LYG14 (H axial)	16.5	-2.004
LYG15 (H equatorial)	14.9	-1.837

2. The calculation method of Tolman angle.

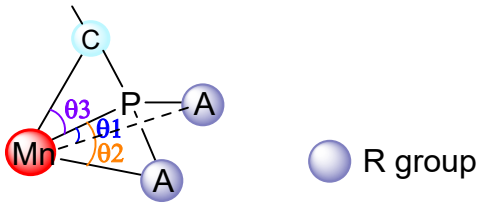

Fig. S1 The model to measure the Tolman angle.

A and C denote the atoms on the R group connected to the P atom and the atoms on the framework directly connected to the P atom, respectively. All atoms A on the connecting group of each P atom are checked, and the maximum angle of P-Mn-A on each substituent is found. The maximum angle of the two substituents and the P-Mn-C angle of the C atom directly connected to the P atom are recorded as three parameters of the cone angle, and the formula is used.

$$\theta = \frac{2}{3}\sum_{i}\frac{\theta_i}{2}$$

3. The multivariate linear relationship between $\Delta G2^{\ddagger}$ and electronic and steric descriptors.

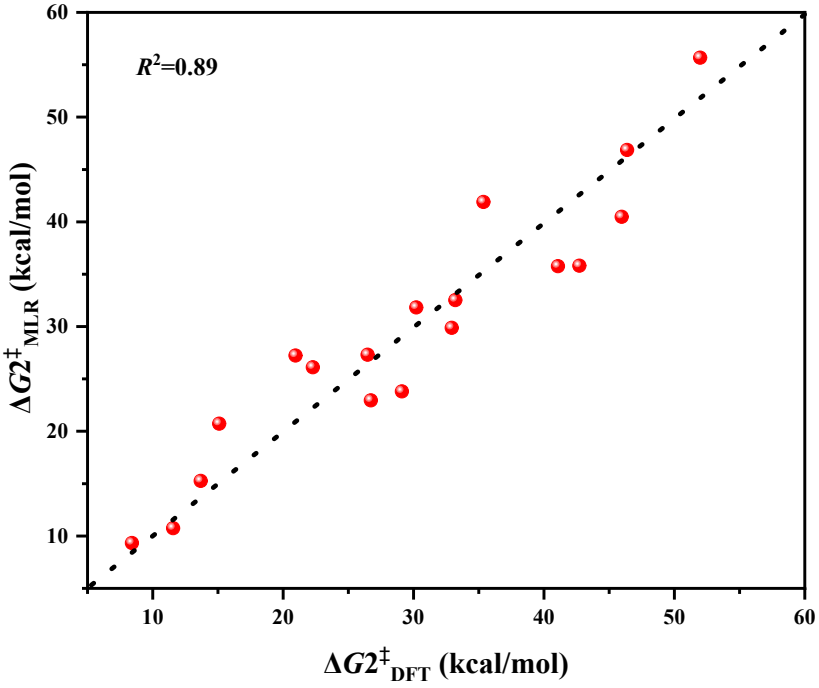

Fig. S2 The comparison between $\Delta G2^{\ddagger}_{DFT}$ and $\Delta G2^{\ddagger}_{MLR}$ ($\Delta G2^{\ddagger}_{DFT}$ denotes the calculated Gibbs free energy barrier for the reverse process of HT step using DFT, $\Delta G2^{\ddagger}_{MLR}$ denotes that predicted using the multivariate linear model of electronic and steric descriptors).

$\Delta G2^{\ddagger}_{MLR}$=-56.919$B_{Mn\text{-}H}$+22.369$A_{P2}$+58.821$A_{P1P3}-23.320C_{P1P3}$+1397.105$\varepsilon_{HOMO\text{-}LUMO}$-357.367
R^2=0.89, MAE=3.49, MSE=17.10.

4. The Gibbs free energy profiles of the acetone hydrogenation catalyzed by Mn(CO)-LYG18.

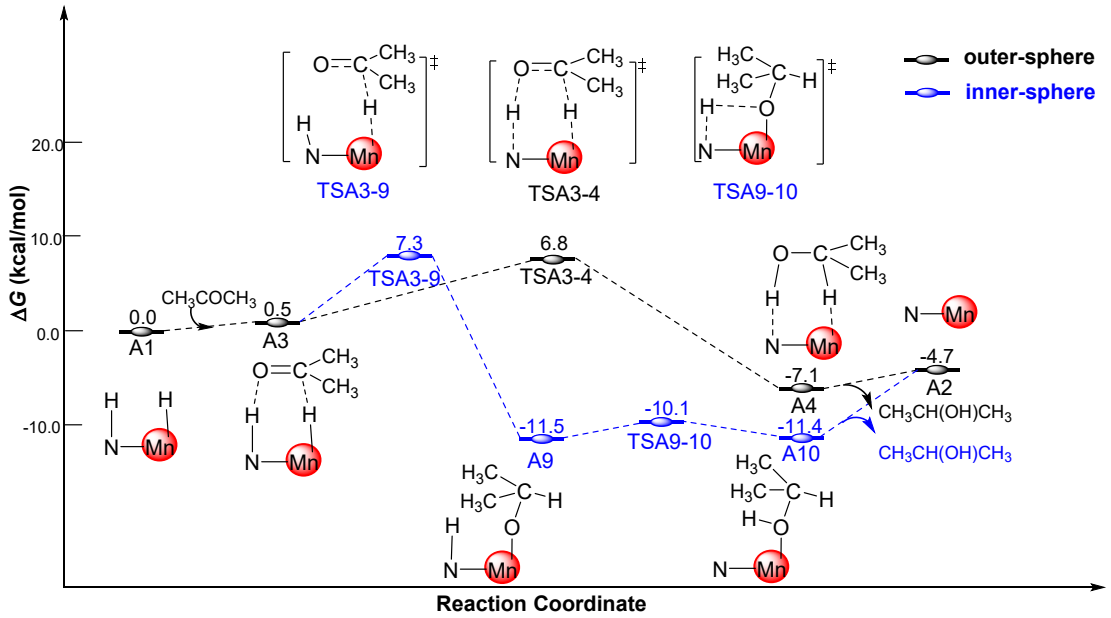

Fig. S3 The Gibbs free energy profiles of acetone hydrogenation catalyzed by Mn(CO)-LYG18 (unit: kcal/mol).

Besides, in the HT step, the outer-sphere mechanism of **A1→A3→A4→A2**+alcohol and the innersphere mechanism of **A1→A9→A10→A2**+alcohol are possibly involved. Fig. S3 shows the Gibbs free energy profiles of the acetone hydrogenation catalyzed by Mn(CO)-LYG18. In the outer-sphere mechanism, acetone coordinates with the Mn center of **A1** to form the intermediate **A3**. Subsequently, the hydride transfers from the Mn center to the C atom and the proton transfers from the N atom to the O atom via six-membered ring transition state **TSA3-4** with an energy barrier of 6.8 kcal/mol. **A2** is then generated with the removal of the propanol product. On the other hand, in the inner-sphere mechanism, the hydride is transferred to the C atom via transition state **TSA3-9**, with an energy barrier of 7.3 kcal/mol in this step, to generate the intermediate **A9**. **A9** then undergoes a proton transfer step via transition state **TSA9-10** to achieve the final propanol product. The energy barrier for this step is 1.4 kcal/mol. The calculation result indicates that the outer-sphere mechanism is more favorable than the inner-sphere mechanism for the HT step.

5. The asymmetric hydrogenation catalyzed by Mn(CO)-LYG complexes.

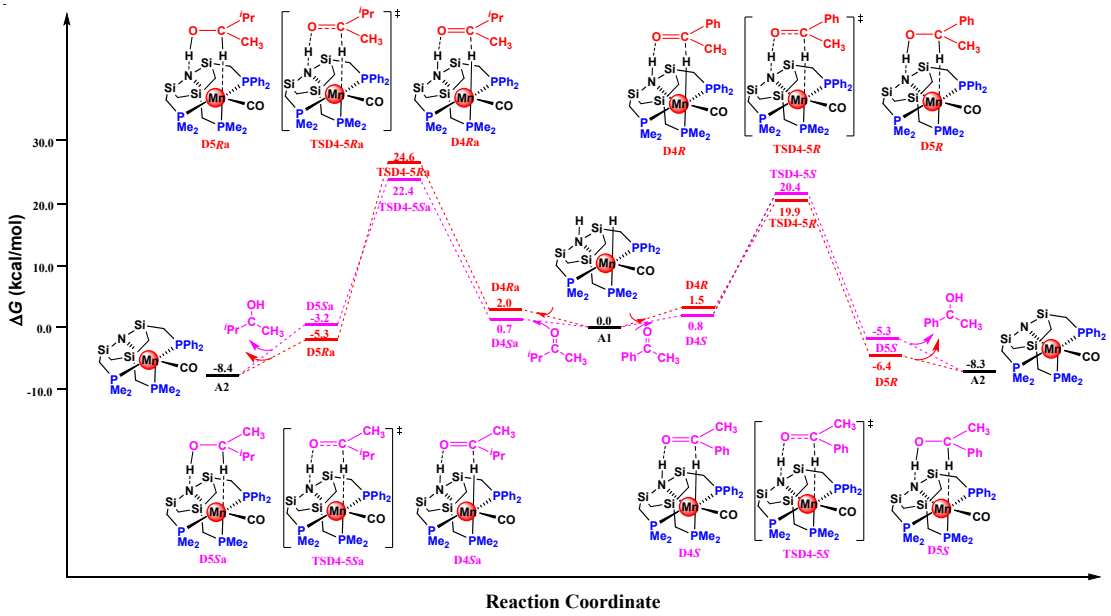

Fig. S4 The calculated Gibbs free energy profile (unit: kcal/mol) for the chirality-determining step (the HT step) of $PhCOCH_3$ and $^iPrCOCH_3$ hydrogenation catalyzed by Mn(CO)-LYG 19 complex.

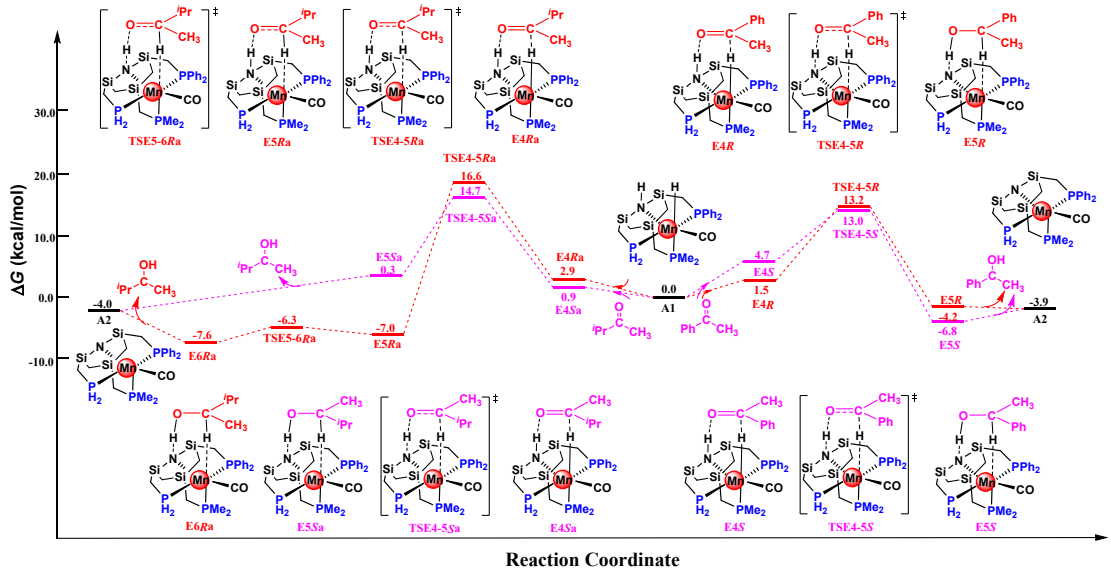

Fig. S5 The calculated Gibbs free energy profile (unit: kcal/mol) for the chirality-determining step (the HT step) of $PhCOCH_3$ and $^iPrCOCH_3$ hydrogenation catalyzed by Mn(CO)-LYG 20 complex.

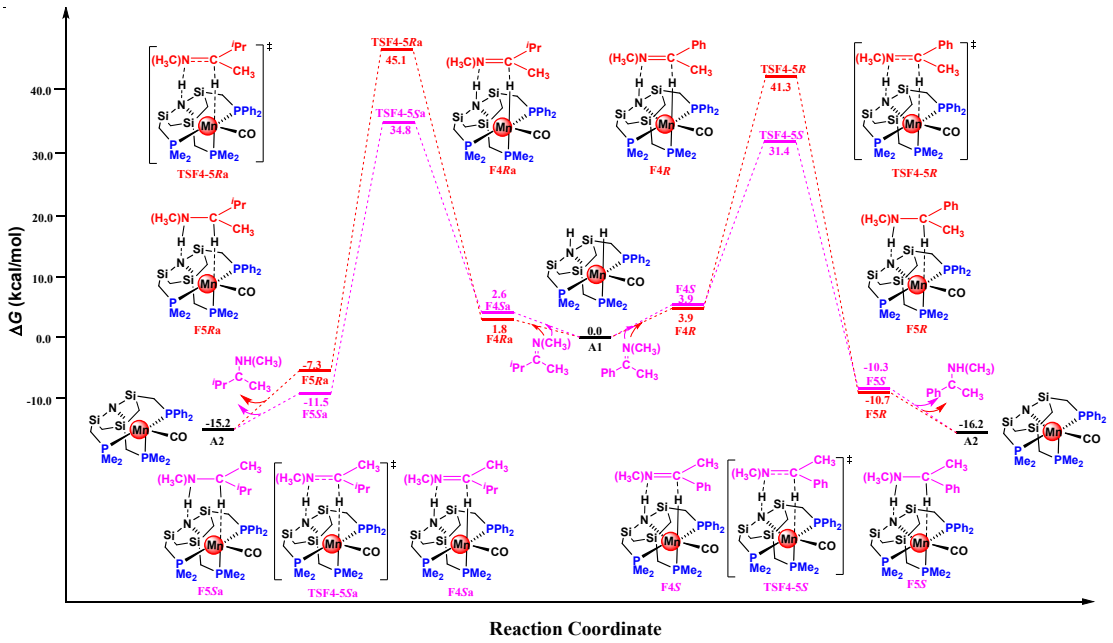

Fig. S6 The calculated Gibbs free energy profile (unit: kcal/mol) for the chirality-determining step (the HT step) of PhCMe=NMe and ^{i}PrCMe=NMe hydrogenation catalyzed by Mn(CO)-LYG 19 complex.

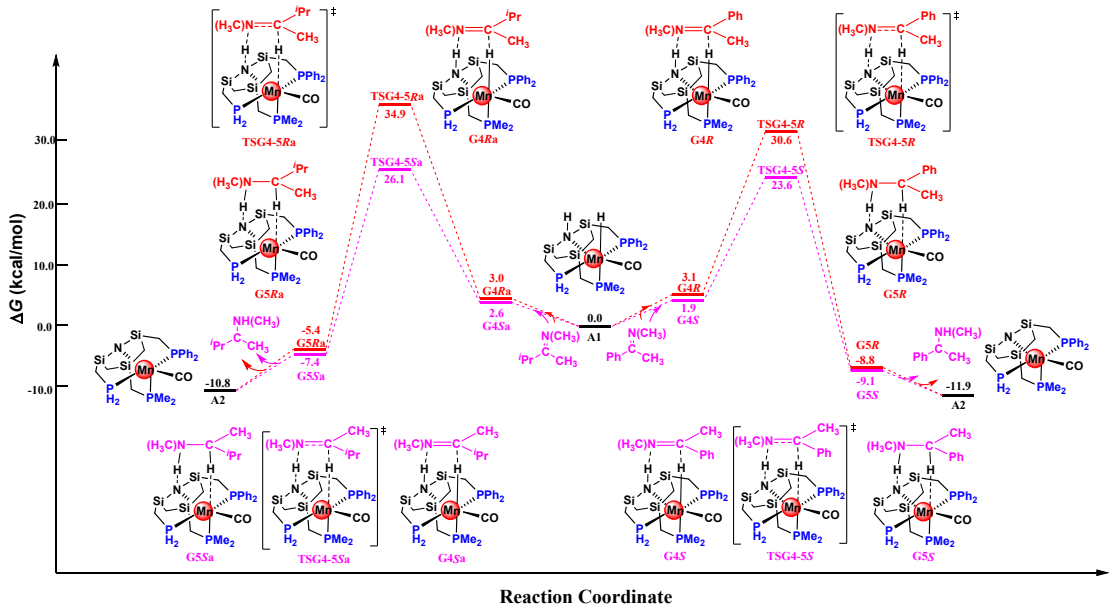

Fig. S7 The calculated Gibbs free energy profile (unit: kcal/mol) for the chirality-determining step (the HT step) of PhCMe=NMe and ^{i}PrCMe=NMe hydrogenation catalyzed by Mn(CO)-LYG 20 complex.

Table S2 The calculated Gibbs free energy barriers (unit: kcal/mol) for the chirality-determining step (the HT step) of the asymmetric hydrogenation catalyzed by Mn(CO)-LYG complexes and those of formic acid-assisted DA step.

	$PhCOCH_3$		$iPrCOCH_3$		PhCMe=NMe		^{i}PrCMe=NMe	
	HT	DA	HT	DA	HT	DA	HT	DA
Mn(CO)-LYG	20.4(S)	16.1	22.4(S)	16.1	31.4(S)	16.1	34.8(S)	16.1
19	19.9(R)		24.6(R)		41.3(R)		45.1(R)	
Mn(CO)-LYG	13.0(S)	19.7	14.7(S)	19.7	23.6(S)	19.7	26.1(S)	19.7
20	13.2(R)		16.6(R)		30.6(R)		34.9(R)	

Interestingly, the calculated Gibbs free energy barrier of the chiral rate-determining step (the HT step) of the asymmetric hydrogenation reaction catalyzed by Mn(CO)-LYG19 is higher than that catalyzed by Mn(CO)-LYG20, in contrast, the calculated Gibbs free energy barrier of the formic acid-assisted DA step is lower.

6. The theoretical ee value is calculated with the following formulas.

$$ee = \frac{R - S}{R + S}$$

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

7. The homo-lumo gap of the corresponding intermediate of AKH/AIH.

For AKHs/AIHs catalyzed by Mn(CO)-LYG19 and Mn(CO)-LYG20, the Homo-Lumo gap of the corresponding intermediate (before the chirality-determining step (the HT step) occurs) were calculated to explain the difference of the energy barriers in AKHs/AIHs as shown in Fig. S7. The lower the HOMO-LUMO gap is, the easier the chemical reaction occurs. We found that the homo-lumo gap of the corresponding intermediate of AKH is smaller than that of AIH, which verifies that the AKHs are easier to occur than the AIHs catalyzed by Mn(CO)-LYG complexes.

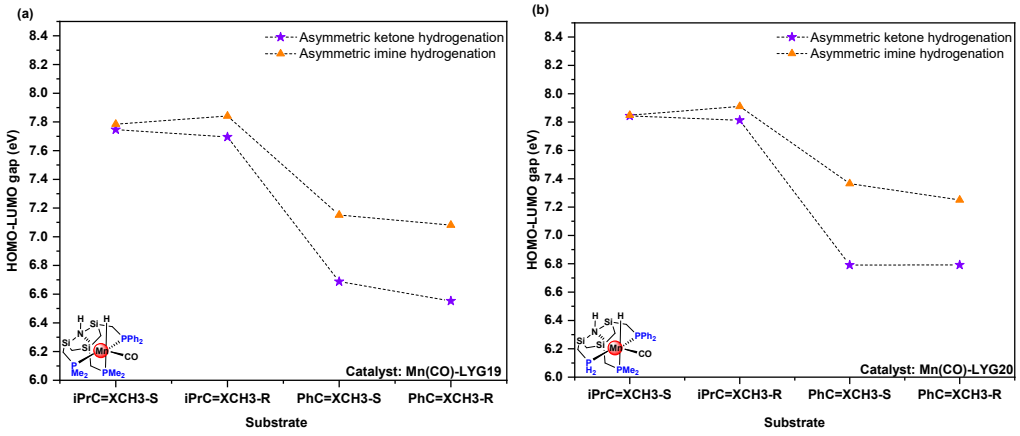

Fig. S8 The homo-lumo gap of the corresponding intermediate of AKH/AIH catalyzed by (a) Mn(CO)-LYG19 (b)Mn(CO)-LYG20.

8. The energy decomposition analysis (EDA).

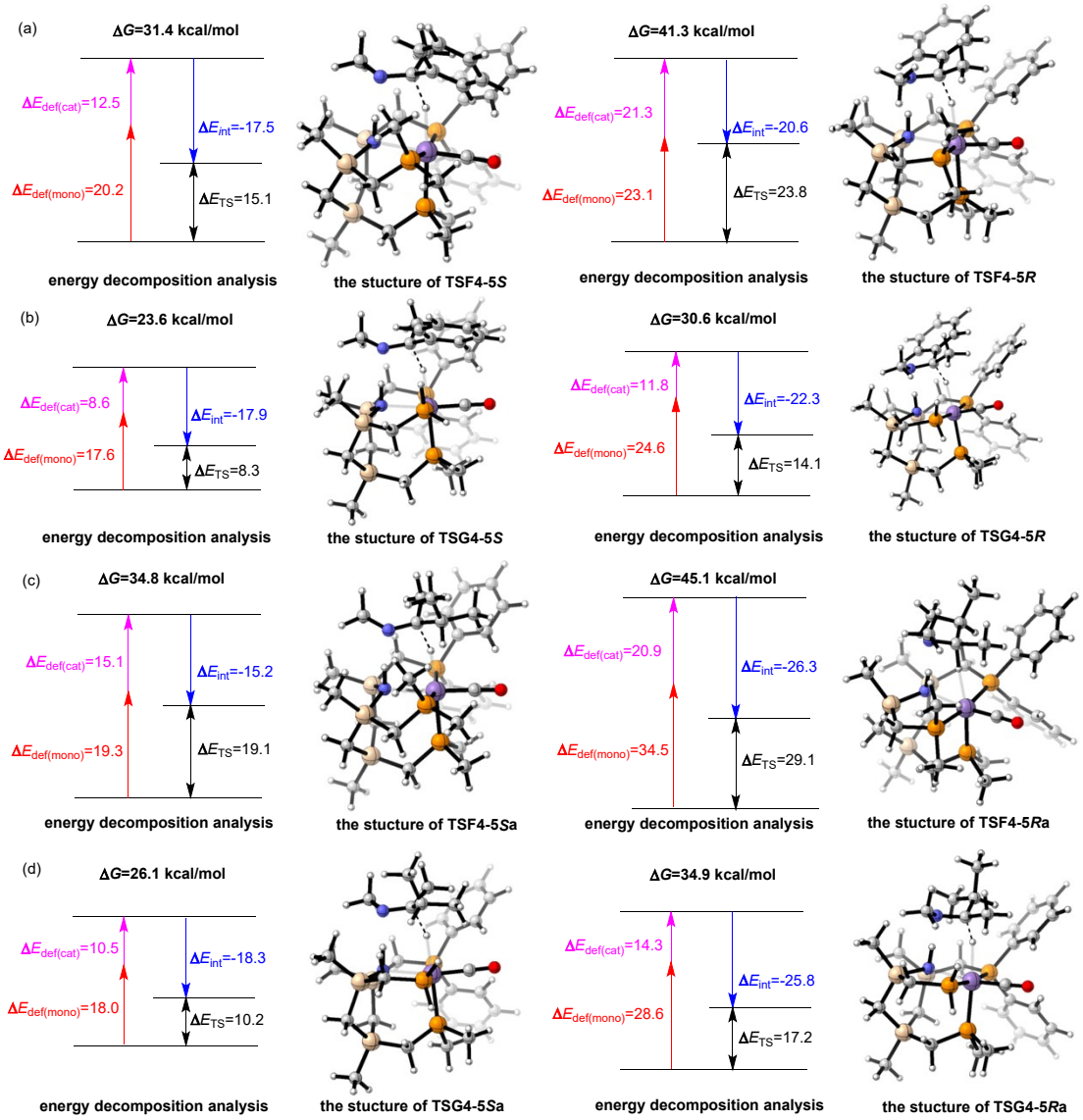

Fig. S9 EDA analysis (unit: kcal/mol) of transition states (a) **TSF4-5*S*** & **TSF4-5*R***, (b) **TSG4-5*S*** & **TSG4-5*R***, (c) **TSF4-5*S*a** & **TSF4-5*R*a**, and (d) **TSFG-5*S*a** & **TSG4-5*R*a** in AIHs catalyzed by Mn(CO)-LYG19 and Mn(CO)-LYG20.

For AIHs catalyzed by Mn(CO)-LYG19 and Mn(CO)-LYG20, the EDA analysis were performed to investigate the nature of the diversity of entioselectivity as shown in Fig. S9 above. For AH of PhCMe=NMe catalyzed by Mn(CO)-LYG19 complex, although the interaction (ΔE_{int}) of **TSF4-5*R*** is higher than that of **TSF4-5*S*** by 3.1 kcal/mol, the total deformation energy of the **TSF4-5*S*** is lower than that of **TSF4-5*R*** (32.7 vs 34.4 kcal/mol). This results **TSF4-5*S*** (ΔE_{TS}=15.1 kcal/mol) being more likely to occur than **TSF4-5*R*** (ΔE_{TS}=23.8 kcal/mol). For AH of PhCMe=NMe catalyzed by Mn(CO)-LYG20, although the interaction (ΔE_{int}) of **TSG4-5*R*** is higher than that of **TSG4-5*S*** by 4.4 kcal/mol, the total deformation energy of the **TSG4-5*S*** is lower than that of **TSG4-5*R*** (26.2 vs 36.4 kcal/mol). This results **TSG4-5*S*** (ΔE_{TS}=8.3 kcal/mol) being more likely to occur than **TSG4-5*R*** (ΔE_{TS}=14.1 kcal/mol). For AH of ^{i}PrCMe=NMe catalyzed by Mn(CO)-LYG19, although the interaction (ΔE_{int}) of **TSF4-5*R*a** is higher than that of **TSF4-5*S*a** by 11.1 kcal/mol, the

total deformation energy of the **TSF4-5*S*a** is lower than that of **TSF4-5*R*a** (34.4 vs 55.4 kcal/mol). This results **TSF4-5*S*a** (ΔE_{TS}=19.1 kcal/mol) being more likely to occur than **TSF4-5*R*a** (ΔE_{TS}=29.1 kcal/mol). For AH of ^{i}PrCMe=NMe catalyzed by Mn(CO)-LYG20 complex, although the interaction (ΔE_{int}) of **TSG4-5*R*a** is higher than that of **TSG4-5*S*a** by 7.5 kcal/mol, the total deformation energy of the **TSG4-5*S*a** is lower than that of **TSG4-5*R*a** (28.5 vs 42.9 kcal/mol). This results **TSG4-5*S*a** (ΔE_{TS}=10.2 kcal/mol) being more likely to occur than **TSG4-5*R*a** (ΔE_{TS}=17.2 kcal/mol).

9. The calculated Gibbs free energy profiles for the DA step of eighteen Mn(CO)-LYG complexes.

Table S3 The calculated Gibbs free energy barriers (unit: kcal/mol) for the forward and reverse HT step of the acetone hydrogenation catalyzed by Mn(CO)-LYG complexes and those of DA step. (Calculated at 298.15 K and 1 atm and Single point calculations at ωB97X-D/SDD&6-311++G** level)

entry	Ligand	R^1	R^2	R^3	$\Delta G1^{\ddagger}$(HT)	$\Delta G2^{\ddagger}$(reverse)	ΔG (DA)
1	LYG1	NMeiPr	NMeiPr	NMeiPr	40.5	52.0	6.3
2	LYG2	CF_3	CF_3	CF_3	43.0	42.7	20.1
3	LYG3	CHF_2	CHF_2	CHF_2	36.4	30.2	23.8
4	LYG4	Ph	Ph	Ph	32.0	41.1	16.7
5	LYG5	iPr	iPr	iPr	29.9	46.4	21.5
6	LYG6	Cy	Cy	Cy	29.9	46.0	13.8
7	LYG7	CH_2F	CH_2F	CH_2F	26.7	26.7	17.1
8	LYG8	Ph	NH_2	Ph	22.4	33.2	15.1
9	LYG9	NMe_2	NMe_2	NMe_2	21.3	35.4	18.3
10	LYG10	OMe	OMe	OMe	21.1	13.7	17.6
11	LYG11	Me	Me	Me	20.4	29.1	15.7
12	LYG12	NH_2	Ph	Ph	20.4	26.5	19.6
13	LYG13	Et	Et	Et	18.4	32.9	17.0
14	LYG14	Ph	H	Ph	16.5	22.3	18.0
15	LYG15	H	Ph	Ph	14.9	20.9	19.8
16	LYG16	F	F	F	15.9	8.4	21.2
17	LYG17	NH_2	NH_2	NH_2	13.2	15.1	19.4
18	LYG18	H	H	H	6.8	11.6	21.5

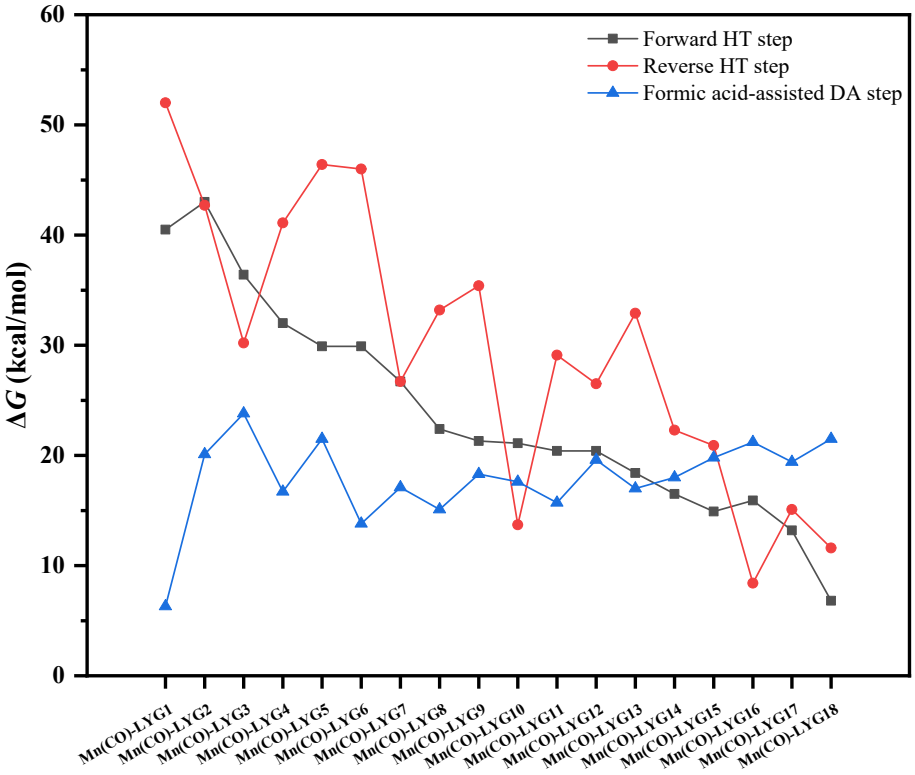

Fig. S10 The calculated barriers of forward and reverse HT, and formic acid-assisted DA steps.

The calculated Gibbs free energy barrier of HT step of the acetone hydrogenation catalyzed by Mn(CO)-LYG complexes and those of formic acid-assisted DA step showed the opposite changing trend.

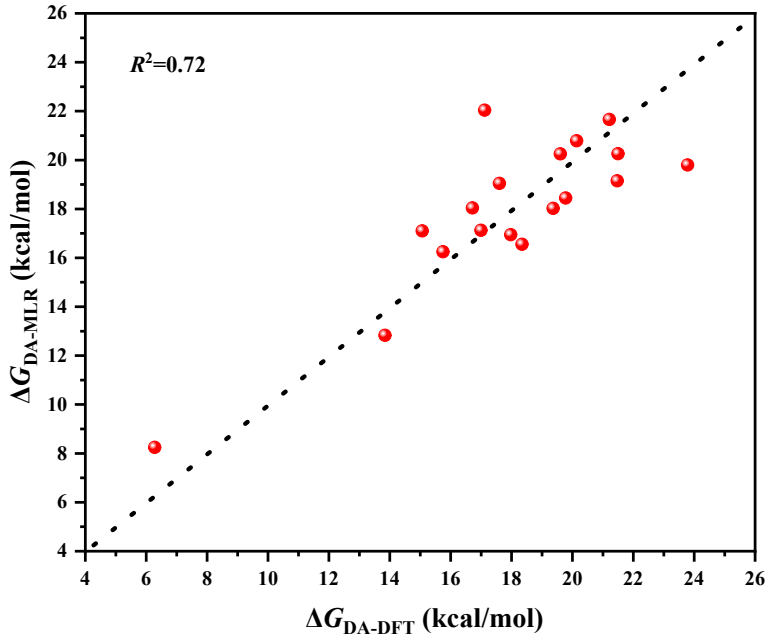

Fig. S11 The comparison between ΔG_{DA-DFT} and ΔG_{DA-MLR} (ΔG_{DA-DFT} denotes the calculated Gibbs free energy barrier for the formic-acid assisted DA step using DFT, ΔG_{DA-DFT} denotes that predicted using the multivariate linear model of electronic and steric descriptors.

ΔG_{DA-DFT}=4.184A_{P2}-7.019A_{P1P3}-9.148C_{P1P3}+178.775B_{N-H}-4.566ΔB_{Mn-N}-98.196

R^2=0.72, MAE=1.56, MSE=3.84.

B_{N-H} denote the Mayer bond order of the N-H[2] bond, ΔB_{Mn-N} denote the difference between **A2**_B_{Mn-N} and **A1**_B_{Mn-N}, which reflect the structure change in the formic acid-assisted DA step.

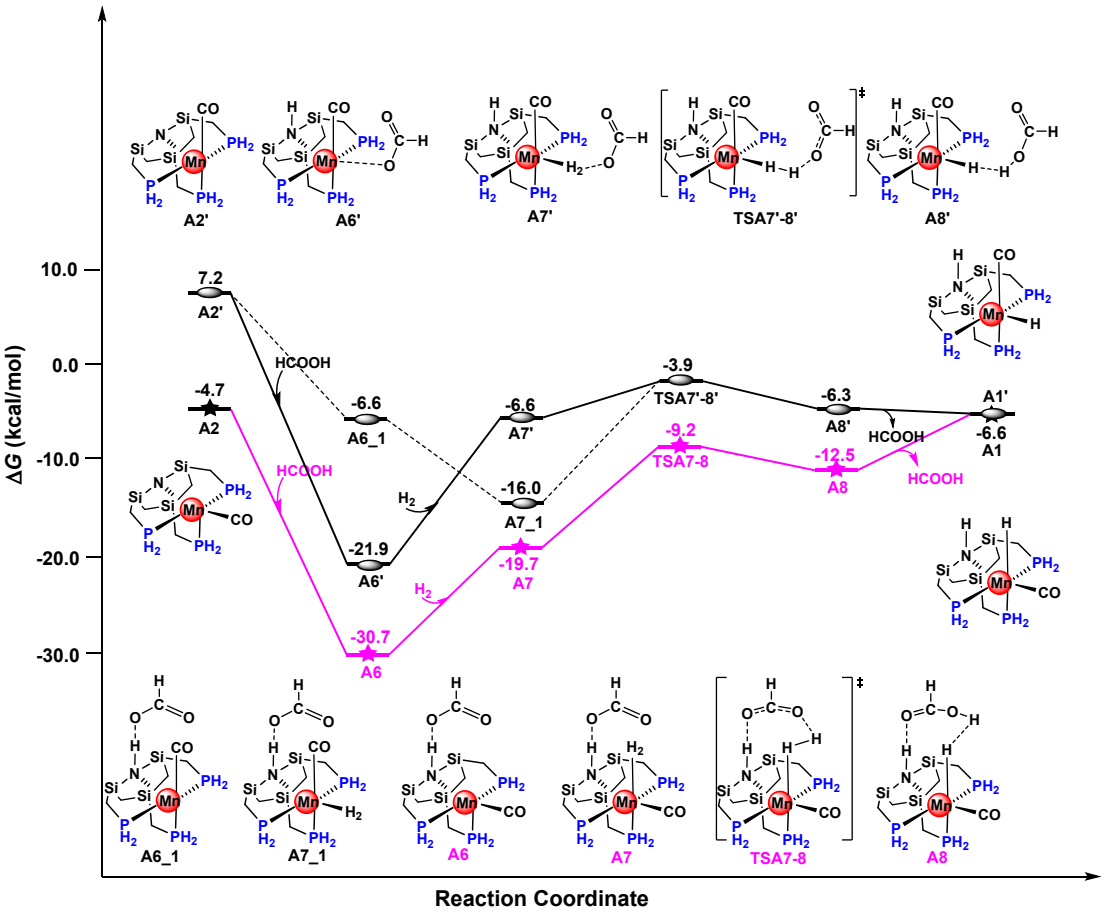

Fig. S12 The calculated Gibbs free energy profiles (unit: kcal/mol) for the DA step of the acetone hydrogenation catalyzed by Mn(CO)-LYG18 (R^1=R^2=R^3=H) in the case of the six coordinate complex with CO cis to nitrogen and H_2 trans to nitrogen.

Besides, we have also considered the case of intermediate with six coordination with CO cis to nitrogen and H_2 trans to nitrogen (**A7'**), the calculated results show that the energy of transtion state **TSA7'-8'** along pathways (**A2'**+HCOOH→**A6'**→**A7'**→**TSA7'-8'**→**A8'**, or **A2'**+HCOOH→**A6_1**→**A7_1**→**TSA7'-8'**→**A8'**) is 5.3 kcal/mol higher than that along the formate-assisted dihydrogen activation pathway (**A2**+HCOOH→**A6**→**A7**→**TSA7-8**→**A8**). Therefore, it is not likely happen compared to the formate-assisted dihydrogen activation pathway in thermodynamics and kinetics.

10. Energies of all the structures.

Table S4 The calculated absolute electronic energies (*E*, in a.u.), thermal free energies (*G*corr, in a.u.), and relative Gibbs energies (Δ*G*, in kcal/mol) (Calculated at 298.15 K and 1 atm and at ωB97X-D/6-31G* level).

In Toluene solvent (6-31G*)

Complex	*E*	*G*corr	*G*	Δ*G*1	Δ*G*2
NMeiPr_A1	-3760.845407	1.062412	-3759.782995	0	10.3
CH3COCH3	-193.097845	0.057767	-193.040078	/	/
A3	-3953.949088	1.143143	-3952.805945	10.7	21
TSA3-4	-3953.898878	1.146311	-3952.752567	44.2	54.5
A4	-3953.97775	1.149517	-3952.828233	-3.2	7
$CH_3CH(OH)CH_3$	-194.299027	0.082193	-194.216834	/	/
A2	-3759.670708	1.04813	-3758.622578	-10.3	0
CF3_A1	-4507.231181	0.313408	-4506.917772	0	-1.1
A3	-4700.340626	0.391723	-4699.948903	5.6	4.5
TSA3-4	-4700.288461	0.39775	-4699.890711	42.1	41.1
A4	-4700.337626	0.396867	-4699.940759	10.7	9.7
A2	-4506.028991	0.289682	-4505.739309	1.1	0
CHF2_A1	-3911.888652	0.364531	-3911.524121	0	-7.6
A3	-4104.999166	0.441359	-4104.557808	4	-3.6
TSA3-4	-4104.958348	0.450112	-4104.508236	35.1	27.5
A4	-4104.990991	0.4509	-4104.540091	15.1	7.5
A2	-3910.682725	0.3475	-3910.335225	7.6	0
Ph_A1	-3871.454128	0.766418	-3870.687709	0	7.8
A3	-4064.567556	0.846142	-4063.721415	4	11.8
TSA3-4	-4064.525799	0.851774	-4063.674025	33.7	41.5
A4	-4064.586541	0.854918	-4063.731623	-2.4	5.4
A2	-3870.271184	0.747869	-3869.523315	-7.8	0
iPr_A1	-3193.02798	0.800517	-3192.227463	0	14.5
A3	-3386.133359	0.880793	-3385.252567	9.4	23.9
TSA3-4	-3386.097466	0.881486	-3385.21598	32.4	46.9
A4	-3386.132921	0.885551	-3385.247371	12.7	27.2
A2	-3191.854755	0.780944	-3191.073811	-14.5	0
Cy_A1	-3893.311096	1.189965	-3892.12113	0	14.2
A3	-4086.42368	1.273525	-4085.150155	6.9	21.2
TSA3-4	-4086.389489	1.278388	-4085.111102	31.4	45.7
A4	-4086.449923	1.280749	-4085.169174	-5	9.2
A2	-3892.136421	1.169353	-3890.967068	-14.2	0
CH2F_A1	-3316.602331	0.416659	-3316.185672	0	-2.7
A3	-3509.718496	0.497533	-3509.220963	3	0.3
TSA3-4	-3509.684504	0.501904	-3509.182601	27.1	24.4
A4	-3509.719041	0.502051	-3509.21699	5.5	2.8
A2	-3315.401286	0.396628	-3315.004658	2.7	0
PhNH2Ph_A1	-3520.199595	0.644038	-3519.555558	0	9.4
A3	-3713.318088	0.72528	-3712.592807	1.8	11.1

TSA3-4	-3713.284317	0.727407	-3712.55691	24.3	33.7
A4	-3713.331791	0.729523	-3712.602268	-4.2	5.2
A2	-3519.013955	0.620219	-3518.393736	-9.4	0
NMe2_A1	-3289.194782	0.729355	-3288.465427	0	11.7
A3	-3482.303061	0.80521	-3481.497851	4.8	16.5
TSA3-4	-3482.282719	0.814118	-3481.468601	23.2	34.9
A4	-3482.340488	0.819276	-3481.521211	-9.9	1.9
A2	-3288.018864	0.711506	-3287.307358	-11.7	0
OMe_A1	-3172.641314	0.492989	-3172.148324	0	-9.6
A3	-3365.745351	0.568087	-3365.177263	7	-2.6
TSA3-4	-3365.729191	0.576363	-3365.152828	22.3	12.7
A4	-3365.759175	0.574556	-3365.184619	2.4	-7.3
A2	-3171.428959	0.472748	-3170.956211	9.6	0
Me_A1	-2721.419406	0.463811	-2720.955594	0	6.4
A3	-2914.535963	0.544617	-2913.991346	5.8	12.2
TSA3-4	-2914.511303	0.550627	-2913.960676	22	28.4
A4	-2914.551923	0.55074	-2914.001183	-3.1	3.3
A2	-2720.233669	0.444606	-2719.789062	-6.4	0
NH2PhPh_A1	-3520.196477	0.646427	-3519.55005	0	4.4
A3	-3713.307321	0.725357	-3712.581964	5.1	9.5
TSA3-4	-3713.285051	0.728708	-3712.556343	21.2	25.6
A4	-3713.327753	0.731438	-3712.596315	-3.9	0.5
A2	-3519.005904	0.625562	-3518.380342	-4.4	0
Et_A1	-2957.223304	0.633117	-2956.590186	0	12.3
A3	-3150.340394	0.714861	-3149.625532	3	15.3
TSA3-4	-3150.316829	0.718791	-3149.598038	20.2	32.5
A4	-3150.363843	0.717221	-3149.646622	-10.3	2
A2	-2956.044104	0.611086	-2955.433018	-12.3	0
PhHPh_A1	-3409.487351	0.609329	-3408.878022	0	4.2
A3	-3602.607515	0.689286	-3601.918228	-0.1	4.1
TSA3-4	-3602.583913	0.694479	-3601.889435	18	22.1
A4	-3602.619766	0.697396	-3601.92237	-2.7	1.5
A2	-3408.296453	0.588556	-3407.707898	-4.2	0
HPhPh_A1	-3409.480962	0.610742	-3408.870221	0	3.9
A3	-3602.59493	0.69256	-3601.90237	5	8.9
TSA3-4	-3602.577505	0.694034	-3601.883472	16.8	20.7
A4	-3602.608274	0.697477	-3601.910797	-0.3	3.6
A2	-3408.290773	0.591095	-3407.699677	-3.9	0
F_A1	-3081.06575	0.258641	-3080.80711	0	-8.4
A3	-3274.182067	0.336263	-3273.845804	0.9	-7.5
TSA3-4	-3274.163553	0.338455	-3273.825099	13.9	5.5
A4	-3274.17739	0.339913	-3273.837477	6.1	-2.3
A2	-3079.852015	0.23506	-3079.616955	8.4	0
NH2_A1	-2817.690314	0.403635	-2817.28668	0	-1

A3	-3010.803377	0.484643	-3010.318734	5	4
TSA3-4	-3010.793537	0.488004	-3010.305533	13.3	12.3
A4	-3010.81477	0.489657	-3010.325113	1	0
A2	-2816.490872	0.382536	-2816.108336	1	0
H_A1	-2485.537681	0.29919	-2485.238491	0	2
A3	-2678.65314	0.377346	-2678.275793	1.9	3.9
TSA3-4	-2678.645308	0.379377	-2678.265931	7.9	9.9
A4	-2678.667336	0.382115	-2678.285221	-3.3	-1.4
A2	-2484.342961	0.278109	-2484.064852	-2	0

Complex	*E*	*G*corr	*G*	Δ*G*
MeMePh_A1	-3104.767219	0.565451	-3104.201769	0
PhCOCH3	-384.776924	0.10752	-384.669404	/
D4S	-3489.560704	0.692985	-3488.867719	2.2
TSD4-5S	-3489.536768	0.699915	-3488.836854	21.5
D5S	-3489.577402	0.701877	-3488.875525	-2.7
PhCH(OH)CH3	-385.974821	0.130499	-385.844322	/
A2	-3103.580005	0.543742	-3103.036263	-5.9
D4R	-3489.564103	0.697211	-3488.866893	2.7
TSD4-5R	-3489.539375	0.701433	-3488.837942	20.9
D5R	-3489.579903	0.702183	-3488.87772	-4.1
iPrCOCH3	-271.706249	0.111687	-271.594562	/
D4Sa	-3376.493034	0.699115	-3375.793919	1.5
TSD4-5Sa	-3376.464982	0.705239	-3375.759743	23
D5Sa	-3376.49921	0.70304	-3375.79617	0.1
iPrCH(OH)CH3	-272.906547	0.136176	-272.770371	/
D4Ra	-3376.49329	0.700995	-3375.792295	2.5
TSD4-5Ra	-3376.460946	0.704696	-3375.75625	25.2
D5Ra	-3376.507792	0.706106	-3375.801686	-3.4
A2’	-3103.580005	0.543742	-3103.036263	-6.5
HMePh_A1	-3026.139566	0.508257	-3025.631309	0
E4S	-3410.932545	0.641918	-3410.290627	6.3
TSE4-5S	-3410.919389	0.641939	-3410.27745	14.6
E5S	-3410.950989	0.643804	-3410.307185	-4.1
A2	-3024.947683	0.489101	-3024.458582	-1.4
E4R	-3410.937074	0.640906	-3410.296168	2.9
TSE4-5R	-3410.921003	0.643742	-3410.277261	14.7
E5R	-3410.948479	0.64545	-3410.303029	-1.5
E4Sa	-3297.864836	0.642144	-3297.222691	2
TSE4-5Sa	-3297.847778	0.647513	-3297.200265	16.1
E5Sa	-3297.86863	0.648747	-3297.219883	3.8
E4Ra	-3297.864535	0.644252	-3297.220283	3.5
TSE4-5Ra	-3297.845824	0.648428	-3297.197397	17.9
E5Ra	-3297.888309	0.651502	-3297.236808	-6.9

TSE5-6Ra	-3297.881429	0.647336	-3297.234094	-5.2
E6Ra	-3297.885718	0.649411	-3297.236307	-6.5
A2’	-3024.947683	0.489101	-3024.458582	-1.9
MeMePh_A1	-3104.767219	0.565451	-3104.201769	0
$PhC=N(CH_3)CH_3$	-404.194006	0.145135	-404.048871	/
F4S	-3508.974455	0.733631	-3508.240824	6.2
TSF4-5S	-3508.938524	0.739583	-3508.198941	32.4
F5S	-3509.005876	0.741098	-3508.264778	-8.9
$PhCHN(CH_3)HCH_3$	-405.410387	0.170468	-405.239919	/
A2	-3103.580005	0.543742	-3103.036263	-16.0
F4R	-3508.978611	0.737309	-3508.241302	5.9
TSF4-5R	-3508.923451	0.741470	-3508.181981	43.1
F5R	-3509.005692	0.740408	-3508.265284	-9.2
$iPrC=N(CH_3)CH_3$	-291.125575	0.150673	-290.974902	/
F4Sa	-3395.909205	0.739998	-3395.169208	4.7
TSF4-5Sa	-3395.864304	0.744115	-3395.120190	35.4
F5Sa	-3395.935212	0.742790	-3395.192422	-9.9
$iPrCHN(CH_3)HCH_3$	-292.340192	0.175675	-292.164517	/
F4Ra	-3395.911321	0.740580	-3395.170741	3.7
TSF4-5Ra	-3395.846474	0.744670	-3395.101804	47.0
F5Ra	-3395.934465	0.747471	-3395.186994	-6.5
A2’	-3103.580005	0.543742	-3103.036263	-15.1
HMePh_A1	-3026.139566	0.508257	-3025.631309	0
G4S	-3430.351337	0.677976	-3429.673361	4.3
TSG4-5S	-3430.321194	0.680780	-3429.640415	25.0
G5S	-3430.376172	0.684522	-3429.691650	-7.2
A2	-3024.947683	0.489101	-3024.458582	-11.5
G4R	-3430.355411	0.683145	-3429.672266	5.0
TSG4-5R	-3430.310865	0.682777	-3429.628088	32.7
G5R	-3430.378044	0.686358	-3429.691686	-7.2
G4Sa	-3317.283751	0.684572	-3316.599179	4.4
TSG4-5Sa	-3317.250777	0.687393	-3316.563384	26.9
G5Sa	-3317.305073	0.690295	-3316.614777	-5.4
G4Ra	-3317.282124	0.683346	-3316.598778	4.7
TSG4-5Ra	-3317.238212	0.690275	-3316.547937	36.6
G5Ra	-3317.305377	0.692001	-3316.613376	-4.5
A2’	-3024.947683	0.489101	-3024.458582	-10.6
NMeiPr_A2	-3759.670708	1.04813	-3758.622578	-10.3
H2	-1.171362	-0.001319	-1.172681	/
A5	-3760.84501	1.057838	-3759.787172	-5.2
TSA5-1	-3760.833727	1.05747	-3759.776258	1.7
A1	-3760.845407	1.062412	-3759.782995	-2.6
HCOOH	-189.699553	0.010444	-189.689109	/

A6	-3949.394906	1.076243	-3948.318664	-14.6
A7	-3950.580813	1.094739	-3949.486074	-11.3
TSA7-8	-3950.57414	1.09173	-3949.48241	-9
A8	-3950.576076	1.09451	-3949.481566	-8.5
CF3_A2	-4506.028991	0.289682	-4505.739309	1.1
A5	-4507.198573	0.307693	-4506.89088	14.3
TSA5-1	-4507.183504	0.307316	-4506.876188	23.5
A1	-4507.231181	0.313408	-4506.917772	-2.6
A6	-4695.775577	0.327885	-4695.447692	-11
A7	-4696.921396	0.341824	-4696.579572	14.6
TSA7-8	-4696.920991	0.339894	-4696.581097	13.6
A8	-4696.949372	0.343375	-4696.605997	-2
CHF2_A2	-3910.682725	0.3475	-3910.335225	7.6
A5	-3911.855988	0.361185	-3911.494804	15.8
TSA5-1	-3911.837986	0.361696	-3911.476289	27.5
A1	-3911.888652	0.364531	-3911.524121	-2.6
A6	-4100.445787	0.381052	-4100.064736	-17.7
A7	-4101.59014	0.395675	-4101.194465	9.2
TSA7-8	-4101.587517	0.394284	-4101.193232	10
A8	-4101.607608	0.398573	-4101.209035	0.1
Ph_A2	-3870.271184	0.747869	-3869.523315	-7.8
A5	-3871.439578	0.765251	-3870.674327	5.8
TSA5-1	-3871.42426	0.763302	-3870.660959	14.2
A1	-3871.454128	0.766418	-3870.687709	-2.6
A6	-4060.016489	0.783132	-4059.233358	-20.9
A7	-4061.174928	0.800091	-4060.374837	-1.3
TSA7-8	-4061.170058	0.796366	-4060.373691	-0.6
A8	-4061.180046	0.79768	-4060.382366	-6
iPr_A2	-3191.854755	0.780944	-3191.073811	-14.5
A5	-3193.02331	0.798574	-3192.224736	-0.8
TSA5-1	-3193.006952	0.797313	-3192.209639	8.6
A1	-3193.02798	0.800517	-3192.227463	-2.6
A6	-3381.597098	0.81352	-3380.783579	-27.5
A7	-3382.764556	0.835131	-3381.929425	-10.6
TSA7-8	-3382.744972	0.82865	-3381.916322	-2.4
A8	-3382.74875	0.8306	-3381.91815	-3.5
Cy_A2	-3892.136421	1.169353	-3890.967068	-14.2
A5	-3893.305872	1.189244	-3892.116628	0.3
TSA5-1	-3893.282527	1.186241	-3892.096287	13
A1	-3893.311096	1.189965	-3892.12113	-2.6
A6	-4081.878099	1.209326	-4080.668774	-22.1
A7	-4083.04775	1.22471	-4081.823041	-10.6
TSA7-8	-4083.03622	1.221279	-4081.814942	-5.5
A8	-4083.039012	1.224301	-4081.814711	-5.4

CH2F_A2	-3315.401286	0.396628	-3315.004658	2.7
A5	-3316.577959	0.412892	-3316.165067	10.4
TSA5-1	-3316.561451	0.41288	-3316.148572	20.7
A1	-3316.602331	0.416659	-3316.185672	-2.6
A6	-3505.158078	0.431883	-3504.726194	-17.7
A7	-3506.312687	0.445969	-3505.866718	2.5
TSA7-8	-3506.303867	0.445598	-3505.858269	7.8
A8	-3506.323376	0.448405	-3505.874971	-2.7
PhNH2Ph_A2	-3519.013955	0.620219	-3518.393736	-9.4
A5	-3520.183651	0.642283	-3519.541368	6.3
TSA5-1	-3520.171901	0.638732	-3519.533169	11.5
A1	-3520.199595	0.644038	-3519.555558	-2.6
A6	-3708.764065	0.659772	-3708.104293	-22.8
A7	-3709.926252	0.67523	-3709.251022	-6.5
TSA7-8	-3709.919836	0.672075	-3709.247761	-4.5
A8	-3709.929074	0.675749	-3709.253325	-8
NMe2_A2	-3288.018864	0.711506	-3287.307358	-11.7
A5	-3289.18625	0.725369	-3288.46088	0.3
TSA5-1	-3289.177576	0.726995	-3288.450581	6.8
A1	-3289.194782	0.729355	-3288.465427	-2.6
A6	-3477.767835	0.744736	-3477.023099	-28.4
A7	-3478.931348	0.760355	-3478.170993	-12.9
TSA7-8	-3478.918257	0.756923	-3478.161335	-6.8
A8	-3478.924849	0.758785	-3478.166064	-9.8
OMe_A2	-3171.428959	0.472748	-3170.956211	9.6
A5	-3172.616899	0.486905	-3172.129993	8.9
TSA5-1	-3172.593454	0.483498	-3172.109956	21.5
A1	-3172.641314	0.492989	-3172.148324	-2.6
A6	-3361.201114	0.50662	-3360.694494	-21.2
A7	-3362.359033	0.518432	-3361.840601	-4.5
TSA7-8	-3362.3517	0.518499	-3361.833201	0.1
A8	-3362.368522	0.524697	-3361.843825	-6.6
Me_A2	-2720.233669	0.444606	-2719.789062	-6.4
A5	-2721.409509	0.462101	-2720.947408	2.6
TSA5-1	-2721.396792	0.46199	-2720.934801	10.5
A1	-2721.419406	0.463811	-2720.955594	-2.6
A6	-2909.991339	0.480642	-2909.510697	-26.8
A7	-2911.155192	0.49246	-2910.662732	-13.9
TSA7-8	-2911.146285	0.493171	-2910.653114	-7.8
A8	-2911.150703	0.495605	-2910.655098	-9.1
NH2PhPh_A2	-3519.005904	0.625562	-3518.380342	-4.4
A5	-3520.179203	0.643237	-3519.535966	6.3
TSA5-1	-3520.171901	0.638732	-3519.533169	8
A1	-3520.196477	0.646427	-3519.55005	-2.6

A6	-3708.764273	0.66123	-3708.103042	-25.5
A7	-3709.916623	0.676764	-3709.239859	-3
TSA7-8	-3709.911522	0.672858	-3709.238663	-2.2
A8	-3709.922873	0.678467	-3709.244406	-5.8
Et_A2	-2956.044104	0.611086	-2955.433018	-12.3
A5	-2957.213481	0.630786	-2956.582695	2.1
TSA5-1	-2957.202497	0.630146	-2956.57235	8.6
A1	-2957.223304	0.633117	-2956.590186	-2.6
A6	-3145.800033	0.649954	-3145.150079	-29.8
A7	-3146.964749	0.661041	-3146.303708	-17.9
TSA7-8	-3146.952185	0.662133	-3146.290052	-9.3
A8	-3146.959013	0.664707	-3146.294306	-12
PhHPh_A2	-3408.296453	0.588556	-3407.707898	-4.2
A5	-3409.471546	0.602804	-3408.868742	3.3
TSA5-1	-3409.460895	0.60298	-3408.857915	10.1
A1	-3409.487351	0.609329	-3408.878022	-2.6
A6	-3598.055716	0.625509	-3597.430207	-25
A7	-3599.216547	0.640764	-3598.575782	-8
TSA7-8	-3599.205362	0.63742	-3598.567941	-3.1
A8	-3599.213617	0.641471	-3598.572146	-5.7
HPhPh_A2	-3408.290773	0.591095	-3407.699677	-3.9
A5	-3409.465468	0.609286	-3408.856182	6.3
TSA5-1	-3409.450657	0.608608	-3408.842048	15.1
A1	-3409.480962	0.610742	-3408.870221	-2.6
A6	-3598.048001	0.62633	-3597.421672	-24.5
A7	-3599.2027	0.643329	-3598.559371	-2.6
TSA7-8	-3599.197501	0.640821	-3598.556679	-0.9
A8	-3599.206999	0.642945	-3598.564054	-5.5
F_A2	-3079.852015	0.23506	-3079.616955	8.4
A5	-3081.03323	0.252087	-3080.781143	13.7
TSA5-1	-3081.021542	0.250195	-3080.771347	19.9
A1	-3081.06575	0.258641	-3080.80711	-2.6
A6	-3269.619908	0.271933	-3269.347975	-17.9
A7	-3270.76915	0.286748	-3270.482402	6.1
TSA7-8	-3270.765547	0.286089	-3270.479458	8
A8	-3270.790042	0.28754	-3270.502503	-6.5
NH2_A2	-2816.490872	0.382536	-2816.108336	1
A5	-2817.669234	0.399789	-2817.269445	8.3
TSA5-1	-2817.658857	0.397549	-2817.261308	13.4
A1	-2817.690314	0.403635	-2817.28668	-2.6
A6	-3006.257316	0.417529	-3005.839786	-25.6
A7	-3007.414984	0.434586	-3006.980398	-5.4
TSA7-8	-3007.408345	0.431253	-3006.977092	-3.4
A8	-3007.416842	0.433922	-3006.982919	-7

H_A2	-2484.342961	0.278109	-2484.064852	-2
A5	-2485.523052	0.291794	-2485.231258	2
TSA5-1	-2485.510461	0.293639	-2485.216822	11
A1	-2485.537681	0.29919	-2485.238491	-2.6
A6	-2674.108446	0.311938	-2673.796509	-28.7
A7	-2675.266962	0.328105	-2674.938857	-9.6
TSA7-8	-2675.255369	0.326663	-2674.928707	-3.3
A8	-2675.265096	0.329373	-2674.935722	-7.7

Table S5 The calculated absolute electronic energies (*E*, in a.u.), thermal free energies (*G*corr, in a.u.), and relative Gibbs energies (Δ*G*, in kcal/mol) (Calculated at 298.15 K and 1 atm and Single point calculations at ωB97X-D/SDD&6-311++G** level).

Single point calculations in Toluene solvent (SDD&6-311++G**)

Complex	*E*	*G*corr	*G*	Δ*G*1	Δ*G*2
NMeiPr_A1	-3761.92637	1.062412	-3760.863958	0.0	11.5
CH3COCH3	-193.155806	0.057767	-193.098039	/	/
A3	-3955.08811	1.143143	-3953.944967	8.8	20.3
TSA3-4	-3955.040768	1.146311	-3953.894457	40.5	52.0
A4	-3955.118177	1.149517	-3953.96866	-6.1	5.4
CH3CH(OH)CH3	-194.364635	0.082193	-194.282442	/	/
A2	-3760.745987	1.04813	-3759.697857	-11.5	0.0
CF3_A1	-4508.602184	0.313408	-4508.288776	0.0	-0.3
A3	-4701.767575	0.391723	-4701.375852	5.0	4.7
TSA3-4	-4701.71306	0.39775	-4701.31531	43.0	42.7
A4	-4701.765278	0.396867	-4701.368411	9.7	9.4
A2	-4507.393644	0.289682	-4507.103962	0.3	0.0
CHF2_A1	-3913.096114	0.364531	-3912.731583	0.0	-6.2
A3	-4106.263644	0.441359	-4105.822285	2.7	-3.5
TSA3-4	-4106.218638	0.450112	-4105.768526	36.4	30.2
A4	-4106.255306	0.4509	-4105.804406	13.9	7.7
A2	-3911.88474	0.3475	-3911.53724	6.2	0.0
Ph_A1	-3872.518855	0.766418	-3871.752437	0.0	9.0
A3	-4065.691042	0.846142	-4064.8449	1.6	10.6
TSA3-4	-4065.648179	0.851774	-4064.796405	32.0	41.1
A4	-4065.710131	0.854918	-4064.855213	-4.9	4.2
A2	-3871.330309	0.747869	-3870.58244	-9.0	0.0
iPr_A1	-3193.953103	0.800517	-3193.152586	0.0	16.5
A3	-3387.117905	0.880793	-3386.237112	6.6	23.1
TSA3-4	-3387.081428	0.881486	-3386.199942	29.9	46.4
A4	-3387.11768	0.885551	-3386.232129	9.7	26.2
A2	-3192.775363	0.780944	-3191.994419	-16.5	0.0
Cy_A1	-3894.396741	1.189965	-3893.206776	0.0	16.0
A3	-4087.566995	1.273525	-4086.29347	5.2	21.3
TSA3-4	-4087.532501	1.278388	-4086.254113	29.9	46.0
A4	-4087.594814	1.280749	-4086.314065	-7.7	8.3
A2	-3893.217293	1.169353	-3892.04794	-16.0	0.0
CH2F_A1	-3317.623636	0.416659	-3317.206977	0.0	0.0
A3	-3510.795332	0.497533	-3510.297799	2.6	2.6
TSA3-4	-3510.761293	0.501904	-3510.259389	26.7	26.7
A4	-3510.79921	0.502051	-3510.297159	3.0	3.0
A2	-3316.419173	0.396628	-3316.022545	0.0	0.0
PhNH2Ph_A1	-3521.200595	0.644038	-3520.556557	0.0	10.8
A3	-3714.376178	0.72528	-3713.650898	0.4	11.3

TSA3-4	-3714.343343	0.727407	-3713.615936	22.4	33.2
A4	-3714.391718	0.729523	-3713.662195	-6.7	4.2
A2	-3520.009654	0.620219	-3519.389435	-10.8	0.0
NMe2_A1	-3290.150795	0.729355	-3289.42144	0.0	14.0
A3	-3483.31936	0.80521	-3482.51415	1.5	15.5
TSA3-4	-3483.296567	0.814118	-3482.482449	21.3	35.4
A4	-3483.355355	0.819276	-3482.536079	-12.3	1.7
A2	-3288.970888	0.711506	-3288.259382	-14.0	0.0
OMe_A1	-3173.581638	0.492989	-3173.088649	0.0	-7.4
A3	-3366.742978	0.568087	-3366.174891	5.5	-1.9
TSA3-4	-3366.726411	0.576363	-3366.150048	21.1	13.7
A4	-3366.757689	0.574556	-3366.183133	0.3	-7.1
A2	-3172.365179	0.472748	-3171.892431	7.4	0.0
Me_A1	-2722.222854	0.463811	-2721.759043	0.0	8.7
A3	-2915.396064	0.544617	-2914.851447	1.6	10.3
TSA3-4	-2915.37212	0.550627	-2914.821493	20.4	29.1
A4	-2915.415262	0.55074	-2914.864522	-6.6	2.1
A2	-2721.033061	0.444606	-2720.588455	-8.7	0.0
NH2PhPh_A1	-3521.197178	0.646427	-3520.550751	0.0	6.1
A3	-3714.364644	0.725357	-3713.639287	4.1	10.2
TSA3-4	-3714.342043	0.728708	-3713.613335	20.4	26.5
A4	-3714.387338	0.731438	-3713.6559	-6.4	-0.2
A2	-3520.001656	0.625562	-3519.376094	-6.1	0.0
Et_A1	-2958.086889	0.633117	-2957.453772	0.0	14.5
A3	-3151.261434	0.714861	-3150.546573	1.4	15.9
TSA3-4	-3151.238218	0.718791	-3150.519427	18.4	32.9
A4	-3151.287253	0.717221	-3150.570032	-13.3	1.2
A2	-2956.903569	0.611086	-2956.292483	-14.5	0.0
PhHPh_A1	-3410.445083	0.609329	-3409.835754	0.0	5.7
A3	-3603.621589	0.689286	-3602.932303	-1.0	4.8
TSA3-4	-3603.59889	0.694479	-3602.904411	16.5	22.3
A4	-3603.636496	0.697396	-3602.9391	-5.2	0.5
A2	-3409.249051	0.588556	-3408.660495	-5.7	0.0
HPhPh_A1	-3410.438239	0.610742	-3409.827497	0.0	6.0
A3	-3603.609548	0.69256	-3602.916988	3.5	9.5
TSA3-4	-3603.592804	0.694034	-3602.89877	14.9	20.9
A4	-3603.625353	0.697477	-3602.927876	-3.4	2.7
A2	-3409.243818	0.591095	-3408.652723	-6.0	0.0
F_A1	-3081.993816	0.258641	-3081.735175	0.0	-7.5
A3	-3275.166451	0.336263	-3274.830188	0.0	-7.4
TSA3-4	-3275.143374	0.338455	-3274.804919	15.9	8.4
A4	-3275.160009	0.339913	-3274.820096	6.3	-1.1
A2	-3080.773953	0.23506	-3080.538893	7.5	0.0
NH2_A1	-2818.563918	0.403635	-2818.160283	0.0	1.9

A3	-3011.734084	0.484643	-3011.249441	3.7	5.6
TSA3-4	-3011.72232	0.488004	-3011.234316	13.2	15.1
A4	-3011.74737	0.489657	-3011.257713	-1.5	0.4
A2	-2817.361492	0.382536	-2816.978956	-1.9	0.0
H_A1	-2486.280853	0.29919	-2485.981663	0.0	4.7
A3	-2679.453194	0.377346	-2679.075848	0.5	5.3
TSA3-4	-2679.445202	0.379377	-2679.065825	6.8	11.6
A4	-2679.470178	0.382115	-2679.088063	-7.1	-2.4
A2	-2485.08293	0.278109	-2484.804821	-4.7	0.0

Complex	*E*	*G*corr	*G*	Δ*G*
MeMePh_A1	-3104.87202	0.565451	-3104.306569	0.0
PhCOCH3	-384.800798	0.10752	-384.693278	/
D4S	-3489.688526	0.692985	-3488.995541	0.8
TSD4-5S	-3489.664217	0.699915	-3488.964302	20.4
D5S	-3489.707138	0.701877	-3489.005261	-5.3
PhCH(OH)CH3	-386.007347	0.130499	-385.876848	/
A2	-3103.67993	0.543742	-3103.136188	-8.3
D4R	-3489.691584	0.697211	-3488.994373	1.5
TSD4-5R	-3489.666507	0.701433	-3488.965074	19.9
D5R	-3489.709141	0.702183	-3489.006958	-6.4
iPrCOCH3	-271.728429	0.111687	-271.616742	/
D4Sa	-3376.618232	0.699115	-3375.919117	0.7
TSD4-5Sa	-3376.589898	0.705239	-3375.884659	22.4
D5Sa	-3376.628514	0.70304	-3375.925474	-3.2
iPrCH(OH)CH3	-272.936633	0.136176	-272.800457	/
D4Ra	-3376.61815	0.700995	-3375.917155	2.0
TSD4-5Ra	-3376.585748	0.704696	-3375.881052	24.6
D5Ra	-3376.634911	0.706106	-3375.928805	-5.3
A2’	-3103.67993	0.543742	-3103.136188	-8.4
HMePh_A1	-3026.237096	0.508257	-3025.728839	0.0
E4S	-3411.053585	0.641918	-3410.411667	4.7
TSE4-5S	-3411.04028	0.641939	-3410.398341	13.0
E5S	-3411.073723	0.643804	-3410.429919	-6.8
A2	-3025.040645	0.489101	-3024.551544	-3.9
E4R	-3411.05756	0.640906	-3410.416654	1.5
TSE4-5R	-3411.041823	0.643742	-3410.398081	13.2
E5R	-3411.071318	0.64545	-3410.425868	-4.2
E4Sa	-3297.983218	0.642144	-3297.341074	0.9
TSE4-5Sa	-3297.966724	0.647513	-3297.319211	14.7
E5Sa	-3297.990885	0.648747	-3297.342138	0.3
E4Ra	-3297.982234	0.644252	-3297.337982	2.9
TSE4-5Ra	-3297.964572	0.648428	-3297.316144	16.6
E5Ra	-3298.005216	0.651502	-3297.353714	-7.0

TSE5-6Ra	-3298.000012	0.647336	-3297.352676	-6.3
E6Ra	-3298.004129	0.649411	-3297.354718	-7.6
A2’	-3025.040645	0.489101	-3024.551544	-4.0
MeMePh_A1	-3104.87202	0.565451	-3104.306569	0.0
$PhC=N(CH_3)CH_3$	-404.220283	0.145135	-404.075148	/
F4S	-3509.106162	0.733631	-3508.372531	3.9
TSF4-5S	-3509.068177	0.739583	-3508.328594	31.4
F5S	-3509.136162	0.741098	-3508.395064	-10.3
$PhCHN(CH_3)HCH_3$	-405.441829	0.170468	-405.271361	/
A2	-3103.67993	0.543742	-3103.136188	-16.2
F4R	-3509.109735	0.737309	-3508.372426	3.9
TSF4-5R	-3509.054315	0.74147	-3508.312845	41.3
F5R	-3509.136149	0.740408	-3508.395741	-10.7
$iPrC=N(CH_3)CH_3$	-291.149879	0.150673	-290.999206	/
F4Sa	-3396.038679	0.739998	-3395.298681	2.6
TSF4-5Sa	-3395.991382	0.744115	-3395.247267	34.8
F5Sa	-3396.063854	0.74279	-3395.321064	-11.5
$iPrCHN(CH_3)HCH_3$	-292.369453	0.175675	-292.193778	/
F4Ra	-3396.040469	0.74058	-3395.299889	1.8
TSF4-5Ra	-3395.975586	0.74467	-3395.230916	45.1
F5Ra	-3396.061807	0.747471	-3395.314336	-7.3
A2’	-3103.67993	0.543742	-3103.136188	-15.2
HMePh_A1	-3026.237096	0.508257	-3025.728839	0.0
G4S	-3430.475983	0.677976	-3429.798007	1.9
TSG4-5S	-3430.444173	0.68078	-3429.763393	23.6
G5S	-3430.499977	0.684522	-3429.815455	-9.1
A2	-3025.040645	0.489101	-3024.551544	-11.9
G4R	-3430.479138	0.683145	-3429.795993	3.1
TSG4-5R	-3430.434912	0.682777	-3429.752135	30.6
G5R	-3430.501393	0.686358	-3429.815035	-8.8
G4Sa	-3317.405383	0.684572	-3316.720811	2.6
TSG4-5Sa	-3317.370781	0.687393	-3316.683388	26.1
G5Sa	-3317.42706	0.690295	-3316.736765	-7.4
G4Ra	-3317.403565	0.683346	-3316.720219	3.0
TSG4-5Ra	-3317.359622	0.690275	-3316.669347	34.9
G5Ra	-3317.425596	0.692001	-3316.733595	-5.4
A2’	-3025.040645	0.489101	-3024.551544	-10.8
CH3COCH3	-193.155806	0.057767	-193.098039	/
CH3CH(OH)CH3	-194.364635	0.082193	-194.282442	/
NMeiPr_A2	-3760.745987	1.04813	-3759.697857	-11.5
HCOOH	-189.766636	0.010444	-189.756192	/
A6	-3950.538577	1.076243	-3949.462334	-18.6
H2	-1.175611	-0.001319	-1.17693	/

A7	-3951.731739	1.094739	-3950.637	-19.0
TSA7-8	-3951.718723	1.09173	-3950.626993	-12.8
A8	-3951.722659	1.09451	-3950.628149	-13.5
A1	-3761.92637	1.062412	-3760.863958	-6.6
CF3_A2	-4507.393644	0.289682	-4507.103962	0.3
A6	-4697.201899	0.327885	-4696.874014	-10.3
A7	-4698.358361	0.341824	-4698.016537	9.4
TSA7-8	-4698.355733	0.339894	-4698.015839	9.8
A8	-4698.384396	0.343375	-4698.041021	-6.0
A1	-4508.602184	0.313408	-4508.288776	-6.6
CHF2_A2	-3911.88474	0.3475	-3911.53724	6.2
A6	-4101.70984	0.381052	-4101.328788	-17.8
A7	-4102.866134	0.395675	-4102.470459	2.4
TSA7-8	-4102.859089	0.394284	-4102.464805	5.9
A8	-4102.879914	0.398573	-4102.481341	-4.4
A1	-3913.096114	0.364531	-3912.731583	-6.6
Ph_A2	-3871.330309	0.747869	-3870.58244	-9.0
A6	-4061.138933	0.783132	-4060.355801	-21.7
A7	-4062.309829	0.800091	-4061.509738	-9.2
TSA7-8	-4062.299448	0.796366	-4061.503082	-5.0
A8	-4062.308986	0.79768	-4061.511306	-10.1
A1	-3872.518855	0.766418	-3871.752437	-6.6
iPr_A2	-3192.775363	0.780944	-3191.994419	-16.5
A6	-3382.580312	0.81352	-3381.766792	-28.5
A7	-3383.760513	0.835131	-3382.925382	-18.9
TSA7-8	-3383.735143	0.82865	-3382.906493	-7.0
A8	-3383.739144	0.8306	-3382.908544	-8.3
A1	-3193.953103	0.800517	-3193.152586	-6.6
Cy_A2	-3893.217293	1.169353	-3892.04794	-16.0
A6	-4083.022352	1.209326	-4081.813026	-23.5
A7	-4084.203262	1.22471	-4082.978552	-18.2
TSA7-8	-4084.186157	1.221279	-4082.964878	-9.7
A8	-4084.189281	1.224301	-4082.96498	-9.7
A1	-3894.396741	1.189965	-3893.206776	-6.6
CH2F_A2	-3316.419173	0.396628	-3316.022545	0.0
A6	-3506.233596	0.431883	-3505.801713	-16.3
A7	-3507.402088	0.445969	-3506.956119	-4.0
TSA7-8	-3507.393952	0.445598	-3506.948354	0.8
A8	-3507.412264	0.448405	-3506.963859	-8.9
A1	-3317.623636	0.416659	-3317.206977	-6.6
PhNH2Ph_A2	-3520.009654	0.620219	-3519.389435	-10.8
A6	-3709.822723	0.659772	-3709.162951	-23.6
A7	-3710.997158	0.67523	-3710.321928	-14.2
TSA7-8	-3710.984933	0.672075	-3710.312858	-8.5

A8	-3710.994074	0.675749	-3710.318325	-12.0
A1	-3521.200595	0.644038	-3520.556557	-6.6
NMe2_A2	-3288.970888	0.711506	-3288.259382	-14.0
A6	-3478.7823	0.744736	-3478.037564	-29.7
A7	-3479.958181	0.760355	-3479.197826	-21.1
TSA7-8	-3479.939169	0.756923	-3479.182246	-11.4
A8	-3479.946422	0.758785	-3479.187637	-14.7
A1	-3290.150795	0.729355	-3289.42144	-6.6
OMe_A2	-3172.365179	0.472748	-3171.892431	7.4
A6	-3362.20009	0.50662	-3361.69347	-22.6
A7	-3363.370216	0.518432	-3362.851784	-12.8
TSA7-8	-3363.357837	0.518499	-3362.839338	-5.0
A8	-3363.373061	0.524697	-3362.848364	-10.7
A1	-3173.581638	0.492989	-3173.088649	-6.6
Me_A2	-2721.033061	0.444606	-2720.588455	-8.7
A6	-2910.853633	0.480642	-2910.372991	-28.3
A7	-2912.029832	0.49246	-2911.537372	-22.4
TSA7-8	-2912.014981	0.493171	-2911.52181	-12.6
A8	-2912.019247	0.495605	-2911.523642	-13.7
A1	-2722.222854	0.463811	-2721.759043	-6.6
NH2PhPh_A2	-3520.001656	0.625562	-3519.376094	-6.1
A6	-3709.823255	0.66123	-3709.162025	-26.7
A7	-3710.988633	0.676764	-3710.311869	-11.6
TSA7-8	-3710.97756	0.672858	-3710.304702	-7.1
A8	-3710.988144	0.678467	-3710.309677	-10.2
A1	-3521.197178	0.646427	-3520.550751	-6.6
Et_A2	-2956.903569	0.611086	-2956.292483	-14.5
A6	-3146.722254	0.649954	-3146.0723	-31.2
A7	-3147.899616	0.661041	-3147.238575	-26.4
TSA7-8	-3147.88126	0.662133	-3147.219127	-14.2
A8	-3147.887932	0.664707	-3147.223225	-16.8
A1	-2958.086889	0.633117	-2957.453772	-6.6
PhHPh_A2	-3409.249051	0.588556	-3408.660495	-5.7
A6	-3599.071327	0.625509	-3598.445818	-25.9
A7	-3600.245117	0.640764	-3599.604353	-16.3
TSA7-8	-3600.228508	0.63742	-3599.591088	-7.9
A8	-3600.236065	0.641471	-3599.594594	-10.1
A1	-3410.445083	0.609329	-3409.835754	-6.6
HPhPh_A2	-3409.243818	0.591095	-3408.652723	-6.0
A6	-3599.063946	0.62633	-3598.437616	-25.9
A7	-3600.231782	0.643329	-3599.588453	-11.5
TSA7-8	-3600.220832	0.640821	-3599.580011	-6.2
A8	-3600.229375	0.642945	-3599.58643	-10.2
A1	-3410.438239	0.610742	-3409.827497	-6.6

F_A2	-3080.773953	0.23506	-3080.538893	7.5
A6	-3270.602464	0.271933	-3270.330531	-16.7
A7	-3271.764368	0.286748	-3271.47762	0.2
TSA7-8	-3271.756729	0.286089	-3271.47064	4.5
A8	-3271.781142	0.28754	-3271.493602	-9.9
A1	-3081.993816	0.258641	-3081.735175	-6.6
NH2_A2	-2817.361492	0.382536	-2816.978956	-1.9
A6	-3007.189415	0.417529	-3006.771886	-26.9
A7	-3008.360017	0.434586	-3007.925431	-14.1
TSA7-8	-3008.346189	0.431253	-3007.914936	-7.5
A8	-3008.355294	0.433922	-3007.921372	-11.5
A1	-2818.563918	0.403635	-2818.160283	-6.6
H_A2	-2485.08293	0.278109	-2484.804821	-4.7
A6	-2674.91125	0.311938	-2674.599312	-30.7
A7	-2676.0838	0.328105	-2675.755695	-19.7
TSA7-8	-2676.065636	0.326663	-2675.738973	-9.2
A8	-2676.073676	0.329373	-2675.744303	-12.5
A1	-2486.280853	0.29919	-2485.981663	-6.6

11. Imaginary frequencies of transition states.

Table S6 Calculated imaginary frequencies of transition states at ωB97X-D/6-31G* level.

In Toluene solvent	
TSA3-4(R^1=R^2=R^3=NMeiPr)	719.88*i*
TSA3-4(R^1=R^2=R^3=CF_3)	536.95*i*
TSA3-4(R^1=R^2=R^3=CHF_2)	519.49*i*
TSA3-4(R^1=R^2=R^3=Ph)	577.03*i*
TSA3-4(R^1=R^2=R^3=iPr)	437.70*i*
TSA3-4(R^1=R^2=R^3=Cy)	608.42*i*
TSA3-4(R^1=R^2=R^3=CH_2F)	604.96*i*
TSA3-4(R^1=R^3=Ph, R^2=NH_2)	591.28*i*
TSA3-4(R^1=R^2=R^3=NMe_2)	585.62*i*
TSA3-4(R^1=R^2=R^3=OMe)	445.02*i*
TSA3-4(R^1=R^2=R^3=Me)	607.27*i*
TSA3-4(R^1=NH_2, R^2=R^3=Ph)	586.76*i*
TSA3-4(R^1=R^2=R^3=Et)	578.46*i*
TSA3-4(R^1=R^3=Ph, R^2=H)	584.80*i*
TSA3-4(R^1=H, R^2=R^3=Ph)	610.98*i*
TSA3-4(R^1=R^2=R^3=F)	588.41*i*
TSA3-4(R^1=R^2=R^3=NH_2)	409.93*i*
TSA3-4(R^1=R^2=R^3=H)	368.99*i*
TSD4-5S	569.93*i*
TSD4-5R	576.54*i*
TSD4-5Sa	586.60*i*
TSD4-5Ra	594.15*i*
TSE4-5S	525.16*i*
TSE4-5R	640.84*i*
TSE4-5Sa	583.84*i*
TSE4-5Ra	545.90*i*
TSE5-6Ra	1149.85*i*
TSF4-5S	928.24*i*
TSF4-5R	648.99*i*
TSF4-5Sa	779.85*i*
TSF4-5Ra	133.93*i*
TSG4-5S	740.54*i*
TSG4-5R	333.57*i*
TSG4-5Sa	694.16*i*
TSG4-5Ra	179.42*i*
TSA5-1(R^1=R^2=R^3=NMeiPr)	1098.36*i*
TSA5-1(R^1=R^2=R^3=CF_3)	1053.73*i*
TSA5-1(R^1=R^2=R^3=CHF_2)	1114.88*i*
TSA5-1(R^1=R^2=R^3=Ph)	1046.69*i*
TSA5-1(R^1=R^2=R^3=iPr)	1174.84*i*
TSA5-1(R^1=R^2=R^3=Cy)	1131.04*i*

TSA5-1(R^1=R^2=R^3=CH_2F)	1157.17*i*
TSA5-1(R^1=R^3=Ph, R^2=NH_2)	1169.24*i*
TSA5-1(R^1=R^2=R^3=NMe_2)	1276.27*i*
TSA5-1(R^1=R^2=R^3=OMe)	1321.34*i*
TSA5-1(R^1=R^2=R^3=Me)	1189.07*i*
TSA5-1(R^1=NH_2, R^2=R^3=Ph)	1169.24*i*
TSA5-1(R^1=R^2=R^3=Et)	1291.19*i*
TSA5-1(R^1=R^3=Ph, R^2=H)	1231.29*i*
TSA5-1(R^1=H, R^2=R^3=Ph)	1176.88*i*
TSA5-1(R^1=R^2=R^3=F)	1182.06*i*
TSA5-1(R^1=R^2=R^3=NH_2)	1269.19*i*
TSA5-1(R^1=R^2=R^3=H)	1181.48*i*
TSA7-8(R^1=R^2=R^3=NMeiPr)	180.12*i*
TSA7-8(R^1=R^2=R^3=CF_3)	255.26*i*
TSA7-8(R^1=R^2=R^3=CHF_2)	364.49*i*
TSA7-8(R^1=R^2=R^3=Ph)	537.71*i*
TSA7-8(R^1=R^2=R^3=iPr)	647.37*i*
TSA7-8(R^1=R^2=R^3=Cy)	975.38*i*
TSA7-8(R^1=R^2=R^3=CH_2F)	355.11*i*
TSA7-8(R^1=R^3=Ph, R^2=NH_2)	534.80*i*
TSA7-8(R^1=R^2=R^3=NMe_2)	421.02*i*
TSA7-8(R^1=R^2=R^3=OMe)	765.14*i*
TSA7-8(R^1=R^2=R^3=Me)	764.56*i*
TSA7-8(R^1=NH_2, R^2=R^3=Ph)	526.81*i*
TSA7-8(R^1=R^2=R^3=Et)	825.04*i*
TSA7-8(R^1=R^3=Ph, R^2=H)	706.28*i*
TSA7-8(R^1=H, R^2=R^3=Ph)	528.56*i*
TSA7-8(R^1=R^2=R^3=F)	455.72*i*
TSA7-8(R^1=R^2=R^3=NH_2)	687.84*i*
TSA7-8(R^1=R^2=R^3=H)	807.24*i*

12. Cartesian coordinates of all the structures.

Table S7 When structure optimization in toluene solvent, the atomic Cartesian coordinates of intermediates and transition states (represented by Å).

R_1=R_2=R_3=NMeiPr

A1

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.177396	-0.250250	-0.673094
N	-0.008421	-0.866393	1.706251
C	2.787118	-0.660960	0.868724
H	3.753893	-1.138868	1.063471
H	2.975836	0.402014	0.684668
C	-2.858982	-0.170228	1.473008
C	-0.357610	-0.261129	-2.395858
O	-0.518548	-0.371524	-3.558804
P	-2.499886	-0.454078	-0.303793
P	1.964152	-1.107514	-0.709567
Si	-1.464527	-0.584914	2.667089
Si	1.630113	-0.701035	2.351490
C	-1.898768	-2.049627	3.766006
H	-1.093715	-2.240313	4.486815
H	-2.808087	-1.834329	4.342306
H	-2.067591	-2.978368	3.213585
C	2.043222	-2.091568	3.555448
H	3.113745	-2.093805	3.799023
H	1.499719	-1.951609	4.498605
H	1.783646	-3.083884	3.173587
H	-2.944044	0.922708	1.521710
H	-3.819542	-0.570615	1.814548
P	0.360441	2.029287	-0.257962
C	-0.251316	2.679758	1.375324
H	-0.083317	3.764652	1.401028
H	-1.339835	2.558808	1.284850
Si	0.202201	2.022960	3.103222
C	0.403286	3.545721	4.199845
H	1.221056	4.188889	3.849688
H	-0.511357	4.152168	4.205728
H	0.623047	3.268020	5.238071
C	-1.177304	0.921540	3.753236
H	-2.120799	1.475661	3.846653
H	-0.900884	0.604077	4.768642

C	1.726953	0.927299	3.284238
H	2.665015	1.435613	3.037796
H	1.782891	0.707769	4.360888
H	-0.470222	-1.816090	-0.714534
H	-0.100725	-1.699414	1.111410
C	-2.756934	-2.606304	-1.910066
H	-2.382009	-1.830729	-2.575438
H	-1.961105	-3.360979	-1.852845
H	-3.634923	-3.056296	-2.392110
C	-3.800258	0.465270	-2.463626
H	-2.805251	0.316923	-2.885441
H	-4.431313	-0.370448	-2.805240
H	-4.197829	1.387177	-2.899569
C	0.092622	4.568460	-1.329967
H	1.170240	4.689948	-1.234489
H	-0.200397	5.063055	-2.261148
H	-0.390064	5.114647	-0.502746
C	2.729367	2.606041	-1.445990
H	2.046234	2.369170	-2.263368
H	3.134452	3.606546	-1.656867
H	3.553385	1.885913	-1.470099
C	1.323726	-3.470675	-1.798881
H	1.082882	-2.742458	-2.577193
H	1.921711	-4.264817	-2.265610
H	0.368682	-3.899572	-1.464380
C	2.758026	-0.164143	-3.167237
H	1.832572	0.399832	-3.084855
H	3.522040	0.514047	-3.569409
H	2.599378	-0.967766	-3.901476
N	-3.112284	-2.053474	-0.610971
N	-3.725593	0.570349	-1.010014
N	-0.262718	3.165675	-1.387661
N	2.011545	2.580890	-0.181001
N	2.056640	-2.828346	-0.722605
N	3.150214	-0.644080	-1.856095
C	-3.399897	-3.068468	0.404104
C	-2.193652	-3.950426	0.758725
C	-4.577013	-3.963340	-0.008601
H	-3.702964	-2.541189	1.313238
H	-1.334995	-3.342642	1.046577
H	-2.440743	-4.624382	1.587638
H	-1.884448	-4.573992	-0.086447
H	-5.435569	-3.371372	-0.338116
H	-4.298797	-4.641736	-0.822940

H	-4.888967	-4.584458	0.838967
C	-5.050143	0.739491	-0.372145
C	-5.919640	-0.524676	-0.324267
C	-5.841432	1.887129	-1.007677
H	-4.860833	1.046532	0.659665
H	-5.492579	-1.279568	0.337972
H	-6.920855	-0.275702	0.047848
H	-6.031905	-0.976169	-1.316000
H	-5.234356	2.792311	-1.092286
H	-6.227911	1.629983	-1.999957
H	-6.705328	2.119631	-0.374809
C	-1.464730	2.859434	-2.163228
C	-1.204523	2.948429	-3.668799
C	-2.657845	3.723911	-1.749321
H	-1.708256	1.826777	-1.922382
H	-0.374374	2.294889	-3.950018
H	-2.091274	2.628739	-4.228952
H	-0.967368	3.971656	-3.986923
H	-2.885051	3.587175	-0.686687
H	-2.475937	4.789971	-1.930431
H	-3.543804	3.445235	-2.327545
C	2.666028	3.314725	0.909260
C	2.600284	4.849094	0.833174
C	4.133050	2.891541	1.070627
H	2.160676	3.034237	1.830246
H	1.574095	5.218889	0.899818
H	3.162112	5.280335	1.670326
H	3.047502	5.236684	-0.089442
H	4.242380	1.805964	1.143670
H	4.749048	3.236704	0.232773
H	4.547488	3.332503	1.984137
C	2.593677	-3.713082	0.306252
C	3.741324	-4.596296	-0.203670
C	1.507210	-4.581621	0.953504
H	3.008896	-3.076820	1.090432
H	4.545832	-3.991393	-0.632339
H	4.159638	-5.185302	0.621101
H	3.402360	-5.302688	-0.969880
H	0.685496	-3.962271	1.325707
H	1.089554	-5.303034	0.242272
H	1.920287	-5.150996	1.794101
C	4.497328	-1.220695	-1.765577
C	5.559039	-0.123767	-1.648512
C	4.813765	-2.196920	-2.902374

H	4.528724	-1.799853	-0.838364
H	5.364766	0.503600	-0.771868
H	6.559198	-0.561408	-1.543743
H	5.571301	0.522363	-2.534391
H	4.033402	-2.960690	-2.984297
H	4.899704	-1.685321	-3.867685
H	5.768543	-2.701459	-2.714241

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.160916	-0.168826	-0.514271
N	-0.121666	-0.641697	1.537033
C	2.799020	-0.980947	1.113469
H	3.396378	-1.845394	1.421658
H	3.462720	-0.111754	1.087656
C	-2.965377	-0.045197	1.467573
C	-0.253506	-0.174519	-2.260960
O	-0.329102	-0.213315	-3.434335
P	-2.523630	-0.437984	-0.248159
P	2.043575	-1.159030	-0.530431
Si	-1.463709	-0.372842	2.582086
Si	1.396758	-0.639062	2.348561
C	-1.892517	-1.763147	3.802767
H	-1.281923	-1.684034	4.709450
H	-2.940191	-1.675161	4.121693
H	-1.744110	-2.769679	3.402690
C	1.535057	-1.929005	3.734193
H	2.585998	-2.101063	4.002732
H	1.021966	-1.606504	4.648256
H	1.099129	-2.890285	3.437789
H	-3.126306	1.039979	1.463298
H	-3.890208	-0.511101	1.823215
P	0.298141	2.079839	-0.324770
C	-0.267923	2.808005	1.271581
H	-0.089474	3.891219	1.246570
H	-1.359402	2.690975	1.213283
Si	0.209679	2.179004	3.012007
C	0.489450	3.746539	4.035357
H	1.343078	4.326051	3.658910
H	-0.389263	4.404046	4.015416

H	0.696278	3.504361	5.085348
C	-1.231037	1.174893	3.670070
H	-2.154013	1.769139	3.709053
H	-1.006953	0.877188	4.704364
C	1.716681	1.058332	3.153450
H	2.626347	1.521624	2.756804
H	1.895051	0.922361	4.231210
C	-2.753491	-2.711581	-1.709085
H	-2.180622	-2.083419	-2.397164
H	-2.279457	-3.700222	-1.721895
H	-3.768633	-2.822814	-2.119566
C	-3.741195	0.224980	-2.589742
H	-2.715472	0.071784	-2.926052
H	-4.346698	-0.603193	-2.987742
H	-4.096285	1.152879	-3.050581
C	-0.031827	4.537885	-1.527027
H	1.049078	4.671684	-1.534837
H	-0.415598	5.002773	-2.439793
H	-0.444754	5.101601	-0.674652
C	2.594972	2.440628	-1.652657
H	1.958226	1.859294	-2.322397
H	2.766429	3.415686	-2.135741
H	3.550410	1.916532	-1.571865
C	0.560238	-3.257734	-1.397678
H	-0.306834	-2.644642	-1.152213
H	0.723011	-3.212938	-2.485348
H	0.291724	-4.286242	-1.140125
C	3.044477	-0.652370	-2.993070
H	2.038605	-0.257059	-3.125236
H	3.737084	0.048165	-3.476541
H	3.099379	-1.608848	-3.534992
N	-2.751887	-2.149703	-0.369866
N	-3.794428	0.317217	-1.135713
N	-0.371601	3.128421	-1.516134
N	1.943972	2.573051	-0.360178
N	1.709127	-2.835356	-0.614990
N	3.350763	-0.781131	-1.578515
C	-2.958402	-3.105974	0.724179
C	-1.682144	-3.900781	1.033446
C	-4.117042	-4.079406	0.466565
H	-3.215931	-2.526268	1.612799
H	-0.833935	-3.225532	1.182429
H	-1.818500	-4.511689	1.933770
H	-1.445671	-4.587530	0.213014

H	-5.050216	-3.565672	0.222256
H	-3.887542	-4.769533	-0.353008
H	-4.289025	-4.684685	1.363591
C	-5.161229	0.422091	-0.581177
C	-5.879743	-0.924992	-0.469959
C	-6.023350	1.419786	-1.357141
H	-5.056178	0.828977	0.427968
H	-5.361931	-1.578759	0.233432
H	-6.906802	-0.785894	-0.112635
H	-5.926826	-1.434769	-1.439450
H	-5.522723	2.385945	-1.465297
H	-6.294030	1.051008	-2.352598
H	-6.956135	1.585551	-0.807436
C	-1.638537	2.796053	-2.168323
C	-1.532447	2.916389	-3.691022
C	-2.817128	3.607541	-1.624801
H	-1.825482	1.751679	-1.928327
H	-0.687300	2.328075	-4.058005
H	-2.444546	2.539412	-4.167635
H	-1.401437	3.955500	-4.017157
H	-2.952896	3.435781	-0.551394
H	-2.680435	4.683346	-1.786804
H	-3.740299	3.316710	-2.134997
C	2.642288	3.386176	0.642203
C	2.656516	4.902342	0.395742
C	4.078977	2.898691	0.849952
H	2.125671	3.230036	1.586881
H	1.657840	5.340236	0.468928
H	3.284468	5.387575	1.152314
H	3.076704	5.152323	-0.585352
H	4.107295	1.814692	0.985054
H	4.725522	3.158442	0.003970
H	4.505912	3.365149	1.744501
C	2.702249	-3.876769	-0.323351
C	2.944222	-4.829713	-1.502059
C	2.310833	-4.659911	0.932737
H	3.651960	-3.372098	-0.121676
H	3.055679	-4.287078	-2.446102
H	3.857828	-5.409898	-1.331688
H	2.122672	-5.544535	-1.622782
H	2.246082	-3.992870	1.797189
H	1.331461	-5.136922	0.804608
H	3.043906	-5.445701	1.152550
C	4.762639	-1.088503	-1.279270

C	5.630949	0.172462	-1.332511
C	5.369264	-2.170558	-2.180546
H	4.800248	-1.460339	-0.252701
H	5.302004	0.905024	-0.592600
H	6.678392	-0.074859	-1.123061
H	5.595539	0.643447	-2.321707
H	4.753990	-3.072494	-2.210155
H	5.502192	-1.814150	-3.208215
H	6.358436	-2.450938	-1.801327

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.054236	0.061807	-0.509049
N	0.131854	0.083415	1.909688
C	1.807826	-2.266285	1.175457
H	1.896426	-3.253263	1.644556
H	2.759503	-2.025342	0.692850
C	-1.133241	2.680912	1.429489
C	-0.242512	-0.058924	-2.227172
O	-0.402091	-0.162961	-3.390683
P	-1.700620	1.655098	0.010589
P	0.506677	-2.158449	-0.118110
Si	-0.241605	1.627024	2.717249
Si	1.471886	-0.950573	2.479175
C	-1.273301	1.302559	4.261490
H	-0.615772	0.971875	5.074775
H	-1.774368	2.215988	4.606524
H	-2.036393	0.529797	4.133766
C	0.955936	-1.727534	4.117391
H	1.665075	-2.501550	4.436782
H	0.924345	-0.969712	4.910372
H	-0.039147	-2.184345	4.062381
H	-0.384831	3.343200	0.976601
H	-1.888396	3.329260	1.887853
P	1.965424	1.183642	-0.786449
C	2.608083	2.342998	0.518431
H	3.525183	2.824462	0.155774
H	1.848656	3.136335	0.516183
Si	2.854353	1.913270	2.340365
C	4.393175	2.827072	2.934043

H	5.292407	2.472522	2.413840
H	4.309887	3.905655	2.751061
H	4.555857	2.682422	4.009119
C	1.329898	2.493189	3.270480
H	1.197372	3.576838	3.150227
H	1.480410	2.311584	4.343617
C	3.012957	0.087361	2.758849
H	3.860493	-0.373837	2.240152
H	3.255412	0.045147	3.831266
H	-1.394781	-0.721752	-0.500580
H	-0.730724	-0.464376	1.921982
C	-4.523478	-2.972908	-1.453047
O	-4.739369	-3.516819	-0.385415
C	-3.148079	-2.947315	-2.076459
H	-3.010100	-3.884068	-2.632947
H	-3.026999	-2.120407	-2.782083
H	-2.373770	-2.892183	-1.306983
C	-5.632656	-2.309267	-2.236566
H	-5.676298	-2.722726	-3.251560
H	-6.593933	-2.448408	-1.737375
H	-5.422565	-1.237707	-2.341263
C	-3.887428	0.163633	-0.313865
H	-3.212634	-0.227638	-1.081075
H	-4.405948	-0.692428	0.131244
H	-4.638775	0.801180	-0.805755
C	-2.493453	2.466885	-2.474402
H	-1.774399	1.703551	-2.763895
H	-3.497282	2.067224	-2.680239
H	-2.338069	3.334902	-3.127063
C	3.272067	2.813024	-2.600206
H	4.025570	2.044234	-2.763495
H	3.135642	3.327523	-3.555617
H	3.681756	3.552713	-1.891451
C	3.316866	-0.523871	-2.321069
H	2.422676	-1.156800	-2.325643
H	3.276032	0.118298	-3.213620
H	4.186169	-1.176559	-2.421046
C	-1.898749	-2.475273	1.309730
H	-2.106918	-1.492093	0.885517
H	-2.809261	-3.072451	1.184646
H	-1.719560	-2.367855	2.394561
C	0.395338	-3.266822	-2.580019
H	-0.267539	-2.408388	-2.660459
H	1.087920	-3.226404	-3.431879

H	-0.220771	-4.171066	-2.684442
N	-3.107170	0.876068	0.684833
N	-2.305130	2.839930	-1.081256
N	2.018177	2.222593	-2.180362
N	3.389539	0.230655	-1.077056
N	-0.782147	-3.078957	0.609051
N	1.110065	-3.226982	-1.315962
C	-3.843552	1.207121	1.910260
C	-4.171236	-0.063195	2.709730
C	-5.134504	2.012394	1.706526
H	-3.180678	1.812285	2.530095
H	-3.286530	-0.693759	2.830145
H	-4.547084	0.202319	3.704510
H	-4.944679	-0.666229	2.221678
H	-4.947161	2.983287	1.243347
H	-5.853561	1.469015	1.083518
H	-5.613750	2.191695	2.676049
C	-3.142030	3.961005	-0.624850
C	-4.556279	3.959786	-1.216492
C	-2.453880	5.302557	-0.886288
H	-3.251666	3.859721	0.457465
H	-5.045458	2.988182	-1.096386
H	-5.170058	4.710477	-0.706225
H	-4.551196	4.210832	-2.282834
H	-1.481722	5.341722	-0.386091
H	-2.293577	5.461130	-1.959141
H	-3.067980	6.132412	-0.515552
C	0.839607	3.008084	-2.552689
C	0.575571	2.940829	-4.060264
C	0.905679	4.465714	-2.080967
H	0.002840	2.538471	-2.039060
H	0.489665	1.900112	-4.380904
H	-0.357838	3.458474	-4.308033
H	1.371397	3.422259	-4.642056
H	1.051238	4.532996	-0.996943
H	1.724299	5.013463	-2.564053
H	-0.026369	4.983182	-2.327117
C	4.708500	0.371684	-0.445881
C	5.764558	1.174563	-1.222892
C	5.322714	-0.987480	-0.077274
H	4.542246	0.893195	0.496814
H	5.528540	2.239802	-1.270676
H	6.739275	1.076161	-0.730335
H	5.875373	0.796140	-2.246300

H	4.600771	-1.636623	0.422801
H	5.707206	-1.518411	-0.955283
H	6.169496	-0.837563	0.602309
C	-0.592229	-4.504409	0.911846
C	-1.583469	-5.366442	0.122912
C	-0.647364	-4.832093	2.408472
H	0.408930	-4.775453	0.577542
H	-1.445298	-5.213468	-0.951637
H	-1.434728	-6.431036	0.341851
H	-2.622268	-5.111933	0.359449
H	0.048491	-4.206934	2.977627
H	-1.650987	-4.693585	2.825231
H	-0.368375	-5.879544	2.570039
C	2.120739	-4.282625	-1.132269
C	3.457304	-3.904907	-1.775439
C	1.669751	-5.656288	-1.647686
H	2.302164	-4.386282	-0.060247
H	3.878605	-3.023594	-1.289581
H	4.178066	-4.726206	-1.680281
H	3.337149	-3.684983	-2.842398
H	0.689404	-5.946022	-1.259889
H	1.623463	-5.682319	-2.741977
H	2.394204	-6.415591	-1.333531

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.030920	0.026944	-0.497555
N	0.175838	0.518363	1.490173
C	-2.267346	2.134640	1.061111
H	-2.481502	3.176419	1.323221
H	-3.214675	1.588387	1.037786
C	2.202235	-1.615306	1.496991
C	0.149997	0.039079	-2.241971
O	0.351217	0.108659	-3.398433
P	2.036968	-1.236354	-0.265963
P	-1.470204	1.934482	-0.562670
Si	1.312978	-0.280347	2.509496
Si	-1.118192	1.302714	2.321742
C	2.575716	0.839281	3.349979
H	2.093202	1.462762	4.112447

H	3.348263	0.249418	3.861715
H	3.065547	1.516780	2.641887
C	-0.531539	2.600891	3.571610
H	-1.364301	3.230605	3.912341
H	-0.107310	2.126862	4.465798
H	0.243428	3.253726	3.152939
H	1.647553	-2.539718	1.683165
H	3.228138	-1.783759	1.837553
P	-1.584060	-1.728755	-0.135985
C	-1.309777	-2.531343	1.505533
H	-1.997947	-3.378178	1.613007
H	-0.320458	-2.991643	1.398353
Si	-1.329214	-1.647990	3.213832
C	-2.215068	-2.875851	4.351246
H	-3.252094	-3.057397	4.039142
H	-1.700984	-3.845461	4.370953
H	-2.244354	-2.498636	5.381154
C	0.413807	-1.311230	3.832589
H	0.978047	-2.227150	4.053659
H	0.318125	-0.763490	4.781387
C	-2.152770	0.036221	3.294387
H	-3.192965	0.025288	2.958946
H	-2.174923	0.314272	4.358927
H	3.760377	3.459146	-1.105725
H	3.654568	1.712267	0.327801
C	4.321835	3.523925	-0.161720
O	3.826456	2.566522	0.760506
C	4.074881	4.891456	0.457038
H	4.611986	4.977118	1.408585
H	4.417525	5.690891	-0.208706
H	3.008134	5.033864	0.656067
C	5.804107	3.309659	-0.464011
H	6.176898	4.079854	-1.149547
H	6.388984	3.355115	0.461552
H	5.982325	2.335188	-0.932858
C	3.482143	0.470689	-1.814666
H	2.517274	0.952932	-1.964248
H	4.244397	1.255440	-1.792777
H	3.679209	-0.151502	-2.697354
C	2.450330	-2.729885	-2.473977
H	1.875342	-1.898167	-2.887805
H	3.487182	-2.614499	-2.823652
H	2.056206	-3.654595	-2.907018
C	-2.431312	-4.212676	-0.997927

H	-2.611997	-4.376402	0.063294
H	-3.406395	-4.076024	-1.490809
H	-1.988677	-5.139153	-1.374988
C	-3.872376	-0.946129	-1.268956
H	-3.218669	-0.273251	-1.823353
H	-4.085273	-1.825649	-1.894867
H	-4.812515	-0.415201	-1.111770
C	1.001744	3.077534	-0.534661
H	1.561776	3.851728	-1.071461
H	1.318811	3.072917	0.514242
H	1.301001	2.117978	-0.963454
C	-2.540481	1.896617	-3.046738
H	-1.872366	1.041289	-3.140138
H	-3.486391	1.628525	-3.533188
H	-2.089767	2.728754	-3.607616
N	3.469088	-0.267676	-0.549998
N	2.343169	-2.746225	-1.025486
N	-1.523436	-3.097422	-1.191050
N	-3.260990	-1.287303	0.004571
N	-0.421422	3.278389	-0.727133
N	-2.762494	2.207800	-1.645219
C	4.764893	-0.902597	-0.167401
C	5.429606	-0.175926	1.002402
C	5.756897	-1.074518	-1.320531
H	4.533129	-1.914096	0.176239
H	4.729231	-0.040086	1.830251
H	6.286440	-0.756720	1.364917
H	5.790687	0.814613	0.715410
H	5.329610	-1.634289	-2.157657
H	6.123420	-0.114684	-1.700805
H	6.626524	-1.632926	-0.957649
C	2.870073	-3.946491	-0.354579
C	4.164406	-4.485512	-0.973984
C	1.814417	-5.055602	-0.283149
H	3.108889	-3.664169	0.671699
H	4.945590	-3.720881	-1.025335
H	4.542749	-5.311090	-0.361051
H	4.002668	-4.877380	-1.984190
H	0.852534	-4.652272	0.050127
H	1.666844	-5.525066	-1.262122
H	2.130593	-5.842849	0.411803
C	-0.991471	-2.960792	-2.559525
C	-1.950605	-2.327732	-3.573990
C	-0.510202	-4.299677	-3.125319

H	-0.125120	-2.311702	-2.460878
H	-2.171533	-1.287960	-3.330326
H	-1.496353	-2.340597	-4.571398
H	-2.894821	-2.883022	-3.631176
H	0.091132	-4.852013	-2.400841
H	-1.344324	-4.936748	-3.442144
H	0.100964	-4.113283	-4.014448
C	-4.224507	-1.730607	1.028156
C	-5.052166	-2.977248	0.680739
C	-5.201953	-0.602662	1.398541
H	-3.652584	-1.955740	1.927440
H	-4.457420	-3.891294	0.667931
H	-5.841706	-3.111947	1.429316
H	-5.540838	-2.871235	-0.294478
H	-4.693284	0.359387	1.489930
H	-6.004405	-0.494167	0.659698
H	-5.679469	-0.827756	2.358743
C	-0.887070	4.657419	-0.548842
C	-0.485349	5.529636	-1.743255
C	-0.430091	5.291217	0.769098
H	-1.978399	4.620297	-0.528835
H	-0.772113	5.048589	-2.683799
H	-0.972513	6.510030	-1.686349
H	0.596694	5.703670	-1.770367
H	-0.708778	4.670909	1.625704
H	0.656448	5.431113	0.794181
H	-0.892072	6.277118	0.895681
C	-3.897712	3.111050	-1.379972
C	-5.221009	2.343492	-1.326046
C	-3.996378	4.272040	-2.378156
H	-3.745681	3.544804	-0.389207
H	-5.213005	1.624446	-0.503070
H	-6.057991	3.034223	-1.168285
H	-5.407441	1.799532	-2.259480
H	-3.042714	4.794664	-2.494383
H	-4.315880	3.929023	-3.368586
H	-4.739067	4.997131	-2.027471

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Coordinates (Angstroms)		
X	Y	Z

Mn	-0.139693	-0.279413	-0.702047
N	0.012441	-0.238046	1.908250
C	2.878430	-0.215962	1.118466
H	3.787481	-0.683851	1.514888
H	3.144348	0.760288	0.705811
C	-2.772021	0.512014	1.468636
C	-0.103269	-0.072506	-2.434591
O	-0.046020	0.072724	-3.595850
P	-2.584243	-0.481352	-0.084351
P	2.132303	-1.144438	-0.278350
Si	-1.415436	0.388144	2.772151
Si	1.655114	0.094636	2.511747
C	-1.778297	-0.678354	4.289638
H	-1.104092	-0.360904	5.094891
H	-2.800907	-0.520911	4.652752
H	-1.630985	-1.753607	4.153502
C	1.966520	-1.000642	4.011770
H	3.014005	-0.957984	4.335586
H	1.352327	-0.664720	4.856945
H	1.714637	-2.050230	3.825006
H	-2.700864	1.543268	1.098617
H	-3.767107	0.404316	1.913440
P	0.349624	2.153548	-0.602997
C	-0.146109	3.220537	0.824245
H	0.078351	4.261426	0.559831
H	-1.241629	3.159206	0.811505
Si	0.320720	2.985163	2.643648
C	0.598119	4.709306	3.352162
H	1.455011	5.203198	2.875498
H	-0.279739	5.347604	3.193206
H	0.794061	4.674429	4.430734
C	-1.123017	2.116646	3.456467
H	-2.045042	2.699826	3.329618
H	-0.938436	2.049484	4.536749
C	1.799258	1.893231	3.039901
H	2.740893	2.304003	2.657583
H	1.884454	1.921511	4.136567
H	-0.503778	-2.007166	-1.295379
H	-0.091936	-1.252382	1.840601
C	-0.760641	-3.243325	-2.038656
O	-1.146837	-4.151058	-1.241725
C	0.618430	-3.438339	-2.680229
H	0.582647	-4.368608	-3.264166
H	0.880178	-2.619864	-3.354438

H	1.386309	-3.540608	-1.912126
C	-1.781129	-2.736263	-3.069898
H	-1.391781	-1.940445	-3.707642
H	-2.045103	-3.590078	-3.709587
H	-2.693253	-2.391402	-2.589429
C	-3.933137	-2.880995	-0.465499
H	-4.299948	-2.313939	-1.319501
H	-3.291693	-3.689294	-0.834340
H	-4.816400	-3.302542	0.035954
C	-3.796610	0.110275	-2.479438
H	-2.756832	0.025927	-2.795208
H	-4.344216	-0.722008	-2.943517
H	-4.205516	1.045320	-2.882533
C	0.052551	4.345108	-2.256717
H	1.134822	4.397792	-2.361192
H	-0.372293	4.638166	-3.220166
H	-0.264315	5.099950	-1.518922
C	2.637103	2.223778	-2.015242
H	1.905489	1.759510	-2.680116
H	3.041960	3.093725	-2.551804
H	3.447009	1.508557	-1.851983
C	0.803522	-3.255750	0.879798
H	-0.039198	-2.748193	0.406112
H	0.670164	-4.313097	0.643022
H	0.739504	-3.143416	1.977242
C	3.098340	-1.138856	-2.834568
H	2.078292	-0.810322	-3.010466
H	3.755458	-0.463580	-3.396605
H	3.209467	-2.146988	-3.254433
N	-3.220512	-1.998729	0.444223
N	-3.877255	0.097962	-1.030810
N	-0.363033	2.993911	-1.935967
N	1.999754	2.624371	-0.766842
N	2.049865	-2.750974	0.334519
N	3.404838	-1.078314	-1.414794
C	-2.892325	-2.604609	1.734596
C	-2.430097	-4.062703	1.630544
C	-4.070591	-2.492864	2.711948
H	-2.047988	-2.049687	2.144986
H	-1.749665	-4.197766	0.785152
H	-1.935761	-4.359477	2.563770
H	-3.281314	-4.738787	1.486107
H	-4.340530	-1.450672	2.905893
H	-4.951119	-2.996694	2.296497

H	-3.837504	-2.971924	3.670090
C	-5.225718	0.256403	-0.447668
C	-6.346124	-0.387603	-1.272809
C	-5.555218	1.733057	-0.208129
H	-5.213192	-0.265248	0.514846
H	-6.167097	-1.447798	-1.467307
H	-7.286192	-0.309215	-0.715906
H	-6.492685	0.120027	-2.232530
H	-4.790935	2.220200	0.402917
H	-5.624797	2.273929	-1.158888
H	-6.520464	1.834765	0.302500
C	-1.732738	2.674905	-2.348500
C	-1.878597	2.699406	-3.874991
C	-2.795638	3.569585	-1.699876
H	-1.906726	1.657831	-1.999890
H	-1.035682	2.191444	-4.348056
H	-2.798671	2.189162	-4.176421
H	-1.942122	3.720907	-4.268798
H	-2.813437	3.457666	-0.610995
H	-2.629040	4.628451	-1.931342
H	-3.789183	3.304970	-2.075902
C	2.726793	3.626867	0.030924
C	2.689363	5.073603	-0.487306
C	4.193894	3.234002	0.240597
H	2.266306	3.638005	1.017903
H	1.682514	5.495062	-0.474716
H	3.316489	5.703022	0.154811
H	3.085642	5.154410	-1.506103
H	4.299218	2.236559	0.673008
H	4.756842	3.262442	-0.698636
H	4.666449	3.943418	0.928391
C	3.232361	-3.560741	0.652400
C	3.225704	-4.890627	-0.110027
C	3.436453	-3.793169	2.153254
H	4.101827	-3.008141	0.304756
H	3.104735	-4.722434	-1.184088
H	4.170421	-5.423068	0.051963
H	2.414976	-5.549698	0.218204
H	3.511382	-2.843643	2.691155
H	2.619944	-4.376304	2.593611
H	4.365332	-4.349887	2.321759
C	4.843859	-1.197599	-1.108994
C	5.622885	0.086336	-1.412835
C	5.501196	-2.387764	-1.821362

H	4.941119	-1.359765	-0.034360
H	5.272903	0.913299	-0.791398
H	6.687561	-0.067208	-1.200704
H	5.538904	0.381730	-2.464353
H	4.914838	-3.305072	-1.714574
H	5.629083	-2.193232	-2.891806
H	6.496418	-2.568114	-1.400165

$R^1=R^2=R^3=CF_3$

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.065031	-0.476142	-0.473572
N	-0.099817	-0.490815	1.840510
C	2.800855	-0.706930	1.370325
H	3.385254	-1.509412	1.830933
H	3.503617	0.086151	1.101837
C	-2.937434	0.104288	1.242101
C	-0.031616	-0.868783	-2.204657
O	0.011485	-1.223528	-3.305837
P	-2.232301	-0.658600	-0.263143
P	1.951728	-1.260936	-0.156084
Si	-1.624772	0.064827	2.609875
Si	1.482090	0.002868	2.532975
C	-2.130164	-1.151651	3.939810
H	-1.365723	-1.240244	4.720481
H	-3.061797	-0.830214	4.421328
H	-2.300808	-2.149284	3.519532
C	1.679923	-0.751323	4.238618
H	2.692154	-0.579556	4.625628
H	0.977681	-0.316130	4.960210
H	1.513806	-1.835130	4.217146
H	-3.147265	1.151347	0.997475
H	-3.883948	-0.354267	1.546877
C	2.006672	-3.120420	0.196426
C	3.324676	-1.259571	-1.460219
C	-2.826606	-2.438952	0.011642
C	-3.509045	-0.171503	-1.587194
P	0.172851	1.691678	-0.715871
C	-0.537978	2.893686	0.480059
H	-0.347007	3.915799	0.137117

H	-1.624248	2.748213	0.420062
Si	-0.053847	2.780305	2.319313
C	1.887768	2.505874	-0.966680
C	-0.548219	2.484690	-2.284218
C	0.046055	4.544022	2.952961
H	0.849159	5.097495	2.451274
H	-0.892096	5.083864	2.775700
H	0.245638	4.569199	4.030980
C	-1.357882	1.798714	3.260565
H	-2.319623	2.328896	3.267130
H	-1.029355	1.746324	4.309056
C	1.566922	1.875479	2.624108
H	2.355221	2.259701	1.970057
H	1.871329	2.131465	3.649501
H	-0.288753	-1.998249	-0.276056
H	-0.131699	-1.513110	1.836972
F	3.254723	-3.593949	0.358800
F	1.416828	-3.857287	-0.742221
F	1.354451	-3.344685	1.365002
F	4.551856	-1.419694	-0.942029
F	3.322113	-0.102984	-2.132833
F	3.122091	-2.245590	-2.346927
F	1.947259	3.794761	-0.584654
F	2.268961	2.448670	-2.248154
F	2.837194	1.865154	-0.250627
F	-0.161611	3.764784	-2.454639
F	-0.220580	1.816979	-3.392886
F	-1.888226	2.498230	-2.197840
F	-4.610200	-0.936000	-1.613236
F	-2.958358	-0.224666	-2.804289
F	-3.917872	1.090790	-1.371811
F	-2.629666	-3.189843	-1.076089
F	-2.125676	-2.986268	1.029029
F	-4.119429	-2.550092	0.356905

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.044372	-0.456437	-0.338900
N	0.027580	-0.324173	1.664307
C	2.958047	-0.451102	1.337771

H	3.573080	-1.217465	1.819033
H	3.615563	0.375199	1.056658
C	-2.908762	-0.085269	1.456577
C	-0.088631	-1.059953	-2.028799
O	-0.097672	-1.485624	-3.103869
P	-2.262138	-0.713240	-0.105166
P	2.109878	-1.076232	-0.132552
Si	-1.394108	-0.022446	2.624894
Si	1.515655	0.168787	2.431146
C	-1.713024	-1.300747	3.964015
H	-0.920698	-1.328796	4.718930
H	-2.658113	-1.094973	4.482644
H	-1.785455	-2.301652	3.521531
C	1.776317	-0.543555	4.153566
H	2.795722	-0.328342	4.499077
H	1.089983	-0.115442	4.893898
H	1.642279	-1.631469	4.157296
H	-3.267767	0.934067	1.276635
H	-3.747931	-0.672300	1.841626
C	2.093126	-2.932284	0.235957
C	3.371464	-1.125511	-1.534526
C	-2.494893	-2.583987	0.055195
C	-3.649560	-0.396495	-1.349022
P	0.030335	1.688839	-0.795918
C	-0.705621	2.815026	0.442747
H	-0.628049	3.843455	0.072998
H	-1.776896	2.575155	0.446172
Si	-0.134286	2.793865	2.283136
C	1.686407	2.563530	-1.138615
C	-0.820104	2.348643	-2.352389
C	-0.188584	4.600541	2.806256
H	0.535543	5.198711	2.239379
H	-1.181048	5.040708	2.647361
H	0.052813	4.709332	3.870654
C	-1.316526	1.741813	3.308532
H	-2.320012	2.184581	3.360758
H	-0.929786	1.736587	4.338666
C	1.576487	2.061006	2.539713
H	2.297544	2.487368	1.834791
H	1.915978	2.356252	3.543133
F	3.314742	-3.487268	0.192398
F	1.316294	-3.591856	-0.631719
F	1.604781	-3.144077	1.467138
F	4.623516	-1.325897	-1.104946

F	3.355330	0.029253	-2.210291
F	3.063667	-2.105816	-2.395473
F	1.680234	3.865580	-0.814913
F	2.020563	2.465299	-2.430203
F	2.684300	2.000584	-0.428294
F	-0.564117	3.646836	-2.590741
F	-0.470657	1.658009	-3.440431
F	-2.149567	2.230765	-2.200954
F	-4.682459	-1.238671	-1.195521
F	-3.213679	-0.507222	-2.605615
F	-4.125005	0.846498	-1.176295
F	-2.505232	-3.154285	-1.157165
F	-1.458777	-3.098511	0.738843
F	-3.611130	-2.950240	0.695992

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.060566	0.043927	-0.653875
N	-0.915399	0.133522	1.427995
C	-0.588933	-2.796904	1.098589
H	-1.487491	-3.412506	1.201954
H	0.265114	-3.452284	1.287470
C	-0.395127	3.014920	0.960174
C	0.397273	-0.040120	-2.393628
O	0.504488	-0.113023	-3.545018
P	-0.353618	2.204344	-0.678359
P	-0.445521	-2.081955	-0.586729
Si	-0.862142	1.718013	2.267237
Si	-0.574308	-1.362576	2.349382
C	-2.523982	2.149230	3.009770
H	-2.862706	1.384569	3.717170
H	-2.451324	3.101982	3.549617
H	-3.293106	2.250924	2.238797
C	-1.924675	-1.642282	3.619892
H	-1.837846	-2.634266	4.080375
H	-1.869643	-0.901400	4.427262
H	-2.914343	-1.556625	3.157548
H	0.618227	3.372303	1.170009
H	-1.052582	3.890624	0.978110
P	2.167544	0.044411	0.025565

C	2.681160	0.979389	1.518854
H	3.768940	0.941247	1.634868
H	2.430407	2.026245	1.308724
Si	1.886248	0.497392	3.187464
C	3.248060	0.600757	4.476147
H	4.022551	-0.153621	4.292176
H	3.732662	1.584562	4.465852
H	2.851780	0.435506	5.485272
C	0.482832	1.685603	3.572311
H	0.858805	2.707238	3.717685
H	0.043217	1.378633	4.532561
C	1.094303	-1.210307	3.205351
H	1.791481	-1.976876	2.856278
H	0.916109	-1.432951	4.268328
H	-1.448048	0.063390	-1.076424
H	-1.877202	0.050252	1.067420
C	-4.932179	-0.287371	0.618470
C	-4.990154	-0.070050	-0.870902
H	-3.993336	0.031302	-1.297225
H	-5.523831	-0.895064	-1.354586
H	-5.561367	0.844745	-1.072360
C	-6.210350	-0.739681	1.281136
H	-7.076500	-0.195289	0.890522
H	-6.366903	-1.801457	1.051169
H	-6.143060	-0.619199	2.364387
O	-3.915584	-0.124960	1.272045
C	-2.100287	2.680854	-1.237719
C	0.618664	3.466424	-1.723963
C	3.479135	0.724789	-1.166837
C	3.178220	-1.561404	0.365978
C	0.508925	-3.366158	-1.624284
C	-2.143958	-2.612749	-1.231838
F	-2.456006	-2.070098	-2.410042
F	-2.263567	-3.948935	-1.352170
F	-3.082454	-2.232716	-0.343176
F	-0.083906	-3.529071	-2.819244
F	0.595212	-4.571443	-1.042293
F	1.754841	-2.947621	-1.872379
F	4.741123	0.533122	-0.732585
F	3.383576	0.178104	-2.382177
F	3.322417	2.049543	-1.298925
F	1.633832	3.959824	-0.991276
F	1.137170	2.870079	-2.803250
F	-0.087604	4.519946	-2.157764

F	4.052127	-1.441215	1.385099
F	2.363697	-2.585885	0.701638
F	3.878334	-1.962695	-0.699834
F	-2.377752	3.993933	-1.173028
F	-2.361979	2.273948	-2.484071
F	-2.977326	2.083162	-0.406479

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.177534	0.033632	-0.557035
N	-0.782372	-0.009688	1.225966
C	-0.371844	-2.945059	1.019924
H	-1.227605	-3.626548	1.046911
H	0.519249	-3.523635	1.277224
C	-0.668561	2.930553	1.028250
C	0.513091	0.024919	-2.320080
O	0.686785	0.002092	-3.462934
P	-0.371356	2.215911	-0.598736
P	-0.157723	-2.185332	-0.611229
Si	-1.063185	1.439634	2.161889
Si	-0.549153	-1.445924	2.201398
C	-2.816806	1.721853	2.774168
H	-3.255990	0.842068	3.252813
H	-2.808177	2.540249	3.506412
H	-3.490414	2.013777	1.961373
C	-1.959553	-1.797330	3.391163
H	-1.821134	-2.775199	3.870363
H	-2.007202	-1.050339	4.193656
H	-2.924847	-1.796660	2.872581
H	0.267275	3.397885	1.353573
H	-1.441326	3.704808	1.024262
P	2.274036	0.193032	0.118845
C	2.542438	1.092985	1.684417
H	3.617816	1.162670	1.879607
H	2.197254	2.117691	1.497128
Si	1.674592	0.480761	3.293920
C	2.966410	0.693527	4.644361
H	3.826684	0.034134	4.476578
H	3.339502	1.724254	4.688359
H	2.547142	0.450697	5.628170

C	0.149050	1.531011	3.611797
H	0.399441	2.578220	3.827776
H	-0.331347	1.136958	4.519934
C	1.054916	-1.290451	3.209453
H	1.831769	-1.975525	2.856957
H	0.836712	-1.590800	4.245085
H	-4.793422	-0.609556	-0.725833
H	-3.370381	-0.269609	0.951320
C	-5.211950	-0.434914	0.274720
O	-4.205935	-0.650197	1.257616
C	-5.746978	0.992586	0.341748
H	-4.959925	1.718218	0.113538
H	-6.555161	1.141894	-0.384041
H	-6.135806	1.204765	1.344009
C	-6.298594	-1.467604	0.528459
H	-6.732907	-1.330313	1.525687
H	-7.099689	-1.379755	-0.213285
H	-5.880011	-2.477396	0.470810
C	3.524456	1.076554	-0.989537
C	3.371695	-1.341707	0.424049
C	0.368740	3.642014	-1.590503
C	-2.085830	2.217965	-1.403498
C	0.853498	-3.357765	-1.708149
C	-1.838903	-2.542522	-1.391328
F	-1.994209	-1.895678	-2.552569
F	-2.047466	-3.849283	-1.613761
F	-2.800880	-2.125597	-0.557868
F	0.295337	-3.469872	-2.921876
F	0.962890	-4.584004	-1.185370
F	2.088794	-2.877000	-1.891236
F	4.117197	-1.642393	-0.642821
F	4.203380	-1.189354	1.466792
F	2.616539	-2.425756	0.697619
F	3.533474	0.568638	-2.224697
F	3.182036	2.371771	-1.080867
F	4.781344	1.033685	-0.516083
F	-2.716787	1.065940	-1.100398
F	-1.978031	2.273149	-2.736007
F	-2.885196	3.215257	-1.006725
F	-0.537422	4.589182	-1.878118
F	0.905271	3.224550	-2.738290
F	1.332217	4.224812	-0.860491

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.026355	-0.409324	-0.427969
N	-0.286711	-0.457444	1.786933
C	2.246586	-1.822846	1.536151
H	1.741345	-2.786782	1.622315
H	3.280764	-1.971640	1.857940
C	-2.679814	1.087030	1.064606
C	-0.037911	-0.684187	-2.195554
O	-0.062950	-0.919744	-3.326255
P	-2.477828	-0.173371	-0.251593
P	2.115419	-1.242522	-0.192554
Si	-1.553175	0.570348	2.522564
Si	1.286218	-0.583376	2.599983
C	-2.445856	-0.417952	3.839747
H	-1.871961	-0.400541	4.773922
H	-3.436782	-0.001524	4.054451
H	-2.572740	-1.461429	3.539070
C	1.105437	-1.287976	4.328816
H	2.081256	-1.580289	4.736402
H	0.671836	-0.556562	5.021930
H	0.461801	-2.175791	4.332757
H	-2.318893	2.043498	0.676742
H	-3.722554	1.234609	1.360944
P	0.386938	1.833919	-0.645251
C	0.508121	3.073745	0.713238
H	1.212415	3.855240	0.407504
H	-0.467941	3.575051	0.762380
Si	0.876969	2.567038	2.509161
C	1.598666	4.098412	3.321897
H	2.573653	4.350547	2.887043
H	0.941655	4.967472	3.196098
H	1.745569	3.944231	4.397616
C	-0.768634	2.094567	3.281471
H	-1.470030	2.938210	3.223292
H	-0.611094	1.902079	4.352238
C	2.068378	1.121199	2.662155
H	2.838354	1.229195	1.893754
H	2.589931	1.217606	3.625129
H	-0.132882	-2.138452	-0.185446
H	-0.740619	-1.403022	1.748894

C	-0.067040	-4.282066	0.780198
H	-0.636435	-5.220535	0.810937
H	0.799217	-4.447510	0.139158
H	0.246060	-4.070952	1.806103
C	-1.033782	-3.202352	0.287427
C	-1.633083	-3.561741	-1.074646
H	-2.391849	-4.336747	-0.912506
H	-2.111739	-2.713148	-1.561557
H	-0.871297	-3.958701	-1.748009
O	-1.764815	-2.680646	1.191284
C	2.043530	2.193972	-1.492190
C	3.949489	-0.679905	-0.336952
C	2.455541	-2.755526	-1.316633
C	-0.623330	2.940422	-1.820290
C	-3.371602	0.429431	-1.829338
C	-4.002426	-1.209496	0.297562
F	3.021150	2.065265	-0.575052
F	2.164023	3.428921	-1.997398
F	2.274994	1.335471	-2.488647
F	4.274158	0.168651	0.654987
F	4.773156	-1.737349	-0.195537
F	4.258452	-0.094667	-1.492254
F	3.043366	-3.763252	-0.652411
F	3.265570	-2.400414	-2.326775
F	1.348861	-3.247097	-1.876544
F	-0.257900	4.230320	-1.800572
F	-0.540228	2.517528	-3.083592
F	-1.918907	2.928816	-1.442321
F	-2.494680	0.802648	-2.766577
F	-4.063420	-0.596488	-2.360200
F	-4.218697	1.445537	-1.634581
F	-4.161090	-2.375269	-0.316565
F	-5.114974	-0.478094	0.034669
F	-4.022810	-1.411714	1.615195

$R^1=R^2=R^3=CHF_2$

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.182175	-0.734407	-0.560366
N	-0.157943	-0.220536	1.688255

C	2.666115	-1.052300	1.329834
H	3.033916	-1.868160	1.959880
H	3.539287	-0.496561	0.979249
C	-2.844949	0.782304	0.898207
C	-0.274891	-1.407055	-2.180640
O	-0.348958	-1.903619	-3.234425
P	-2.353357	-0.466993	-0.343973
P	1.745557	-1.698454	-0.120721
Si	-1.527555	0.793319	2.263427
Si	1.510002	0.121393	2.259699
C	-2.229935	0.080758	3.847985
H	-1.457006	-0.016899	4.619544
H	-3.013364	0.738078	4.245357
H	-2.674456	-0.906022	3.684836
C	1.616998	-0.223490	4.101986
H	2.654772	-0.153183	4.451684
H	1.026518	0.491798	4.687651
H	1.255588	-1.231493	4.339093
H	-2.853385	1.758535	0.399196
H	-3.852853	0.603686	1.287339
P	0.425030	1.281426	-1.257136
C	0.016386	2.853868	-0.396262
H	0.424806	3.696074	-0.963640
H	-1.075101	2.948596	-0.448090
Si	0.526944	3.037165	1.424091
C	0.996126	4.838146	1.681217
H	1.876414	5.102162	1.082350
H	0.180780	5.511388	1.389148
H	1.234170	5.042233	2.732340
C	-0.915099	2.544794	2.527849
H	-1.760690	3.233219	2.394928
H	-0.589504	2.654855	3.572619
C	1.952069	1.911996	1.906634
H	2.739844	1.959341	1.148684
H	2.386799	2.321579	2.830168
H	-0.641285	-2.156957	-0.053717
H	-0.381249	-1.193693	1.912308
C	-3.207471	-1.982658	0.364124
H	-3.057959	-2.870835	-0.253380
C	-3.528631	-0.187497	-1.779330
H	-3.146731	0.548947	-2.487705
C	-0.237234	1.736356	-2.957577
H	-0.143022	0.929477	-3.690337
C	2.231811	1.624712	-1.729143

H	2.458852	1.290342	-2.744315
C	1.531915	-3.463881	0.469091
H	0.913032	-4.068005	-0.200151
C	3.049975	-2.075542	-1.436515
H	2.956373	-3.094422	-1.825325
F	-2.671942	-2.231737	1.604298
F	-4.542027	-1.793171	0.551889
F	-3.665628	-1.380535	-2.434036
F	-4.765507	0.208981	-1.375196
F	-1.567381	2.044872	-2.831607
F	0.371414	2.844796	-3.469730
F	2.560532	2.944003	-1.633391
F	3.080795	0.963276	-0.882530
F	0.932598	-3.428006	1.699415
F	2.733519	-4.094974	0.637572
F	4.312062	-1.915536	-0.960860
F	2.898018	-1.227551	-2.494858

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.054203	-0.622994	-0.564749
N	-0.057878	-0.545921	1.431415
C	2.870051	-0.808835	1.207025
H	3.340356	-1.678041	1.677750
H	3.646204	-0.058846	1.039573
C	-2.987084	-0.247451	1.164174
C	-0.111325	-1.194961	-2.239909
O	-0.168735	-1.605381	-3.331577
P	-2.305198	-0.733246	-0.439810
P	2.089025	-1.256706	-0.371013
Si	-1.495068	-0.197501	2.347287
Si	1.424655	-0.108153	2.233952
C	-1.865432	-1.448770	3.702318
H	-1.098153	-1.475711	4.482463
H	-2.824552	-1.226403	4.187489
H	-1.934891	-2.455237	3.270788
C	1.617558	-0.800157	3.977009
H	2.638683	-0.618037	4.337418
H	0.935891	-0.333903	4.698325
H	1.443889	-1.882523	3.996964

H	-3.423656	0.751466	1.058421
H	-3.782180	-0.924841	1.489688
P	0.182741	1.522171	-1.014705
C	-0.640358	2.653004	0.160182
H	-0.524835	3.683565	-0.191710
H	-1.710196	2.417387	0.091475
Si	-0.137086	2.583972	2.019853
C	-0.138799	4.384376	2.574735
H	0.619260	4.966526	2.036448
H	-1.112292	4.859587	2.399508
H	0.079037	4.466403	3.646773
C	-1.385848	1.575556	3.011702
H	-2.376392	2.048919	3.027736
H	-1.029482	1.573232	4.053101
C	1.538047	1.785133	2.332135
H	2.294471	2.178840	1.646633
H	1.856100	2.077478	3.343600
C	-2.696509	-2.566738	-0.569972
H	-2.802080	-2.896197	-1.608366
C	-3.555153	-0.095013	-1.681301
H	-3.207668	-0.140038	-2.716275
C	-0.396971	2.144139	-2.684906
H	0.131950	1.647460	-3.506068
C	1.887475	2.325808	-1.208029
H	2.206612	2.370499	-2.252254
C	2.122557	-3.127338	-0.295917
H	1.653774	-3.595252	-1.167779
C	3.367236	-1.067246	-1.746378
H	3.534532	-1.997735	-2.296850
F	-1.656924	-3.256376	-0.009841
F	-3.819219	-2.915626	0.107167
F	-4.723423	-0.792247	-1.592128
F	-3.828826	1.200787	-1.365034
F	-1.728148	1.905053	-2.830839
F	-0.210187	3.490391	-2.813853
F	1.899501	3.591691	-0.708619
F	2.842633	1.628627	-0.524349
F	1.462399	-3.532381	0.820294
F	3.405936	-3.590559	-0.204351
F	4.557776	-0.644125	-1.256669
F	2.932874	-0.137239	-2.648779

A3

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.088456	-0.013544	-0.731811
N	0.817593	0.305085	1.447514
C	0.073152	3.052400	0.825065
H	0.854360	3.799077	1.002921
H	-0.878102	3.586384	0.786214
C	1.663558	-2.376725	1.025093
C	0.017577	-0.111014	-2.488794
O	0.104749	-0.140469	-3.650526
P	0.650643	-2.134267	-0.475753
P	0.338469	2.183064	-0.771929
Si	1.001542	-1.217135	2.354188
Si	0.043960	1.729310	2.182881
C	2.283326	-1.070742	3.717308
H	1.914124	-0.497367	4.575238
H	2.561931	-2.067000	4.084503
H	3.191220	-0.587647	3.341651
C	1.045759	2.360308	3.640669
H	0.671349	3.336794	3.973701
H	0.993926	1.681078	4.499454
H	2.102511	2.482679	3.374002
H	1.760936	-3.427845	1.313261
H	2.667501	-1.982152	0.823170
P	-2.119005	-0.150016	-0.451942
C	-2.834026	-1.075810	0.959241
H	-3.923426	-0.980142	0.963714
H	-2.620102	-2.136673	0.785087
Si	-2.153412	-0.592999	2.663490
C	-3.535533	-0.926884	3.895227
H	-4.407593	-0.296885	3.680808
H	-3.864012	-1.972801	3.852689
H	-3.221152	-0.719100	4.925236
C	-0.666428	-1.674948	3.093407
H	-0.914110	-2.724446	2.882360
H	-0.546937	-1.625013	4.185967
C	-1.677379	1.233964	2.753304
H	-2.433788	1.819406	2.218596
H	-1.763196	1.531588	3.808526
H	1.676394	-0.070771	-0.950290
H	1.756648	0.554782	1.124189
C	4.775665	0.090554	0.091480

O	4.136718	-0.230742	1.077371
C	5.691421	1.289130	0.097815
H	5.542293	1.879309	1.003305
H	6.732391	0.944529	0.055736
H	5.521252	1.910427	-0.787743
C	4.689365	-0.686362	-1.198757
H	4.012370	-0.150101	-1.876272
H	5.664290	-0.755572	-1.692197
H	4.286912	-1.686549	-1.025694
C	1.698103	-2.803913	-1.884929
H	2.240594	-1.992642	-2.376893
C	-0.461660	-3.634556	-0.230516
H	-0.893342	-3.626000	0.776823
C	-2.989714	-1.009758	-1.879268
H	-2.545444	-1.978804	-2.108622
C	-3.297386	1.343668	-0.490394
H	-3.650557	1.548547	-1.502211
C	2.109809	2.692956	-1.099789
H	2.537319	2.193216	-1.973926
C	-0.428852	3.283744	-2.096860
H	0.236596	3.403079	-2.958154
F	2.606872	-3.729684	-1.467890
F	0.883389	-3.397118	-2.801648
F	-1.497299	-3.650822	-1.122909
F	0.213365	-4.808002	-0.377441
F	-4.318582	-1.193896	-1.613237
F	-2.916837	-0.220838	-2.991087
F	-4.386417	1.171796	0.313245
F	-2.670576	2.472200	-0.035348
F	2.856332	2.352455	-0.000986
F	2.250794	4.041387	-1.263672
F	-0.724642	4.518737	-1.612803
F	-1.586495	2.729678	-2.551392

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.066703	-0.042122	-0.644680
N	0.716866	0.458402	1.199693
C	-0.493947	3.091919	0.572477
H	0.238946	3.905579	0.572480

H	-1.485965	3.535646	0.694013
C	1.703612	-2.301128	1.351006
C	0.061256	-0.266992	-2.415179
O	0.100207	-0.355101	-3.572669
P	1.131982	-2.023254	-0.356906
P	-0.401858	2.150063	-0.982595
Si	1.251728	-0.747581	2.357692
Si	-0.118048	1.813714	1.937822
C	2.751809	-0.281957	3.396977
H	2.475946	0.378058	4.226899
H	3.192506	-1.187293	3.834950
H	3.518332	0.236034	2.813855
C	0.901582	2.694142	3.253443
H	0.455384	3.669910	3.485590
H	0.949096	2.131128	4.193106
H	1.928042	2.864606	2.907848
H	1.206444	-3.187802	1.762971
H	2.775355	-2.523177	1.369925
P	-2.004808	-0.786874	-0.281020
C	-2.199259	-1.642477	1.319293
H	-3.205219	-2.067856	1.391213
H	-1.494638	-2.484444	1.305482
Si	-1.829548	-0.655330	2.929056
C	-3.209633	-1.123822	4.119374
H	-4.184139	-0.791285	3.741139
H	-3.262369	-2.208953	4.271820
H	-3.058417	-0.658618	5.101201
C	-0.148584	-1.209124	3.553371
H	-0.134895	-2.287107	3.763708
H	0.032090	-0.710133	4.516768
C	-1.736566	1.213056	2.727917
H	-2.608794	1.591890	2.187685
H	-1.801833	1.635330	3.741992
H	3.642652	1.019329	-0.970250
H	2.570939	1.295398	0.917302
C	4.262301	1.231400	-0.082717
O	3.443118	1.734772	0.955790
C	5.256460	2.321596	-0.453863
H	4.728615	3.215574	-0.797416
H	5.858448	2.593087	0.421234
H	5.933560	1.985521	-1.247081
C	4.967611	-0.053442	0.349523
H	5.563254	-0.480222	-0.466317
H	5.635125	0.149596	1.194710

H	4.245295	-0.810418	0.673836
C	2.702529	-2.076571	-1.395687
H	3.167938	-1.089035	-1.456597
C	0.422727	-3.697671	-0.800867
H	-0.381094	-3.970602	-0.106000
C	-2.750364	-2.033466	-1.466651
H	-2.155813	-2.943388	-1.560591
C	-3.534253	0.331773	-0.270395
H	-4.052522	0.328739	-1.230198
C	0.974133	3.029216	-1.898775
H	1.175146	2.591340	-2.882545
C	-1.744466	2.765038	-2.170098
H	-1.318493	3.227296	-3.064671
F	3.622081	-2.950389	-0.909780
F	2.370981	-2.470433	-2.653586
F	-0.093888	-3.682204	-2.061605
F	1.367814	-4.669526	-0.750877
F	-4.011879	-2.387096	-1.077353
F	-2.854488	-1.456671	-2.695532
F	-4.415981	-0.050227	0.693991
F	-3.185315	1.621022	0.015368
F	2.108585	2.979137	-1.159641
F	0.663914	4.348120	-2.077272
F	-2.556495	3.673193	-1.579096
F	-2.508711	1.717737	-2.591831

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.208721	0.495597	-0.580604
N	-0.024696	0.577312	1.624695
C	-2.850909	1.045591	0.929155
H	-3.224177	2.003174	1.308048
H	-3.720901	0.413090	0.738047
C	2.866710	-0.167128	1.443158
C	0.407655	0.822909	-2.311506
O	0.538331	1.134272	-3.423196
P	2.381661	-0.051467	-0.328581
P	-1.927349	1.353348	-0.626290
Si	1.352964	-0.019000	2.590014
Si	-1.684651	0.279508	2.215052

C	1.715617	1.215203	3.956824
H	1.023696	1.086335	4.797045
H	2.734967	1.109131	4.347291
H	1.588347	2.237738	3.583385
C	-1.942454	1.172566	3.845465
H	-3.003565	1.168509	4.125589
H	-1.388479	0.699661	4.665399
H	-1.616441	2.216659	3.773695
H	3.366043	-1.128659	1.616657
H	3.624361	0.589031	1.670323
P	-0.447338	-1.694696	-0.767824
C	0.200588	-2.844102	0.509694
H	0.007682	-3.877379	0.206783
H	1.287449	-2.724050	0.547569
Si	-0.410032	-2.619394	2.305937
C	-0.700840	-4.342211	2.995138
H	-1.515226	-4.847435	2.462268
H	0.196575	-4.966423	2.904653
H	-0.970476	-4.302436	4.057531
C	0.934005	-1.721537	3.271091
H	1.843864	-2.333190	3.335269
H	0.572258	-1.605178	4.303161
C	-1.957577	-1.565927	2.456865
H	-2.748471	-1.938475	1.800829
H	-2.323465	-1.703310	3.484924
H	0.937367	2.074128	-0.218513
H	0.059615	1.629456	1.658522
C	1.031842	3.351072	0.553364
O	0.185018	3.268319	1.498630
C	0.792980	4.324871	-0.603425
H	-0.268822	4.481905	-0.769780
H	1.224893	5.295386	-0.323606
H	1.272596	3.993904	-1.530175
C	2.501070	3.384316	0.994426
H	3.216528	3.532250	0.182542
H	2.584755	4.250164	1.662314
H	2.782583	2.505901	1.574693
C	3.529562	1.225258	-1.129430
H	3.002099	2.167238	-1.277486
C	3.324608	-1.560346	-0.962264
H	2.998413	-2.487377	-0.479899
C	0.152053	-2.547967	-2.332963
H	1.225704	-2.457152	-2.488128
C	-2.199182	-2.426345	-0.937922

H	-2.459223	-2.610347	-1.980112
C	-2.411092	3.152309	-0.930084
H	-1.858685	3.598619	-1.763326
C	-3.013997	0.788412	-2.077432
H	-3.059167	1.566266	-2.844614
F	4.647054	1.455135	-0.390837
F	3.922673	0.774860	-2.349124
F	3.168952	-1.718280	-2.307701
F	4.655339	-1.422420	-0.719157
F	-0.165045	-3.879344	-2.311920
F	-0.483539	-2.005693	-3.407349
F	-2.318537	-3.605027	-0.261885
F	-3.136949	-1.588746	-0.409908
F	-2.238607	3.903538	0.178505
F	-3.746223	3.218858	-1.234778
F	-4.280027	0.493695	-1.695204
F	-2.494978	-0.317020	-2.682494

$R^1=R^2=R^3$=Ph

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.096774	0.535204	-0.282600
N	-0.600756	0.966685	1.992666
C	-2.881559	-0.690978	1.167458
H	-3.951790	-0.690158	1.399058
H	-2.603017	-1.723316	0.929465
C	1.924474	2.350522	1.670444
C	0.026340	0.580808	-2.018572
O	0.072245	0.711328	-3.185852
P	1.889989	1.522123	0.012087
P	-2.390355	0.325364	-0.283232
Si	0.810762	1.504048	2.927018
Si	-1.850456	-0.119577	2.643302
C	0.277194	2.791675	4.192392
H	-0.330873	2.350382	4.991135
H	1.146837	3.265336	4.665831
H	-0.316317	3.586140	3.722953
C	-2.945680	0.813174	3.855260
H	-3.803214	0.201579	4.164213
H	-2.399115	1.095593	4.763169

H	-3.339182	1.732235	3.404334
H	2.940162	2.544215	2.033814
H	1.469335	3.335298	1.499025
P	0.596004	-1.649533	-0.004608
C	1.496930	-2.069500	1.550145
H	1.754601	-3.135336	1.557798
H	2.452502	-1.534487	1.468318
Si	0.862408	-1.646716	3.280649
C	1.548790	-2.986703	4.415929
H	1.111944	-3.967815	4.190220
H	2.637155	-3.078027	4.311837
H	1.333805	-2.766253	5.468850
C	1.555347	0.022699	3.805952
H	2.646697	0.012473	3.695160
H	1.361834	0.141612	4.881758
C	-1.006907	-1.570656	3.481524
H	-1.466274	-2.504734	3.135701
H	-1.201266	-1.512501	4.562518
H	-0.372345	2.102300	-0.321699
H	-1.042898	1.809146	1.616401
C	3.507394	0.630821	-0.077171
C	3.958340	0.240573	-1.345608
C	4.278442	0.287372	1.035360
C	5.154351	-0.448981	-1.496166
H	3.368957	0.482424	-2.226427
C	5.470726	-0.423201	0.888882
H	3.962650	0.579546	2.032480
C	5.914528	-0.787657	-0.377373
H	5.484146	-0.738566	-2.489243
H	6.055698	-0.678680	1.768432
H	6.847554	-1.331326	-0.495056
C	2.342085	2.968418	-1.061798
C	3.604134	3.564558	-0.933275
C	1.431026	3.527198	-1.959470
C	3.944171	4.686403	-1.681054
H	4.333354	3.144972	-0.245167
C	1.773311	4.645510	-2.718501
H	0.448786	3.083677	-2.063532
C	3.027928	5.229190	-2.580744
H	4.926272	5.136171	-1.564123
H	1.053125	5.057221	-3.420304
H	3.293669	6.102001	-3.170850
C	1.799141	-2.324888	-1.260896
C	2.949797	-3.040093	-0.914394

C	1.526792	-2.149020	-2.623032
C	3.800690	-3.553829	-1.890103
H	3.218579	-3.192634	0.123794
C	2.375159	-2.658997	-3.600448
H	0.648444	-1.600008	-2.936115
C	3.519584	-3.364704	-3.238441
H	4.693401	-4.094688	-1.588189
H	2.138974	-2.499210	-4.648734
H	4.185992	-3.760062	-3.999980
C	-0.633584	-3.037846	-0.113909
C	-1.465815	-3.070869	-1.238979
C	-0.790467	-4.037955	0.850555
C	-2.416927	-4.072195	-1.401122
H	-1.382578	-2.292488	-1.992076
C	-1.757486	-5.031736	0.702649
H	-0.159954	-4.058426	1.733485
C	-2.572764	-5.053594	-0.424530
H	-3.048524	-4.071084	-2.284412
H	-1.865577	-5.793711	1.469806
H	-3.323622	-5.829718	-0.542179
C	-3.405742	-0.319763	-1.678146
C	-4.381005	-1.307254	-1.521162
C	-3.209149	0.238162	-2.946717
C	-5.139550	-1.732831	-2.609745
H	-4.547728	-1.763129	-0.550479
C	-3.966547	-0.185703	-4.033764
H	-2.457085	1.007955	-3.087169
C	-4.933864	-1.174853	-3.868225
H	-5.892193	-2.504346	-2.471789
H	-3.799556	0.258118	-5.010956
H	-5.525331	-1.507787	-4.716379
C	-3.341412	1.901828	0.008377
C	-2.873184	3.096588	-0.548939
C	-4.553099	1.932118	0.709981
C	-3.578170	4.287270	-0.392768
H	-1.933667	3.090072	-1.090436
C	-5.254155	3.123461	0.879774
H	-4.968378	1.023962	1.134611
C	-4.766520	4.306817	0.331588
H	-3.190688	5.201642	-0.833394
H	-6.186389	3.123752	1.437770
H	-5.311291	5.237102	0.465326

A2

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.146812	0.309941	-0.202762
N	0.119090	1.005520	1.720707
C	-2.791378	1.216689	1.278525
H	-3.468135	2.061158	1.448789
H	-3.373150	0.288411	1.332932
C	2.940016	0.113376	1.708124
C	0.283352	0.192437	-1.950429
O	0.415917	0.182495	-3.116499
P	2.442590	0.267194	-0.035832
P	-1.990021	1.256190	-0.360786
Si	1.536733	0.922452	2.707263
Si	-1.391811	1.104223	2.559947
C	2.165615	2.606093	3.281553
H	1.423408	3.150314	3.876844
H	3.074213	2.506202	3.889328
H	2.415594	3.229137	2.412616
C	-1.525700	2.592983	3.717959
H	-2.526869	2.648648	4.165154
H	-0.806642	2.531619	4.544492
H	-1.346014	3.536623	3.188457
H	2.962662	-0.947615	1.976242
H	3.931418	0.529290	1.917271
P	-0.270593	-1.877372	0.304670
C	0.300524	-2.389621	1.992323
H	0.029348	-3.442750	2.141080
H	1.395748	-2.398697	1.912843
Si	-0.118427	-1.486180	3.635046
C	-0.250698	-2.882631	4.902937
H	-1.081066	-3.564460	4.677358
H	0.668700	-3.481190	4.938654
H	-0.420143	-2.478523	5.908700
C	1.232676	-0.272211	4.146693
H	2.164194	-0.774780	4.438395
H	0.864013	0.249837	5.042007
C	-1.686311	-0.457639	3.601042
H	-2.549186	-1.019709	3.228871
H	-1.916346	-0.178279	4.639670
C	3.547762	-0.838920	-0.998482
C	3.757765	-0.576891	-2.357925

C	4.111984	-1.987685	-0.439329
C	4.515032	-1.445112	-3.137094
H	3.324674	0.309940	-2.812025
C	4.870397	-2.857199	-1.219165
H	3.961400	-2.218830	0.610664
C	5.073811	-2.588999	-2.569021
H	4.670000	-1.227028	-4.189825
H	5.299710	-3.747389	-0.768753
H	5.665611	-3.266706	-3.177527
C	3.103428	1.923092	-0.494071
C	4.443077	2.263056	-0.266044
C	2.254886	2.873128	-1.064875
C	4.914725	3.530446	-0.586655
H	5.125623	1.529094	0.155318
C	2.724078	4.146567	-1.383558
H	1.216718	2.625236	-1.265346
C	4.052842	4.477164	-1.141585
H	5.955929	3.781051	-0.404969
H	2.043469	4.874062	-1.816032
H	4.421984	5.468759	-1.387947
C	0.424614	-3.268236	-0.705765
C	0.182434	-4.604568	-0.356961
C	1.173939	-3.006894	-1.852031
C	0.697159	-5.644926	-1.120527
H	-0.433147	-4.839800	0.507630
C	1.689418	-4.047740	-2.623680
H	1.362422	-1.985521	-2.151927
C	1.457611	-5.367810	-2.257137
H	0.497606	-6.674264	-0.835866
H	2.276054	-3.815615	-3.507366
H	1.858538	-6.181141	-2.855589
C	-2.036863	-2.401604	0.263767
C	-2.701235	-2.253052	-0.958526
C	-2.735947	-2.949064	1.341706
C	-4.036484	-2.612173	-1.095465
H	-2.166056	-1.842276	-1.809883
C	-4.078685	-3.303477	1.211037
H	-2.242023	-3.112108	2.293954
C	-4.733057	-3.129506	-0.004835
H	-4.534106	-2.468973	-2.050030
H	-4.608587	-3.720782	2.062732
H	-5.780232	-3.400344	-0.105182
C	-3.321196	0.858316	-1.562170
C	-4.669608	0.866735	-1.193689

C	-2.988846	0.548049	-2.886065
C	-5.661463	0.559618	-2.121683
H	-4.956057	1.107776	-0.175172
C	-3.979186	0.243574	-3.814949
H	-1.949874	0.537249	-3.197157
C	-5.319658	0.245208	-3.434013
H	-6.703972	0.565752	-1.816397
H	-3.701634	0.002709	-4.837074
H	-6.092946	0.003898	-4.157659
C	-1.738656	3.065745	-0.669343
C	-2.419695	3.761864	-1.673948
C	-0.816368	3.766332	0.120860
C	-2.187333	5.119966	-1.880435
H	-3.138620	3.249990	-2.305042
C	-0.594396	5.125703	-0.079081
H	-0.252492	3.233300	0.881566
C	-1.277245	5.808014	-1.083220
H	-2.724079	5.639967	-2.669046
H	0.127053	5.646010	0.544772
H	-1.099357	6.867317	-1.245411

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.045494	-0.151877	-0.366823
N	-0.560957	-0.855240	1.840687
C	1.920534	-2.337099	1.343807
H	2.191769	-3.369102	1.591030
H	2.855425	-1.766810	1.282342
C	-2.806011	0.861563	1.279554
C	0.039698	0.047821	-2.092612
O	-0.005597	0.125601	-3.265437
P	-1.825201	1.211768	-0.251788
P	1.108955	-2.138425	-0.296255
Si	-1.743101	0.182991	2.673453
Si	0.840237	-1.550420	2.681241
C	-2.835025	-0.842329	3.806084
H	-2.267037	-1.272184	4.639724
H	-3.630305	-0.219828	4.236603
H	-3.327745	-1.662290	3.270161
C	0.273828	-2.859612	3.912415

H	1.111927	-3.488279	4.239631
H	-0.156921	-2.400534	4.810340
H	-0.492247	-3.517092	3.484514
H	-3.467788	1.685261	1.569676
H	-3.470713	0.032235	1.008688
P	1.604295	1.375246	0.177516
C	1.348492	2.378837	1.699524
H	2.168235	3.095209	1.831407
H	0.453030	2.980885	1.498034
Si	1.035638	1.559904	3.377580
C	1.824566	2.695268	4.660695
H	2.913818	2.746707	4.536039
H	1.433962	3.717329	4.577844
H	1.625960	2.345978	5.681312
C	-0.818148	1.467213	3.684305
H	-1.258610	2.462586	3.542463
H	-0.968867	1.220368	4.745295
C	1.740577	-0.174542	3.585830
H	2.802532	-0.185293	3.313561
H	1.700302	-0.394328	4.662863
H	-1.279596	-1.119813	-0.632947
H	-1.088144	-1.603394	1.382981
C	-5.046992	-2.140648	0.741477
C	-5.920973	-1.284202	-0.145461
H	-5.360247	-0.399069	-0.470671
H	-6.209583	-1.824209	-1.053399
H	-6.811798	-0.964997	0.399819
C	-3.840504	-2.776697	0.096297
H	-4.112555	-3.277116	-0.838894
H	-3.101941	-2.007573	-0.170711
H	-3.374687	-3.494129	0.776240
O	-5.289355	-2.279804	1.926577
C	3.369295	0.827108	0.390124
C	3.919782	0.017491	-0.609236
C	4.182503	1.168110	1.475649
C	5.224331	-0.457091	-0.522708
H	3.314947	-0.263208	-1.464071
C	5.487706	0.687324	1.574584
H	3.812981	1.815685	2.263862
C	6.012219	-0.130661	0.578621
H	5.613372	-1.095069	-1.310902
H	6.094720	0.959130	2.433952
H	7.027587	-0.508316	0.658617
C	1.933883	2.712557	-1.073954

C	1.960573	4.073019	-0.756449
C	2.199078	2.343639	-2.398880
C	2.240171	5.032550	-1.727461
H	1.739002	4.412973	0.248537
C	2.476268	3.298268	-3.370996
H	2.181407	1.299038	-2.685573
C	2.498067	4.651008	-3.039113
H	2.242712	6.084099	-1.453450
H	2.672283	2.982158	-4.391725
H	2.711906	5.398898	-3.797478
C	2.392374	-2.730371	-1.488789
C	3.450688	-3.555138	-1.095785
C	2.291704	-2.368759	-2.836563
C	4.389363	-4.000300	-2.022826
H	3.559065	-3.849929	-0.056941
C	3.228221	-2.815547	-3.765379
H	1.487763	-1.720156	-3.166510
C	4.282121	-3.630603	-3.361288
H	5.206702	-4.637405	-1.696451
H	3.133109	-2.520859	-4.806657
H	5.015167	-3.976031	-4.084564
C	-0.021196	-3.602042	-0.400281
C	-0.779477	-3.733407	-1.572114
C	-0.164573	-4.569620	0.594669
C	-1.638726	-4.808371	-1.749891
H	-0.699723	-2.975798	-2.347156
C	-1.052913	-5.636147	0.431723
H	0.413082	-4.514119	1.511875
C	-1.785568	-5.762638	-0.741428
H	-2.206323	-4.897085	-2.672084
H	-1.157525	-6.372937	1.223337
H	-2.471064	-6.594952	-0.872231
C	-3.164762	1.013700	-1.525607
C	-4.214181	1.940460	-1.596835
C	-3.197470	-0.092791	-2.377973
C	-5.262180	1.766726	-2.495465
H	-4.212717	2.811805	-0.947509
C	-4.242859	-0.264913	-3.283754
H	-2.403670	-0.827853	-2.321022
C	-5.277755	0.662304	-3.346022
H	-6.064810	2.497845	-2.533911
H	-4.243038	-1.128516	-3.943261
H	-6.090776	0.529351	-4.054244
C	-1.693285	3.052796	-0.285918

C	-1.300565	3.645580	-1.492801
C	-1.922763	3.877627	0.818206
C	-1.171431	5.024843	-1.598976
H	-1.091921	3.021820	-2.358437
C	-1.770894	5.261051	0.720255
H	-2.228555	3.449316	1.767937
C	-1.403438	5.838224	-0.490758
H	-0.868170	5.463279	-2.544640
H	-1.954154	5.884938	1.590843
H	-1.293569	6.915805	-0.572350

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.064698	-0.112689	-0.155916
N	1.024949	0.037062	1.667310
C	1.524592	2.792239	1.048984
H	2.610463	2.668097	0.974036
H	1.324256	3.854541	1.212249
C	0.307520	-2.796203	1.907236
C	-0.252343	-0.215078	-1.881455
O	-0.439189	-0.240007	-3.040267
P	0.302915	-2.393144	0.128004
P	0.763619	2.145180	-0.496965
Si	0.929619	-1.247464	2.828140
Si	0.939402	1.615319	2.397201
C	2.564048	-1.680781	3.664042
H	2.860393	-0.908387	4.382416
H	2.484128	-2.629521	4.211592
H	3.378459	-1.762805	2.936403
C	2.042821	1.886340	3.905840
H	2.035756	2.951245	4.175926
H	1.719195	1.328516	4.792554
H	3.074285	1.603442	3.670733
H	-0.738515	-2.971351	2.182911
H	0.854041	-3.710210	2.161399
P	-2.163714	-0.085104	0.336903
C	-2.544436	-0.514477	2.082136
H	-3.629485	-0.493099	2.240215
H	-2.254896	-1.563904	2.198694
Si	-1.653999	0.387392	3.509861

C	-2.961144	0.730757	4.828272
H	-3.717731	1.442530	4.474108
H	-3.480146	-0.187855	5.129423
H	-2.504272	1.161265	5.728180
C	-0.356896	-0.816827	4.164468
H	-0.848517	-1.729815	4.529937
H	0.145659	-0.373129	5.035344
C	-0.835386	1.983406	2.938187
H	-1.424972	2.402184	2.111979
H	-0.842762	2.727737	3.746284
H	4.289895	1.525848	-0.076748
H	3.099531	0.202483	1.384728
C	4.810961	0.799444	0.564646
O	3.998136	0.458478	1.675365
C	5.136972	-0.435859	-0.263803
H	4.220204	-0.895644	-0.645417
H	5.772040	-0.185289	-1.121664
H	5.657163	-1.175670	0.355015
C	6.059824	1.464872	1.121341
H	6.604034	0.771251	1.773034
H	6.727834	1.776054	0.310573
H	5.793559	2.349276	1.710197
C	-0.677278	-3.735438	-0.663412
C	-1.151660	-3.570993	-1.968174
C	-0.911460	-4.949093	-0.009804
C	-1.834265	-4.600551	-2.607691
H	-1.007902	-2.628871	-2.485357
C	-1.604190	-5.975681	-0.645847
H	-0.547739	-5.105322	1.001128
C	-2.064104	-5.804987	-1.948146
H	-2.202902	-4.451919	-3.618186
H	-1.777944	-6.912445	-0.123684
H	-2.602593	-6.606382	-2.446036
C	1.984098	-2.856848	-0.477211
C	2.973433	-3.414610	0.335788
C	2.255461	-2.685769	-1.841869
C	4.195515	-3.812067	-0.204020
H	2.805271	-3.550453	1.398533
C	3.473830	-3.084534	-2.381130
H	1.501462	-2.254044	-2.494723
C	4.447769	-3.653414	-1.562255
H	4.952169	-4.242168	0.445713
H	3.660266	-2.952602	-3.443081
H	5.399512	-3.965706	-1.981753

C	-3.238173	-1.297308	-0.579838
C	-3.796847	-2.421466	0.036372
C	-3.492992	-1.105233	-1.943632
C	-4.591553	-3.314556	-0.679560
H	-3.622931	-2.620761	1.087725
C	-4.297184	-1.985981	-2.657292
H	-3.060937	-0.262009	-2.467967
C	-4.852768	-3.096110	-2.026918
H	-5.004956	-4.184083	-0.177015
H	-4.482357	-1.805438	-3.712374
H	-5.475872	-3.788981	-2.584949
C	-3.160332	1.442273	0.050191
C	-3.090527	2.050289	-1.208674
C	-4.036859	1.980517	0.997423
C	-3.912293	3.122765	-1.532349
H	-2.377290	1.691499	-1.943483
C	-4.834653	3.080284	0.687920
H	-4.114761	1.545479	1.988045
C	-4.787309	3.643603	-0.582827
H	-3.845273	3.569983	-2.518578
H	-5.505695	3.484285	1.440759
H	-5.419961	4.491293	-0.830163
C	-0.257250	3.552159	-1.093403
C	-0.890906	4.417202	-0.196345
C	-0.417500	3.769623	-2.466806
C	-1.640043	5.494732	-0.659519
H	-0.805546	4.256906	0.874231
C	-1.165409	4.848090	-2.929188
H	0.061645	3.106099	-3.181463
C	-1.771129	5.719548	-2.026600
H	-2.123469	6.157299	0.052293
H	-1.268982	5.010960	-3.998214
H	-2.349570	6.564847	-2.388171
C	2.177058	2.214787	-1.679089
C	2.687137	1.049582	-2.251666
C	2.826742	3.431144	-1.933179
C	3.814381	1.092582	-3.071471
H	2.219720	0.092611	-2.044845
C	3.952481	3.475627	-2.745798
H	2.448270	4.348361	-1.489407
C	4.449438	2.303682	-3.318351
H	4.201374	0.172389	-3.498931
H	4.446944	4.424805	-2.931237
H	5.331037	2.339073	-3.952054

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.105246	-0.438153	-0.270931
N	-0.287848	-1.253370	1.846130
C	2.257595	-2.393056	1.135028
H	1.764906	-3.338747	0.900824
H	3.297002	-2.633858	1.377619
C	-2.692110	0.428546	1.772801
C	-0.121073	-0.071076	-1.976393
O	-0.144541	0.136641	-3.133098
P	-2.534073	-0.100437	0.011762
P	2.085678	-1.323810	-0.357842
Si	-1.550188	-0.585247	2.901481
Si	1.304882	-1.597547	2.537272
C	-2.419374	-2.002950	3.778734
H	-1.782033	-2.372310	4.591564
H	-3.372557	-1.698081	4.228444
H	-2.599233	-2.840056	3.096435
C	1.182766	-2.789336	3.989342
H	2.176386	-3.151567	4.282861
H	0.735680	-2.317955	4.873328
H	0.572386	-3.663446	3.731677
H	-2.327338	1.461884	1.798805
H	-3.730556	0.453092	2.122005
P	0.362341	1.835434	0.313417
C	0.345153	2.404182	2.079525
H	0.894804	3.350511	2.141420
H	-0.697676	2.664578	2.296121
Si	0.840750	1.332672	3.557917
C	1.546165	2.501081	4.856810
H	2.467059	2.981669	4.503072
H	0.832098	3.295220	5.107529
H	1.786985	1.967065	5.784188
C	-0.741525	0.530038	4.181909
H	-1.449762	1.310388	4.493650
H	-0.522591	-0.064332	5.080094
C	2.092204	0.008310	3.105716
H	2.743703	0.410971	2.321605
H	2.735427	-0.203386	3.971049

H	-0.280067	-2.149277	-0.590564
H	-0.712719	-2.136892	1.489207
C	-0.030489	-4.584326	-0.286481
H	-0.519912	-5.535100	-0.541480
H	0.784898	-4.433543	-0.996083
H	0.355208	-4.688404	0.730700
C	-1.118026	-3.512355	-0.340564
C	-1.801777	-3.464541	-1.705272
H	-2.596230	-4.222211	-1.716096
H	-2.247642	-2.493842	-1.899415
H	-1.089637	-3.693787	-2.503812
O	-1.766148	-3.316181	0.721514
C	3.743544	-0.489507	-0.423104
C	4.655879	-0.463896	0.635525
C	4.141790	0.051226	-1.651372
C	5.931881	0.073024	0.468904
H	4.394005	-0.875795	1.604072
C	5.416673	0.574444	-1.823825
H	3.450772	0.043103	-2.490387
C	6.320386	0.584322	-0.763321
H	6.625907	0.075933	1.305010
H	5.703707	0.981608	-2.788894
H	7.317686	0.993226	-0.898024
C	2.435926	-2.535447	-1.718750
C	1.571878	-2.703206	-2.800049
C	3.587154	-3.331902	-1.654541
C	1.843400	-3.644088	-3.792602
H	0.664866	-2.118957	-2.858897
C	3.854411	-4.280119	-2.635546
H	4.288008	-3.207644	-0.833145
C	2.980724	-4.439249	-3.710694
H	1.153095	-3.757576	-4.623744
H	4.748916	-4.892383	-2.563801
H	3.188966	-5.178729	-4.478655
C	2.014262	2.478878	-0.242421
C	2.222966	2.723646	-1.605336
C	3.042877	2.798448	0.646401
C	3.388654	3.330887	-2.054139
H	1.466114	2.451526	-2.332295
C	4.225061	3.383218	0.195705
H	2.936618	2.607157	1.709017
C	4.393064	3.672921	-1.152539
H	3.516063	3.527040	-3.114974
H	5.010680	3.617678	0.908053

H	5.307795	4.142182	-1.502732
C	-0.628668	3.235797	-0.433480
C	-0.960108	4.398290	0.273537
C	-0.965205	3.187517	-1.790743
C	-1.597868	5.467837	-0.351120
H	-0.715949	4.503756	1.323395
C	-1.581361	4.261548	-2.422713
H	-0.755342	2.298676	-2.371818
C	-1.904570	5.408267	-1.705099
H	-1.843105	6.354808	0.226814
H	-1.825071	4.188561	-3.478106
H	-2.394373	6.244558	-2.195647
C	-3.353976	1.240700	-0.955680
C	-3.298900	1.170792	-2.353271
C	-4.112866	2.255501	-0.369825
C	-4.024765	2.055444	-3.142632
H	-2.673520	0.425632	-2.835573
C	-4.811281	3.166051	-1.159624
H	-4.171891	2.343891	0.710628
C	-4.785162	3.057680	-2.546615
H	-3.977186	1.972520	-4.224832
H	-5.386584	3.956118	-0.685512
H	-5.344336	3.758506	-3.159869
C	-3.946176	-1.314446	-0.136714
C	-4.506110	-1.925239	0.986672
C	-4.509828	-1.612945	-1.382316
C	-5.574160	-2.810269	0.876122
H	-4.108166	-1.728641	1.971593
C	-5.574475	-2.500255	-1.501562
H	-4.124818	-1.154340	-2.285528
C	-6.113362	-3.106067	-0.370782
H	-5.981526	-3.269456	1.772481
H	-5.985981	-2.710654	-2.484669
H	-6.944918	-3.799150	-0.460745

$R^1=R^2=R^3$=iPr

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.169198	-0.638224	-0.603832
N	-0.280427	-0.050273	1.704186

C	2.498312	-1.081829	1.559416
H	2.916952	-1.821177	2.253240
H	3.346582	-0.491364	1.194771
C	-2.805118	1.128907	0.689446
C	-0.100031	-1.200878	-2.244068
O	-0.043428	-1.579503	-3.360422
P	-2.497758	-0.304524	-0.437663
P	1.666420	-1.860554	0.090982
Si	-1.620085	1.036903	2.151857
Si	1.336398	0.123828	2.424264
C	-2.468304	0.314694	3.670010
H	-1.799860	0.354525	4.538871
H	-3.381134	0.863979	3.931428
H	-2.743944	-0.736160	3.519724
C	1.249789	-0.257951	4.269162
H	2.255283	-0.308813	4.706284
H	0.698803	0.519691	4.813212
H	0.754704	-1.216131	4.468699
H	-2.562182	2.026902	0.107754
H	-3.844725	1.237517	1.019726
P	0.736593	1.421888	-1.261193
C	0.356590	2.980323	-0.318430
H	0.884141	3.824918	-0.777536
H	-0.712342	3.178212	-0.478604
Si	0.660551	3.103325	1.546127
C	1.221810	4.869904	1.895195
H	2.172248	5.095433	1.395225
H	0.482215	5.598779	1.540745
H	1.366202	5.039020	2.969479
C	-0.918003	2.737963	2.506961
H	-1.687276	3.489828	2.284709
H	-0.689081	2.832072	3.578294
C	1.940514	1.890108	2.203559
H	2.844938	1.895207	1.585403
H	2.250745	2.259377	3.192063
H	-0.755189	-2.039915	-0.176048
H	-0.587929	-1.012677	1.845932
C	-3.271462	-1.718131	0.549703
C	-3.390069	-2.990979	-0.293695
C	-4.572159	-1.475734	1.324925
H	-2.488350	-1.906344	1.294759
H	-2.490428	-3.160039	-0.893429
H	-3.534868	-3.862961	0.356744
H	-4.256075	-2.940744	-0.963228

H	-4.564537	-0.550002	1.906538
H	-5.448325	-1.453486	0.672721
H	-4.723350	-2.299177	2.035350
C	-3.707044	0.049162	-1.833112
C	-5.191109	0.154330	-1.471266
C	-3.524722	-0.886643	-3.035389
H	-3.389746	1.050897	-2.141475
H	-5.369425	0.755841	-0.574259
H	-5.734397	0.628144	-2.299221
H	-5.639741	-0.832316	-1.318393
H	-2.475067	-1.062200	-3.281021
H	-3.984410	-1.863402	-2.854077
H	-4.012171	-0.456477	-3.919479
C	0.286120	1.995973	-3.007400
C	0.796813	3.371460	-3.446918
C	-1.218843	1.925947	-3.236812
H	0.736286	1.237623	-3.657589
H	1.876390	3.492106	-3.340836
H	0.559110	3.525990	-4.507055
H	0.310829	4.180113	-2.888488
H	-1.573648	0.906852	-3.103621
H	-1.766911	2.583975	-2.549582
H	-1.465659	2.241431	-4.258581
C	2.636777	1.478649	-1.365614
C	3.358873	2.798806	-1.069997
C	3.135158	0.909350	-2.703230
H	2.937415	0.772814	-0.583611
H	3.123175	3.202752	-0.081933
H	4.443996	2.633376	-1.098877
H	3.132806	3.578869	-1.802223
H	2.564704	0.033984	-3.029651
H	3.074031	1.656182	-3.501798
H	4.188375	0.612991	-2.619510
C	1.238967	-3.564265	0.789854
C	0.269455	-3.470737	1.972364
C	2.419443	-4.451760	1.198506
H	0.701133	-4.047408	-0.035814
H	-0.664200	-2.981571	1.684384
H	0.010781	-4.477073	2.323984
H	0.714783	-2.941440	2.825075
H	3.049384	-4.737328	0.354513
H	3.056843	-3.971425	1.950554
H	2.042028	-5.380755	1.644400
C	3.080973	-2.220439	-1.097396

C	2.692142	-3.306416	-2.108138
C	4.486471	-2.449183	-0.531842
H	3.124522	-1.284225	-1.655406
H	1.715532	-3.112450	-2.559305
H	3.430980	-3.337441	-2.918665
H	2.664499	-4.303473	-1.656076
H	4.800840	-1.642449	0.137915
H	4.584432	-3.390331	0.014837
H	5.206655	-2.477811	-1.360201

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.139107	-0.527449	-0.505179
N	-0.249996	-0.055416	1.519032
C	2.524146	-1.089183	1.638646
H	2.830909	-1.876218	2.337970
H	3.425275	-0.516758	1.387650
C	-2.911298	0.989542	0.851425
C	-0.222618	-1.266460	-2.093066
O	-0.305984	-1.755316	-3.159572
P	-2.530093	-0.283283	-0.400065
P	1.808448	-1.763322	0.088424
Si	-1.555501	0.862108	2.173217
Si	1.239195	0.104237	2.371457
C	-2.379398	0.092328	3.696177
H	-1.685645	-0.011818	4.537808
H	-3.220209	0.711141	4.037416
H	-2.775001	-0.907906	3.476253
C	1.127909	-0.259641	4.229038
H	2.133080	-0.318472	4.667695
H	0.586726	0.523475	4.774634
H	0.622116	-1.213172	4.424280
H	-2.849772	1.964525	0.351970
H	-3.915927	0.902988	1.280535
P	0.695636	1.478056	-1.290159
C	0.188649	2.937547	-0.276473
H	0.604112	3.846575	-0.728581
H	-0.901426	3.019533	-0.388313
Si	0.553958	3.042179	1.600282
C	1.047914	4.842878	1.905546

H	1.965258	5.116887	1.368688
H	0.258811	5.535190	1.584895
H	1.227717	5.022123	2.973173
C	-0.991029	2.625363	2.592312
H	-1.799813	3.345838	2.409024
H	-0.737308	2.706695	3.659850
C	1.905876	1.881133	2.208597
H	2.790024	1.916001	1.561307
H	2.239319	2.241442	3.193340
C	-3.017617	-1.872953	0.469917
C	-2.540972	-3.125764	-0.274111
C	-4.480253	-2.021415	0.893789
H	-2.417647	-1.801369	1.384930
H	-1.485221	-3.057733	-0.552531
H	-2.665755	-4.008082	0.365622
H	-3.108794	-3.301583	-1.192736
H	-4.871676	-1.124830	1.384943
H	-5.124382	-2.255241	0.039348
H	-4.572253	-2.851308	1.605947
C	-3.784922	0.024857	-1.758831
C	-5.190798	0.439110	-1.310680
C	-3.848752	-1.120723	-2.773771
H	-3.361754	0.893516	-2.270018
H	-5.172990	1.297789	-0.632799
H	-5.775743	0.730470	-2.192584
H	-5.730254	-0.372470	-0.815888
H	-2.856120	-1.468200	-3.076314
H	-4.400903	-1.976192	-2.369141
H	-4.377787	-0.790971	-3.676351
C	0.239525	2.017016	-3.037279
C	0.664604	3.426750	-3.456571
C	-1.252902	1.833824	-3.294116
H	0.759570	1.294364	-3.677285
H	1.738027	3.599961	-3.355645
H	0.409709	3.588412	-4.511384
H	0.141335	4.195466	-2.876444
H	-1.539337	0.789489	-3.169322
H	-1.857545	2.453400	-2.619442
H	-1.500883	2.130381	-4.320974
C	2.579541	1.604985	-1.330332
C	3.219873	2.967353	-1.040957
C	3.141034	1.030062	-2.638442
H	2.879020	0.934708	-0.516207
H	2.913128	3.382486	-0.078042

H	4.311368	2.854916	-1.010809
H	2.991338	3.712816	-1.807571
H	2.646510	0.099436	-2.936018
H	3.032598	1.742990	-3.462804
H	4.213199	0.823665	-2.532241
C	1.202190	-3.474919	0.572265
C	0.267540	-3.391400	1.786023
C	2.275558	-4.532603	0.842758
H	0.612422	-3.798336	-0.295577
H	-0.456971	-2.578912	1.708997
H	-0.270385	-4.339353	1.906128
H	0.843025	-3.222642	2.704685
H	2.814012	-4.826276	-0.061400
H	3.005832	-4.186904	1.583670
H	1.803127	-5.436934	1.246872
C	3.296447	-2.025224	-1.017760
C	2.938965	-2.803191	-2.287298
C	4.583534	-2.562931	-0.379118
H	3.516118	-0.997736	-1.320173
H	2.070600	-2.381188	-2.798970
H	3.782319	-2.785634	-2.988856
H	2.718373	-3.854680	-2.069905
H	4.816063	-2.074405	0.572189
H	4.547983	-3.640015	-0.202751
H	5.424550	-2.373802	-1.058421

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.228196	0.183376	-0.570505
N	-0.207802	0.267926	1.802937
C	-1.385509	2.823452	1.009023
H	-1.258340	3.786692	1.515642
H	-2.340301	2.886333	0.479182
C	1.514494	-1.967951	1.631362
C	0.846309	0.518997	-2.156437
O	1.322897	0.862358	-3.179177
P	1.253585	-1.887807	-0.203307
P	-0.042763	2.468263	-0.225421
Si	0.068827	-1.279177	2.603657
Si	-1.490465	1.397867	2.245268

C	0.640052	-1.040149	4.384803
H	-0.168494	-0.703607	5.044545
H	1.028372	-1.980138	4.798349
H	1.446910	-0.298651	4.439233
C	-1.275015	2.082980	3.989123
H	-2.038549	2.845837	4.191602
H	-1.385893	1.301744	4.750312
H	-0.295442	2.551285	4.140949
H	1.844699	-2.947276	1.988645
H	2.334395	-1.264930	1.838765
P	-1.951946	-0.500301	-1.254407
C	-2.831786	-1.679540	-0.124536
H	-3.833661	-1.891385	-0.514891
H	-2.290356	-2.629384	-0.195150
Si	-2.994811	-1.375817	1.729389
C	-4.589614	-2.232385	2.264308
H	-5.469045	-1.776751	1.791707
H	-4.578834	-3.294484	1.988174
H	-4.732881	-2.176099	3.350618
C	-1.547965	-2.233753	2.591687
H	-1.420086	-3.214594	2.113686
H	-1.825602	-2.440927	3.634550
C	-3.113501	0.450270	2.189312
H	-3.817292	0.935181	1.500262
H	-3.578029	0.517643	3.183527
H	1.715706	0.476844	-0.035629
H	0.697195	0.736483	1.756438
C	5.138840	0.658639	0.510965
O	4.726995	0.591559	1.653914
C	4.595448	1.673342	-0.468990
H	4.465864	2.638147	0.029495
H	5.232095	1.791338	-1.350484
H	3.601177	1.333447	-0.793304
C	6.202610	-0.283344	-0.002754
H	5.892682	-0.728290	-0.955028
H	7.123463	0.280380	-0.200314
H	6.407159	-1.066319	0.730353
C	3.052862	-1.973619	-0.755338
C	3.285994	-1.807451	-2.259556
C	3.872405	-3.150090	-0.218273
H	3.420881	-1.062254	-0.272147
H	2.710422	-0.983780	-2.681729
H	4.347987	-1.597873	-2.446051
H	3.042888	-2.716720	-2.817137

H	3.795447	-3.255954	0.867966
H	3.576382	-4.098797	-0.678123
H	4.933237	-2.997940	-0.455148
C	0.531077	-3.603255	-0.557303
C	0.805559	-4.724677	0.450252
C	0.858182	-4.083612	-1.975386
H	-0.545958	-3.408357	-0.521686
H	0.401832	-4.500635	1.442426
H	0.323934	-5.649812	0.107035
H	1.873728	-4.934787	0.563501
H	0.730698	-3.297016	-2.725566
H	1.887848	-4.449266	-2.041283
H	0.203390	-4.918869	-2.254610
C	-2.230735	-1.410940	-2.911357
C	-2.408841	-2.929318	-2.818317
C	-1.156401	-1.078276	-3.946604
H	-3.184038	-1.022411	-3.288403
H	-3.308520	-3.214827	-2.266215
H	-2.506168	-3.343884	-3.829839
H	-1.553790	-3.421101	-2.351461
H	-1.031941	-0.003916	-4.097361
H	-0.182466	-1.474532	-3.644960
H	-1.419269	-1.524280	-4.914846
C	-3.294026	0.826142	-1.479871
C	-4.746611	0.369894	-1.315666
C	-3.153917	1.553148	-2.825474
H	-3.081088	1.548479	-0.687865
H	-4.973275	0.023721	-0.302789
H	-5.424136	1.205792	-1.533411
H	-5.000470	-0.439538	-2.011972
H	-2.114279	1.703346	-3.120295
H	-3.641546	0.994995	-3.632468
H	-3.636418	2.536711	-2.781194
C	1.405925	3.403634	0.545229
C	2.032196	2.728361	1.766903
C	1.119036	4.868636	0.901164
H	2.157873	3.379579	-0.251934
H	2.417975	1.731108	1.542847
H	2.883428	3.323595	2.119787
H	1.326998	2.672970	2.605397
H	0.595633	5.418700	0.116993
H	0.522564	4.945213	1.818043
H	2.064127	5.392038	1.093381
C	-0.415689	3.531816	-1.743151

C	0.846052	4.094697	-2.411780
C	-1.498528	4.601782	-1.588933
H	-0.799871	2.784395	-2.438110
H	1.614595	3.326690	-2.536917
H	0.588399	4.460439	-3.413462
H	1.280634	4.935067	-1.860910
H	-2.453151	4.175772	-1.264670
H	-1.224049	5.381429	-0.871139
H	-1.673064	5.089634	-2.556552

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.963271	0.333786	-0.656321
N	0.622193	0.103869	1.412469
C	-0.963584	2.567417	0.992617
H	-1.088060	3.557038	1.448960
H	-1.950070	2.259025	0.631008
C	1.950836	-2.458456	1.075917
C	1.200222	0.453259	-2.398582
O	1.327042	0.490428	-3.562493
P	1.679261	-1.929814	-0.658135
P	0.130047	2.569401	-0.478855
Si	0.892362	-1.397435	2.233707
Si	-0.412589	1.227560	2.226413
C	1.886304	-1.221044	3.835518
H	1.298698	-0.768533	4.643683
H	2.215039	-2.207663	4.190742
H	2.776377	-0.601578	3.678955
C	0.422414	2.045084	3.719441
H	-0.093216	2.967218	4.019471
H	0.406972	1.375338	4.587836
H	1.471713	2.288560	3.521738
H	1.843229	-3.536099	1.237034
H	2.995439	-2.207403	1.307007
P	-2.783063	-0.524025	-0.633623
C	-2.901939	-1.786294	0.706084
H	-3.923775	-2.178396	0.783937
H	-2.284367	-2.634379	0.383254
Si	-2.291302	-1.392497	2.471991
C	-3.619746	-2.088170	3.625180

H	-4.578122	-1.566090	3.507532
H	-3.797437	-3.153858	3.431949
H	-3.320438	-1.989504	4.676194
C	-0.685379	-2.334772	2.731794
H	-0.751109	-3.295591	2.203562
H	-0.594571	-2.584541	3.798685
C	-2.008445	0.420053	2.901272
H	-2.886170	1.027338	2.640280
H	-1.959047	0.446782	4.001397
H	3.466916	-0.080642	-0.070501
H	2.436078	0.709175	1.617655
C	4.098448	0.578122	0.546976
O	3.390657	0.936757	1.720494
C	4.439722	1.801694	-0.301488
H	3.530925	2.275525	-0.687123
H	4.989428	2.539739	0.293879
H	5.058561	1.518407	-1.161419
C	5.347134	-0.195013	0.951272
H	5.923275	-0.510155	0.073455
H	5.990684	0.435167	1.576597
H	5.080853	-1.083739	1.534019
C	3.293550	-2.473793	-1.446120
C	3.601959	-1.808757	-2.789254
C	3.506430	-3.989805	-1.498707
H	4.024800	-2.081649	-0.726827
H	3.616596	-0.718801	-2.701652
H	4.591991	-2.128493	-3.138675
H	2.877178	-2.071045	-3.564965
H	3.309514	-4.466643	-0.532866
H	2.873279	-4.467530	-2.253163
H	4.548628	-4.205726	-1.764920
C	0.292074	-2.982259	-1.337959
C	0.130496	-4.390511	-0.764299
C	0.316293	-2.999309	-2.870870
H	-0.586688	-2.397556	-1.036437
H	0.003619	-4.380472	0.322513
H	-0.764819	-4.859717	-1.192433
H	0.982529	-5.035057	-1.000660
H	0.424636	-1.996191	-3.293256
H	1.134056	-3.618547	-3.253040
H	-0.616188	-3.424225	-3.259838
C	-3.554244	-1.397995	-2.124832
C	-3.436732	-2.923467	-2.090674
C	-2.920883	-0.831994	-3.401508

H	-4.626307	-1.162311	-2.137112
H	-4.002346	-3.361560	-1.262843
H	-3.831509	-3.347320	-3.022535
H	-2.398025	-3.255491	-1.996288
H	-3.053838	0.252646	-3.480263
H	-1.842614	-1.029570	-3.425434
H	-3.369263	-1.287148	-4.294004
C	-4.171146	0.665076	-0.175508
C	-5.423391	0.021631	0.423834
C	-4.545175	1.543441	-1.375275
H	-3.736429	1.318863	0.590164
H	-5.226130	-0.446853	1.392858
H	-6.197981	0.782958	0.581576
H	-5.846026	-0.742066	-0.240799
H	-3.665458	1.949476	-1.881169
H	-5.126603	0.982242	-2.115823
H	-5.163815	2.388281	-1.050290
C	1.285193	4.018383	-0.207101
C	1.997043	3.883790	1.142532
C	0.647574	5.410070	-0.288394
H	2.031941	3.932878	-1.007706
H	2.435460	2.898041	1.312044
H	2.807633	4.620310	1.204963
H	1.301703	4.096916	1.962064
H	0.321684	5.674796	-1.296387
H	-0.212452	5.498444	0.385599
H	1.382942	6.162394	0.022583
C	-0.977487	3.052351	-1.914468
C	-0.171826	3.474935	-3.149131
C	-2.090307	4.067486	-1.627799
H	-1.451470	2.088186	-2.147848
H	0.613195	2.760451	-3.402618
H	-0.839223	3.548631	-4.016558
H	0.293690	4.456978	-3.014589
H	-2.666705	3.824554	-0.730044
H	-1.699822	5.080942	-1.508766
H	-2.792588	4.088478	-2.470786

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Coordinates (Angstroms)		
X	Y	Z

Mn	1.178308	0.076008	-0.659507
N	0.709521	0.075758	1.587271
C	-0.526477	2.654812	0.755695
H	-0.609489	3.692115	1.103496
H	-1.491398	2.392542	0.308941
C	1.349738	-2.793349	1.204942
C	1.443400	0.063697	-2.382091
O	1.626665	0.031948	-3.543763
P	1.286711	-2.230783	-0.556319
P	0.709381	2.429644	-0.599679
Si	0.630119	-1.518407	2.389067
Si	-0.282263	1.436440	2.180761
C	1.719066	-1.442333	3.920351
H	1.281876	-0.805133	4.699000
H	1.876484	-2.437326	4.355943
H	2.693847	-1.015569	3.655402
C	0.597703	2.193440	3.665153
H	0.205173	3.189138	3.907154
H	0.442446	1.561058	4.548525
H	1.677604	2.276001	3.510796
H	0.911416	-3.784800	1.361171
H	2.412399	-2.890191	1.458046
P	-2.821221	-0.081034	-0.655485
C	-3.177836	-1.287118	0.698571
H	-4.248452	-1.518046	0.761296
H	-2.684871	-2.226659	0.418652
Si	-2.562686	-0.888113	2.453755
C	-4.004217	-1.261428	3.614261
H	-4.860056	-0.602787	3.418620
H	-4.351591	-2.295964	3.499828
H	-3.718362	-1.122252	4.664148
C	-1.119290	-2.009847	2.894802
H	-1.323988	-3.027537	2.536093
H	-1.107223	-2.081815	3.992867
C	-1.986185	0.873984	2.774482
H	-2.739353	1.601732	2.446958
H	-1.969797	0.952619	3.872468
H	2.818798	0.155340	-0.342205
H	1.700846	0.365991	1.702641
C	4.095598	0.387043	0.816416
O	3.547610	0.707683	1.893916
C	4.807319	1.422888	-0.040628
H	4.261400	2.362655	-0.075487
H	5.789308	1.614163	0.416636

H	4.961310	1.059094	-1.059645
C	4.712229	-0.995841	0.700974
H	4.867397	-1.296977	-0.337357
H	5.691762	-0.955451	1.198649
H	4.104833	-1.732215	1.228684
C	2.736336	-3.207083	-1.239722
C	3.248403	-2.712006	-2.593418
C	2.582608	-4.730879	-1.208160
H	3.512150	-2.959618	-0.509251
H	3.493553	-1.647816	-2.554956
H	4.159977	-3.261245	-2.862941
H	2.522901	-2.860526	-3.398335
H	2.248353	-5.091722	-0.229321
H	1.879300	-5.093850	-1.964043
H	3.551925	-5.201717	-1.415681
C	-0.278514	-2.994689	-1.259404
C	-0.796191	-4.283953	-0.618518
C	-0.183201	-3.125702	-2.784638
H	-1.012733	-2.204322	-1.057663
H	-1.035807	-4.148153	0.441537
H	-1.717339	-4.607438	-1.119989
H	-0.077708	-5.104896	-0.698641
H	0.203768	-2.214635	-3.250680
H	0.464302	-3.957467	-3.079228
H	-1.173747	-3.322829	-3.211826
C	-3.644839	-0.844175	-2.178255
C	-3.862948	-2.355885	-2.099915
C	-2.812322	-0.466016	-3.409498
H	-4.636018	-0.385598	-2.280111
H	-4.549786	-2.631713	-1.293685
H	-4.295670	-2.717303	-3.041075
H	-2.926789	-2.898011	-1.942752
H	-2.746714	0.620150	-3.537785
H	-1.786954	-0.843783	-3.324363
H	-3.255034	-0.881789	-4.323695
C	-4.030734	1.314148	-0.282267
C	-5.399014	0.884155	0.250034
C	-4.188762	2.215855	-1.512646
H	-3.540322	1.908856	0.497754
H	-5.328432	0.401817	1.230020
H	-6.050846	1.759582	0.363014
H	-5.901255	0.188037	-0.433225
H	-3.231049	2.427451	-1.995342
H	-4.844675	1.759297	-2.262497

H	-4.640645	3.173396	-1.228533
C	1.956015	3.788053	-0.258208
C	2.468527	3.685956	1.182135
C	1.489529	5.227742	-0.500385
H	2.780408	3.571841	-0.949160
H	2.749742	2.671093	1.477206
H	3.353720	4.322692	1.306049
H	1.708678	4.056578	1.880138
H	1.320613	5.452737	-1.554970
H	0.569111	5.454472	0.050888
H	2.260770	5.921210	-0.141574
C	-0.211409	2.971859	-2.144507
C	0.755827	3.224928	-3.308662
C	-1.211708	4.127008	-2.018549
H	-0.776601	2.059176	-2.382120
H	1.497239	2.430941	-3.416139
H	0.196902	3.282197	-4.250913
H	1.288809	4.174227	-3.190183
H	-1.867182	4.030461	-1.147965
H	-0.713898	5.097050	-1.951460
H	-1.851240	4.156027	-2.910237

R^1=R^2=R^3=Cy

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.011833	-0.352170	-0.183751
N	0.428202	-0.891147	2.110234
C	3.092927	0.098205	1.322131
H	4.090759	-0.293507	1.549436
H	3.211721	1.176088	1.156539
C	-2.537605	-1.151725	1.970738
C	-0.208719	-0.252718	-1.903239
O	-0.375328	-0.230675	-3.070368
P	-2.130341	-1.160958	0.161784
P	2.363158	-0.578631	-0.238536
Si	-1.025473	-1.161507	3.087600
Si	1.898815	-0.137490	2.758735
C	-0.891650	-2.833348	3.940478
H	0.012459	-2.907097	4.556382
H	-1.756389	-3.027084	4.587157

H	-0.852257	-3.639643	3.195990
C	2.670147	-1.265820	4.056670
H	3.644443	-0.885802	4.389633
H	2.033585	-1.354203	4.946156
H	2.825634	-2.277448	3.660274
H	-3.068649	-0.212583	2.165252
H	-3.232583	-1.953958	2.244941
P	-0.422013	1.895289	0.221009
C	-1.229032	2.246161	1.864154
H	-1.509409	3.304114	1.918007
H	-2.180149	1.698828	1.849947
Si	-0.420834	1.850793	3.541036
C	-0.777215	3.327103	4.659054
H	-0.293581	4.237242	4.281497
H	-1.853665	3.527907	4.727681
H	-0.406058	3.154456	5.676736
C	-1.164144	0.280654	4.280326
H	-2.220535	0.428173	4.541203
H	-0.635666	0.068018	5.220420
C	1.431698	1.512123	3.535548
H	1.995603	2.333517	3.078529
H	1.734526	1.489952	4.593045
H	0.196988	-1.934599	-0.284816
H	0.644427	-1.762338	1.619248
C	-2.250025	-3.001070	-0.217692
C	-3.578333	-3.722467	0.055854
C	-1.747864	-3.389693	-1.618878
H	-1.506621	-3.393562	0.495390
C	-3.394200	-5.243509	-0.027012
H	-4.318714	-3.421325	-0.696538
H	-3.993677	-3.455472	1.034034
C	-1.556318	-4.905810	-1.724737
H	-2.471185	-3.068384	-2.378897
H	-0.807067	-2.878122	-1.828457
C	-2.842904	-5.664916	-1.391900
H	-4.349055	-5.746787	0.169052
H	-2.697818	-5.564037	0.761510
H	-1.208558	-5.167720	-2.731461
H	-0.763687	-5.212598	-1.026743
H	-2.668783	-6.747625	-1.414672
H	-3.596697	-5.449115	-2.162980
C	-3.692888	-0.378308	-0.538162
C	-3.793398	-0.573873	-2.060015
C	-5.050282	-0.679537	0.120819

H	-3.511050	0.689736	-0.352772
C	-4.903226	0.283215	-2.674968
H	-4.015481	-1.629373	-2.265033
H	-2.836424	-0.355452	-2.544491
C	-6.139751	0.221307	-0.474945
H	-5.331665	-1.725832	-0.037691
H	-5.002921	-0.525788	1.203982
C	-6.250203	0.039827	-1.991041
H	-4.978028	0.078679	-3.749828
H	-4.634391	1.343015	-2.576076
H	-7.103224	0.009497	0.004835
H	-5.900205	1.272000	-0.252512
H	-7.012626	0.713543	-2.400461
H	-6.584412	-0.985671	-2.204829
C	-1.691679	2.634104	-0.974553
C	-2.671825	3.679015	-0.417352
C	-1.093796	3.143425	-2.295010
H	-2.274782	1.749232	-1.249091
C	-3.759707	4.036311	-1.438659
H	-2.122324	4.586966	-0.131095
H	-3.162858	3.309946	0.488689
C	-2.197280	3.412233	-3.321939
H	-0.561396	4.086112	-2.117217
H	-0.373368	2.423620	-2.694777
C	-3.184461	4.455028	-2.793021
H	-4.398419	4.831411	-1.034388
H	-4.406765	3.160145	-1.579574
H	-1.753612	3.754076	-4.264706
H	-2.724250	2.473306	-3.541051
H	-3.995349	4.618714	-3.513149
H	-2.661248	5.416016	-2.681582
C	0.992055	3.133677	0.303495
C	1.842538	3.196846	-0.972609
C	0.728645	4.564196	0.796468
H	1.624536	2.653310	1.062526
C	3.195375	3.853136	-0.687919
H	1.336630	3.800500	-1.730753
H	1.951328	2.199511	-1.401924
C	2.058529	5.282413	1.071194
H	0.160848	5.117691	0.035570
H	0.126024	4.573020	1.710966
C	2.989647	5.271417	-0.145187
H	3.803283	3.882564	-1.600827
H	3.755420	3.254124	0.046276

H	1.868978	6.314704	1.389750
H	2.558900	4.780948	1.913004
H	3.952080	5.729452	0.112635
H	2.547988	5.890792	-0.938835
C	2.789645	-2.409432	-0.116242
C	2.597845	-3.099278	-1.475358
C	4.096169	-2.867241	0.551309
H	1.974638	-2.782537	0.519168
C	2.615824	-4.622543	-1.323397
H	3.403827	-2.800238	-2.158987
H	1.651999	-2.772420	-1.921401
C	4.102855	-4.394236	0.706497
H	4.967483	-2.569986	-0.041421
H	4.212128	-2.407056	1.539251
C	3.899353	-5.098257	-0.637538
H	2.506042	-5.100679	-2.304343
H	1.746974	-4.927672	-0.722515
H	5.044669	-4.717291	1.166550
H	3.297387	-4.690095	1.394851
H	3.877850	-6.185689	-0.496438
H	4.757510	-4.879287	-1.289448
C	3.555210	0.155407	-1.489243
C	5.011948	-0.328150	-1.449164
C	3.027082	0.152121	-2.930755
H	3.585057	1.203898	-1.167272
C	5.897075	0.546794	-2.345126
H	5.071210	-1.364822	-1.802837
H	5.397035	-0.314101	-0.422943
C	3.914370	1.010485	-3.838607
H	2.993334	-0.874949	-3.317002
H	2.000856	0.525255	-2.960108
C	5.379503	0.571568	-3.785385
H	6.931091	0.181476	-2.317852
H	5.911814	1.571019	-1.944945
H	3.540929	0.969404	-4.868703
H	3.838846	2.060097	-3.517467
H	5.999828	1.234030	-4.401279
H	5.469527	-0.436168	-4.216379

A2

Coordinates (Angstroms)		
X	Y	Z

Mn	-0.046206	-0.277286	-0.048123
N	0.146586	-0.822970	1.952368
C	3.034757	-0.580274	1.442635
H	3.823286	-1.290611	1.710424
H	3.512227	0.403101	1.345535
C	-2.793306	-0.550152	1.997610
C	-0.204121	-0.276874	-1.793265
O	-0.317127	-0.313505	-2.963942
P	-2.349153	-0.715596	0.231190
P	2.219349	-0.935019	-0.160149
Si	-1.218417	-0.865093	3.006467
Si	1.648081	-0.479320	2.731923
C	-1.455898	-2.514731	3.903700
H	-0.625386	-2.745619	4.580716
H	-2.378230	-2.513149	4.499668
H	-1.527600	-3.340262	3.183023
C	2.077661	-1.666768	4.145354
H	3.105198	-1.497210	4.493696
H	1.418185	-1.526376	5.011037
H	1.996043	-2.716259	3.836482
H	-3.121984	0.479764	2.176013
H	-3.623185	-1.202285	2.292168
P	-0.070356	2.003739	0.193493
C	-0.820555	2.497556	1.814328
H	-0.903145	3.589512	1.855500
H	-1.854612	2.132154	1.781607
Si	-0.109117	1.953604	3.510668
C	-0.196507	3.501044	4.596176
H	0.474923	4.289772	4.232326
H	-1.211414	3.917603	4.628899
H	0.096959	3.270172	5.627957
C	-1.141644	0.564766	4.255624
H	-2.155245	0.890321	4.525573
H	-0.649424	0.259892	5.190993
C	1.642104	1.271991	3.489929
H	2.346623	1.949825	2.993952
H	1.969576	1.211378	4.538802
C	-2.597411	-2.558693	-0.006020
C	-4.040382	-3.074135	0.110438
C	-1.934268	-3.121298	-1.272539
H	-2.033666	-2.963134	0.850047
C	-4.090933	-4.604685	0.109068
H	-4.622673	-2.711043	-0.746253

H	-4.523710	-2.686569	1.013588
C	-2.011071	-4.652026	-1.302924
H	-2.421117	-2.710766	-2.166691
H	-0.887071	-2.804114	-1.317926
C	-3.443722	-5.167019	-1.156953
H	-5.131288	-4.941542	0.191442
H	-3.561995	-4.988175	0.993513
H	-1.561782	-5.027429	-2.229775
H	-1.409090	-5.051562	-0.473675
H	-3.452378	-6.263371	-1.138943
H	-4.033519	-4.857619	-2.031872
C	-3.724732	0.202273	-0.646155
C	-3.742832	-0.044732	-2.162379
C	-5.142603	0.097183	-0.058278
H	-3.420691	1.248433	-0.492254
C	-4.715843	0.905385	-2.869089
H	-4.050534	-1.081691	-2.355826
H	-2.740073	0.069774	-2.584965
C	-6.090453	1.075804	-0.761657
H	-5.536672	-0.916313	-0.182141
H	-5.129062	0.302720	1.017235
C	-6.121936	0.827558	-2.271470
H	-4.741160	0.680627	-3.942121
H	-4.340689	1.934142	-2.771619
H	-7.097698	0.984182	-0.337765
H	-5.758557	2.106857	-0.569605
H	-6.784810	1.549305	-2.763417
H	-6.542314	-0.170474	-2.461885
C	-1.162672	2.911460	-1.041224
C	-1.877336	4.193585	-0.588813
C	-0.509556	3.146664	-2.412419
H	-1.938110	2.155116	-1.212334
C	-2.918629	4.630969	-1.628219
H	-1.141659	4.996618	-0.439055
H	-2.383117	4.045146	0.370288
C	-1.564036	3.527516	-3.454831
H	0.205136	3.974561	-2.336192
H	0.045710	2.263406	-2.740679
C	-2.318756	4.788604	-3.027367
H	-3.392009	5.567370	-1.309085
H	-3.714362	3.872866	-1.662850
H	-1.085753	3.683307	-4.429240
H	-2.269119	2.693683	-3.578194
H	-3.106389	5.029873	-3.751334

H	-1.619452	5.637136	-3.025254
C	1.584052	2.880337	0.285555
C	2.402730	2.877301	-1.013643
C	1.625820	4.287367	0.900805
H	2.113480	2.211072	0.976883
C	3.862045	3.243033	-0.726283
H	2.006268	3.623317	-1.708625
H	2.320017	1.911706	-1.517430
C	3.075345	4.717600	1.167927
H	1.147411	5.001655	0.215641
H	1.070854	4.328913	1.842738
C	3.949173	4.631679	-0.086209
H	4.448544	3.212752	-1.652887
H	4.304752	2.501369	-0.044700
H	3.092964	5.735943	1.574608
H	3.495962	4.062243	1.944631
H	4.989403	4.876659	0.158940
H	3.609627	5.380826	-0.815389
C	2.032052	-2.803443	-0.210946
C	1.958252	-3.330707	-1.653330
C	3.035679	-3.618518	0.619694
H	1.044059	-2.957938	0.249617
C	1.640645	-4.827507	-1.689636
H	2.923120	-3.174084	-2.150095
H	1.213451	-2.768330	-2.228403
C	2.714959	-5.116239	0.564995
H	4.055176	-3.452707	0.248289
H	3.017961	-3.289097	1.663365
C	2.655902	-5.629830	-0.874537
H	1.616490	-5.176588	-2.728963
H	0.640161	-4.995171	-1.274246
H	3.461033	-5.675248	1.142584
H	1.743244	-5.289648	1.050108
H	2.400513	-6.696206	-0.889037
H	3.649867	-5.533842	-1.335688
C	3.563968	-0.455735	-1.365146
C	4.887597	-1.228538	-1.249759
C	3.133722	-0.327255	-2.834676
H	3.783588	0.562860	-1.018332
C	5.983579	-0.537718	-2.069976
H	4.758140	-2.253884	-1.618922
H	5.199453	-1.303720	-0.201847
C	4.230167	0.361079	-3.654773
H	2.936516	-1.317054	-3.262194

H	2.197601	0.232310	-2.914590
C	5.567767	-0.374083	-3.534323
H	6.918753	-1.106476	-2.000525
H	6.182138	0.452900	-1.636114
H	3.924755	0.425644	-4.705937
H	4.350337	1.393743	-3.295645
H	6.347247	0.158387	-4.092559
H	5.472126	-1.368649	-3.993598

A3

Coordinates (Angstroms)

	X	Y	Z
Mn	-0.076548	-0.250413	-0.248712
N	-0.206025	-1.025468	2.042482
C	2.670954	-1.352918	1.572473
H	3.266552	-2.233318	1.833477
H	3.373368	-0.511006	1.559868
C	-2.982560	-0.611010	1.515758
C	-0.001230	-0.205538	-1.977996
O	0.046981	-0.308738	-3.152963
P	-2.379939	0.083032	-0.103265
P	1.925241	-1.460229	-0.128129
Si	-1.705980	-0.603467	2.881348
Si	1.352630	-1.007315	2.871163
C	-2.185156	-1.923399	4.139063
H	-2.018427	-2.920960	3.718338
H	-1.607212	-1.844555	5.067404
H	-3.246251	-1.834351	4.408361
C	1.429985	-2.350270	4.190583
H	2.443928	-2.442743	4.601151
H	0.753602	-2.146167	5.028941
H	1.149159	-3.325018	3.772757
H	-3.946221	-0.204327	1.835689
H	-3.153221	-1.677446	1.326541
P	0.697821	1.960882	0.211323
C	0.003640	2.730380	1.753809
H	0.386578	3.749225	1.870703
H	-1.074023	2.843781	1.582774
Si	0.135559	1.905954	3.449277
C	0.349536	3.296598	4.710482
H	1.303167	3.823241	4.577516

H	-0.452940	4.040250	4.624798
H	0.329403	2.907132	5.736051
C	-1.496043	1.031971	3.779451
H	-2.313748	1.717265	3.517024
H	-1.590743	0.840855	4.857199
C	1.560152	0.687251	3.666806
H	2.495213	1.148431	3.324040
H	1.684182	0.540066	4.749974
H	-0.715664	-1.719632	-0.472788
H	-0.368117	-1.930954	1.590306
C	-2.438014	-4.258111	0.879975
O	-1.463641	-3.988422	1.561051
C	-2.305841	-4.559801	-0.592109
H	-1.877199	-5.563185	-0.702486
H	-3.269397	-4.543120	-1.108571
H	-1.620144	-3.838244	-1.048426
C	-3.825629	-4.327561	1.467713
H	-4.479814	-3.609630	0.956927
H	-4.254115	-5.321865	1.290538
H	-3.812172	-4.117102	2.538907
C	-3.448620	-1.012082	-1.210294
C	-4.965670	-0.932548	-0.972639
C	-3.143428	-0.988311	-2.713940
H	-3.114197	-1.997682	-0.857371
C	-5.698873	-2.069225	-1.694474
H	-5.352371	0.023504	-1.348967
H	-5.198516	-0.967714	0.097449
C	-3.888989	-2.110867	-3.446557
H	-3.433637	-0.025763	-3.151911
H	-2.073465	-1.103280	-2.878517
C	-5.396686	-2.061348	-3.193752
H	-6.778814	-1.988105	-1.519776
H	-5.380929	-3.032180	-1.266737
H	-3.681559	-2.049011	-4.521701
H	-3.495614	-3.079869	-3.106749
H	-5.897595	-2.902434	-3.688805
H	-5.807924	-1.142239	-3.636045
C	-3.170730	1.795529	-0.161112
C	-3.356324	2.264451	-1.613238
C	-4.429296	2.085491	0.671788
H	-2.381923	2.426912	0.264180
C	-3.742219	3.744082	-1.683865
H	-4.152958	1.679587	-2.088305
H	-2.441284	2.076665	-2.189256

C	-4.818580	3.567206	0.584838
H	-5.269584	1.468791	0.331256
H	-4.255660	1.833091	1.723790
C	-5.001335	4.026512	-0.862756
H	-3.889538	4.042141	-2.729017
H	-2.916445	4.355366	-1.294364
H	-5.735206	3.744998	1.160532
H	-4.027530	4.170640	1.054402
H	-5.245678	5.095104	-0.894578
H	-5.852811	3.492303	-1.308490
C	0.156822	3.315755	-1.001101
C	0.587169	4.760153	-0.683880
C	0.420572	3.005615	-2.483563
H	-0.933149	3.280366	-0.874616
C	-0.104951	5.772262	-1.604944
H	1.671269	4.864466	-0.813883
H	0.367848	5.018927	0.356453
C	-0.261469	4.023202	-3.405086
H	1.497445	3.013056	-2.688412
H	0.062753	2.006591	-2.726375
C	0.153512	5.457879	-3.078547
H	0.238915	6.785747	-1.363341
H	-1.187349	5.753978	-1.415218
H	-0.027930	3.785380	-4.450067
H	-1.351340	3.931163	-3.297864
H	-0.381880	6.168216	-3.720243
H	1.225546	5.582992	-3.290250
C	2.549379	2.277574	0.491868
C	3.332202	2.455666	-0.819597
C	2.965224	3.381789	1.480842
H	2.885011	1.329717	0.931186
C	4.846031	2.432239	-0.583940
H	3.075972	3.421590	-1.269037
H	3.043423	1.691668	-1.546512
C	4.479279	3.363740	1.723640
H	2.672396	4.365948	1.095386
H	2.460621	3.260827	2.443218
C	5.266644	3.505167	0.420806
H	5.372889	2.572599	-1.535580
H	5.145327	1.446010	-0.200735
H	4.752396	4.161373	2.424973
H	4.750318	2.412968	2.206928
H	6.343842	3.444266	0.616144
H	5.077105	4.498321	-0.010866

C	1.591492	-3.305800	-0.328429
C	1.532231	-3.669156	-1.822672
C	2.457524	-4.297529	0.464979
H	0.570217	-3.400874	0.060010
C	1.138351	-5.129720	-2.062856
H	2.516532	-3.514203	-2.279156
H	0.832345	-2.997520	-2.334354
C	2.017157	-5.744007	0.209903
H	3.517556	-4.196488	0.204624
H	2.372323	-4.093523	1.538281
C	2.039163	-6.085597	-1.280226
H	1.185796	-5.348437	-3.136827
H	0.098402	-5.286064	-1.754789
H	2.663007	-6.430047	0.771871
H	0.997372	-5.878104	0.597462
H	1.726275	-7.124759	-1.440051
H	3.069840	-6.003460	-1.655648
C	3.473166	-1.079853	-1.130559
C	4.651466	-2.052470	-0.959133
C	3.237989	-0.764175	-2.616839
H	3.782740	-0.136085	-0.663369
C	5.922843	-1.510199	-1.621958
H	4.409446	-3.018780	-1.418339
H	4.840934	-2.243296	0.103228
C	4.517315	-0.250120	-3.287698
H	2.890281	-1.656555	-3.148777
H	2.444991	-0.021064	-2.721269
C	5.688050	-1.217168	-3.104856
H	6.741284	-2.230190	-1.498430
H	6.232585	-0.585393	-1.114155
H	4.327501	-0.076117	-4.353638
H	4.787689	0.721939	-2.852710
H	6.596853	-0.807320	-3.562112
H	5.466235	-2.159486	-3.626362

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.147986	0.028885	-0.105376
N	-1.013334	-0.375090	1.778647
C	0.176780	-3.053485	1.325967

H	-0.356931	-3.998246	1.462400
H	1.244121	-3.279352	1.441675
C	-1.561703	2.528730	1.822974
C	-0.019804	0.215610	-1.841577
O	0.000697	0.326842	-3.012180
P	-1.158091	2.171094	0.068418
P	-0.047005	-2.304094	-0.335095
Si	-1.480738	0.927863	2.831974
Si	-0.302412	-1.734162	2.604572
C	-3.122012	0.707944	3.761689
H	-3.365245	-0.348071	3.916521
H	-3.045410	1.184759	4.747305
H	-3.970324	1.173957	3.248385
C	-1.459898	-2.534285	3.868618
H	-1.030815	-3.470005	4.250794
H	-1.636531	-1.882761	4.734308
H	-2.433603	-2.756585	3.417320
H	-0.783067	3.189270	2.221095
H	-2.511622	3.063360	1.936372
P	2.072115	0.587334	0.403764
C	2.072196	1.483766	2.025138
H	3.069443	1.890214	2.228253
H	1.417409	2.353828	1.882164
Si	1.507693	0.622120	3.643390
C	2.782911	1.085087	4.963324
H	3.778141	0.663307	4.777565
H	2.894203	2.174340	5.040282
H	2.452721	0.721268	5.944712
C	-0.174897	1.247778	4.173228
H	-0.166897	2.313526	4.439294
H	-0.440351	0.702644	5.091312
C	1.281301	-1.240762	3.549483
H	2.163416	-1.756528	3.155516
H	1.175046	-1.584218	4.589947
H	-4.538941	0.206101	1.519560
H	-2.872162	-1.172119	1.513620
C	-4.819865	-0.836979	1.320447
O	-3.708502	-1.683656	1.558991
C	-5.271457	-0.924499	-0.131996
H	-5.666215	-1.919565	-0.364285
H	-6.056282	-0.188552	-0.344383
H	-4.424178	-0.729825	-0.795455
C	-5.929982	-1.233488	2.282764
H	-6.836962	-0.643617	2.107387

H	-6.176474	-2.293163	2.147195
H	-5.613790	-1.086508	3.320155
C	-2.869460	2.142989	-0.721183
C	-3.592632	3.497444	-0.773293
C	-2.872743	1.472748	-2.107800
H	-3.435053	1.489945	-0.036616
C	-5.001801	3.373726	-1.358270
H	-3.026820	4.179430	-1.418865
H	-3.631635	3.955737	0.221157
C	-4.254021	1.447080	-2.775611
H	-2.168528	1.991919	-2.768696
H	-2.502478	0.446707	-2.014800
C	-4.936388	2.814182	-2.779188
H	-5.490118	4.355608	-1.352054
H	-5.610662	2.710792	-0.726638
H	-4.145761	1.065300	-3.797936
H	-4.904099	0.741467	-2.246502
H	-5.940471	2.733800	-3.212255
H	-4.370048	3.511412	-3.413594
C	-0.275636	3.741049	-0.456549
C	-0.031685	3.825791	-1.970707
C	-0.800070	5.083687	0.088814
H	0.705369	3.587840	0.018957
C	0.892746	4.997837	-2.320121
H	-0.991027	3.961490	-2.488087
H	0.395954	2.888476	-2.342532
C	0.158524	6.228161	-0.256870
H	-1.777268	5.316444	-0.342671
H	-0.939666	5.034678	1.173096
C	0.371759	6.325170	-1.768032
H	1.026264	5.055847	-3.406985
H	1.885424	4.807706	-1.888481
H	-0.237793	7.171651	0.137369
H	1.126989	6.059742	0.236808
H	1.071263	7.135036	-2.006853
H	-0.582935	6.574157	-2.252916
C	2.968910	1.821413	-0.704697
C	4.321088	2.356587	-0.204595
C	3.103198	1.375223	-2.174379
H	2.266674	2.666612	-0.700987
C	4.821773	3.504753	-1.089154
H	5.065417	1.549607	-0.220707
H	4.251890	2.705586	0.830461
C	3.623487	2.505709	-3.068893

H	3.805272	0.540075	-2.248893
H	2.148380	1.018864	-2.559292
C	4.946476	3.071875	-2.550759
H	5.786089	3.868862	-0.713806
H	4.116859	4.345970	-1.016864
H	3.745640	2.129533	-4.091826
H	2.876900	3.307492	-3.117571
H	5.272761	3.914388	-3.172286
H	5.725040	2.299061	-2.628781
C	3.313298	-0.801232	0.730797
C	4.032572	-1.329291	-0.520119
C	4.367450	-0.562104	1.826342
H	2.660590	-1.610622	1.083583
C	4.772910	-2.637120	-0.220798
H	4.773151	-0.590731	-0.849634
H	3.333129	-1.461957	-1.347957
C	5.133708	-1.851911	2.143259
H	5.075147	0.210661	1.500773
H	3.910173	-0.195669	2.745842
C	5.797197	-2.442213	0.898096
H	5.263645	-3.005151	-1.129971
H	4.050652	-3.409074	0.081579
H	5.882948	-1.656250	2.919519
H	4.430338	-2.587483	2.561113
H	6.287624	-3.392645	1.139048
H	6.583333	-1.757676	0.549114
C	-1.774435	-2.809848	-0.873854
C	-1.945891	-2.755276	-2.401911
C	-2.308691	-4.135007	-0.306597
H	-2.406223	-2.021264	-0.445709
C	-3.402563	-2.988504	-2.812670
H	-1.334365	-3.537042	-2.869525
H	-1.590552	-1.797291	-2.796884
C	-3.751746	-4.395939	-0.748392
H	-1.670947	-4.969956	-0.622710
H	-2.290989	-4.104677	0.786391
C	-3.921583	-4.319792	-2.266495
H	-3.483818	-2.966091	-3.906319
H	-4.027161	-2.170139	-2.432759
H	-4.075507	-5.376836	-0.378309
H	-4.391278	-3.648266	-0.266414
H	-4.975745	-4.458413	-2.536374
H	-3.363732	-5.142807	-2.737414
C	1.183741	-3.263115	-1.361346

C	0.952693	-4.780599	-1.431877
C	1.461960	-2.679522	-2.756014
H	2.099630	-3.117989	-0.773225
C	2.134787	-5.486007	-2.106147
H	0.042576	-4.992406	-2.006669
H	0.796712	-5.189766	-0.426794
C	2.627833	-3.403007	-3.438530
H	0.572826	-2.764493	-3.389596
H	1.678802	-1.610713	-2.679270
C	2.398278	-4.914483	-3.501087
H	1.941226	-6.563843	-2.165063
H	3.034473	-5.357588	-1.487205
H	2.773022	-2.995417	-4.446093
H	3.555161	-3.205835	-2.881982
H	3.261503	-5.411339	-3.959916
H	1.531987	-5.123639	-4.145141

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.068904	-0.565683	-0.140224
N	0.317789	-1.090429	2.073571
C	2.939886	0.199896	1.658347
H	3.930678	-0.101979	2.008407
H	2.977931	1.291029	1.569422
C	-2.421416	-2.024073	1.545172
C	0.190819	-0.753817	-1.872204
O	0.373022	-1.036939	-2.999103
P	-2.357606	-1.044485	-0.019909
P	2.537179	-0.448433	-0.030800
Si	-1.226040	-1.445694	2.873207
Si	1.607146	-0.214940	2.919955
C	-0.980369	-2.879896	4.072542
H	-0.291492	-3.614744	3.637997
H	-0.551194	-2.550626	5.026287
H	-1.926785	-3.388881	4.295410
C	2.332361	-1.310563	4.267642
H	3.245194	-0.871318	4.689733
H	1.628407	-1.464782	5.094296
H	2.588451	-2.298435	3.865625
H	-3.424773	-2.191043	1.945617

H	-2.045560	-3.006936	1.267669
P	-0.315909	1.836957	0.114730
C	-1.375071	2.187678	1.597833
H	-1.627127	3.252291	1.632759
H	-2.323582	1.675879	1.427859
Si	-0.909533	1.675214	3.360254
C	-1.521923	3.058113	4.489872
H	-0.999473	4.004202	4.299687
H	-2.594712	3.238788	4.345550
H	-1.368286	2.804964	5.546164
C	-1.815754	0.085065	3.795076
H	-2.894729	0.226768	3.647022
H	-1.677954	-0.092539	4.871592
C	0.920774	1.374869	3.662005
H	1.512521	2.233356	3.318808
H	1.056525	1.331542	4.752613
H	-0.068283	-2.348512	-0.106540
H	0.713975	-2.010417	1.803187
C	0.494845	-3.915823	0.277553
O	1.304363	-3.723304	1.219904
C	0.949332	-4.155981	-1.157975
H	1.452368	-5.132648	-1.202968
H	0.091093	-4.181468	-1.836875
H	1.629333	-3.387071	-1.507651
C	-0.737459	-4.757907	0.608031
H	-1.589458	-4.596048	-0.055439
H	-0.424290	-5.803382	0.476421
H	-1.034814	-4.642751	1.652170
C	-2.798445	-2.346412	-1.294025
C	-3.997166	-3.254300	-0.980891
C	-2.859946	-1.880425	-2.759948
H	-1.889812	-2.957365	-1.226151
C	-4.016006	-4.463779	-1.926342
H	-4.934646	-2.692960	-1.095092
H	-3.964666	-3.604998	0.056815
C	-2.830142	-3.095291	-3.693633
H	-3.787249	-1.333511	-2.952979
H	-2.032619	-1.206807	-2.990889
C	-3.999098	-4.039463	-3.397513
H	-4.895268	-5.086201	-1.718999
H	-3.133055	-5.086864	-1.723009
H	-2.866566	-2.763265	-4.738302
H	-1.878686	-3.629941	-3.564201
H	-3.953004	-4.923470	-4.044824

H	-4.941811	-3.524042	-3.632549
C	-3.906734	0.067018	0.121733
C	-4.626264	0.345737	-1.208339
C	-4.939566	-0.347229	1.185207
H	-3.517769	1.038156	0.440514
C	-5.709538	1.415771	-1.041104
H	-5.105367	-0.570937	-1.569402
H	-3.913906	0.657288	-1.979272
C	-6.055627	0.693846	1.332846
H	-5.376035	-1.320304	0.920792
H	-4.458878	-0.469725	2.159701
C	-6.743182	0.992855	0.001743
H	-6.190140	1.609746	-2.007430
H	-5.245980	2.358914	-0.719378
H	-6.784934	0.345789	2.074207
H	-5.621578	1.623705	1.729480
H	-7.503011	1.772858	0.129904
H	-7.266090	0.092226	-0.350051
C	-1.452941	2.471495	-1.250587
C	-2.068894	3.870808	-1.082288
C	-0.891332	2.303342	-2.674321
H	-2.273878	1.748103	-1.169957
C	-3.124923	4.147963	-2.161551
H	-1.286728	4.637971	-1.148374
H	-2.533143	3.977802	-0.095906
C	-1.967882	2.561600	-3.732664
H	-0.072223	3.008037	-2.849279
H	-0.482134	1.301220	-2.800809
C	-2.569444	3.958466	-3.573559
H	-3.523948	5.162200	-2.036893
H	-3.967139	3.457798	-2.021781
H	-1.534606	2.441023	-4.732831
H	-2.762505	1.806867	-3.640905
H	-3.358900	4.125888	-4.316327
H	-1.789500	4.710374	-3.763150
C	1.000732	3.186399	0.350701
C	1.550437	3.752048	-0.968647
C	0.662413	4.362233	1.285330
H	1.823614	2.645172	0.834074
C	2.795064	4.610710	-0.730375
H	0.785741	4.380689	-1.439268
H	1.768470	2.950456	-1.677629
C	1.887254	5.254359	1.522207
H	-0.150746	4.962024	0.855727

H	0.310600	4.005314	2.256277
C	2.485552	5.772107	0.214178
H	3.182269	4.984154	-1.686303
H	3.586420	3.987893	-0.289839
H	1.611639	6.090557	2.176029
H	2.650054	4.672010	2.060107
H	3.391778	6.355818	0.414633
H	1.769076	6.450954	-0.269922
C	3.528874	-2.044708	-0.139128
C	3.944165	-2.381925	-1.583657
C	4.715758	-2.216641	0.825352
H	2.792017	-2.786444	0.186225
C	4.549612	-3.785498	-1.685428
H	4.694016	-1.667271	-1.940686
H	3.091109	-2.289846	-2.265911
C	5.323169	-3.619709	0.698667
H	5.495214	-1.465544	0.642392
H	4.379554	-2.084196	1.859409
C	5.739979	-3.935907	-0.737714
H	4.853521	-3.981484	-2.721102
H	3.788624	-4.533138	-1.427248
H	6.180556	-3.711457	1.376983
H	4.576735	-4.356327	1.025886
H	6.154871	-4.949250	-0.800770
H	6.539261	-3.245603	-1.046118
C	3.486964	0.813433	-1.054258
C	5.002776	0.862360	-0.788515
C	3.166623	0.789411	-2.558397
H	3.081250	1.754616	-0.668289
C	5.687629	1.993454	-1.563427
H	5.472596	-0.081151	-1.083861
H	5.191538	0.983786	0.284477
C	3.889871	1.908554	-3.318446
H	3.452176	-0.171585	-2.998105
H	2.086308	0.883402	-2.702503
C	5.397068	1.892433	-3.061031
H	6.768445	1.961062	-1.378892
H	5.332805	2.964778	-1.192529
H	3.682860	1.811106	-4.390947
H	3.490446	2.884057	-3.008292
H	5.884575	2.713703	-3.600292
H	5.824257	0.957173	-3.451565

$R^1=R^2=R^3=CH_2F$

A1

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.012743	-1.113590	0.050944
N	0.189216	0.659513	-1.436071
C	-2.550231	-0.058855	-1.891281
H	-2.354422	-0.495680	-2.879453
H	-3.616372	0.186359	-1.856473
C	2.904621	0.626084	-0.265242
C	-0.032968	-2.607085	0.957449
O	-0.061597	-3.620662	1.545857
P	2.230969	-1.078336	-0.226507
P	-2.115056	-1.305989	-0.607672
Si	1.667988	1.655904	-1.264863
Si	-1.411776	1.417765	-1.648514
C	2.400865	1.967335	-2.965302
H	1.654706	2.350025	-3.671898
H	3.211459	2.704545	-2.906787
H	2.831548	1.048706	-3.382451
C	-1.428815	2.508273	-3.182310
H	-2.434678	2.907407	-3.364012
H	-0.752494	3.365954	-3.079430
H	-1.129367	1.951256	-4.078440
H	2.955978	0.974326	0.772356
H	3.912684	0.665806	-0.690688
C	-2.423250	-2.929186	-1.442393
H	-2.184428	-3.740601	-0.744223
H	-1.752521	-3.005771	-2.303805
C	-3.602235	-1.237399	0.501773
H	-3.619400	-2.140514	1.125643
H	-3.535613	-0.360606	1.149204
C	2.712616	-1.701558	-1.909104
H	2.671807	-2.797147	-1.902822
H	1.991879	-1.345738	-2.651746
C	3.381244	-2.067658	0.823457
H	3.075547	-3.120040	0.777442
H	3.319540	-1.719419	1.856567
P	-0.077165	0.056083	1.958242
C	0.253894	1.865115	2.173493
H	-0.172851	2.199600	3.128389
H	1.341458	1.969899	2.275839

Si	-0.282317	3.056983	0.802799
C	-1.612711	-0.052859	3.027527
H	-2.064249	-1.047282	2.954587
H	-1.401575	0.170452	4.079522
C	1.076192	-0.545596	3.308293
H	0.826386	-0.122976	4.287731
H	1.078217	-1.638409	3.370140
C	-0.646635	4.713530	1.616983
H	-1.480775	4.631166	2.324746
H	0.224391	5.084807	2.171069
H	-0.914851	5.474111	0.873678
C	1.160171	3.241064	-0.402966
H	2.027708	3.660709	0.124688
H	0.880971	3.980415	-1.168066
C	-1.800077	2.453039	-0.139376
H	-2.441464	1.901903	0.556691
H	-2.375695	3.329607	-0.468466
H	0.107511	-1.982166	-1.305033
H	0.312545	-0.000070	-2.205356
F	3.979050	-1.297291	-2.315134
F	4.701371	-1.972957	0.401703
F	2.375089	-0.124266	3.009323
F	-2.554350	0.887741	2.600254
F	-3.732023	-3.088246	-1.875381
F	-4.804215	-1.160881	-0.191427

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.070284	-0.938186	0.175022
N	0.011922	0.494770	-1.237230
C	-2.949550	0.400141	-1.144445
H	-3.488207	0.109004	-2.051684
H	-3.654920	0.925142	-0.492108
C	2.917850	0.350094	-0.690820
C	-0.157135	-2.486564	1.014116
O	-0.212621	-3.517616	1.567529
P	2.136143	-1.211796	-0.221461
P	-2.291804	-1.064521	-0.290005
Si	1.520617	1.294319	-1.588629
Si	-1.412118	1.478178	-1.452376

C	1.985364	1.290538	-3.415763
H	1.195857	1.700465	-4.055204
H	2.894319	1.882073	-3.585168
H	2.195224	0.268469	-3.755980
C	-1.559449	2.239537	-3.174022
H	-2.528487	2.743984	-3.283304
H	-0.782398	2.987962	-3.372698
H	-1.495460	1.472947	-3.955857
H	3.204690	0.874803	0.227720
H	3.815041	0.209069	-1.301126
C	-2.336857	-2.358207	-1.613735
H	-2.156914	-3.344622	-1.170498
H	-1.535348	-2.137984	-2.328754
C	-3.572944	-1.666103	0.890547
H	-3.240359	-2.616820	1.324637
H	-3.689852	-0.927710	1.688416
C	2.197355	-2.192545	-1.791997
H	1.988221	-3.247199	-1.575881
H	1.423684	-1.811174	-2.467338
C	3.289187	-2.151727	0.866112
H	2.883728	-3.157721	1.029920
H	3.370850	-1.643205	1.829782
P	0.028701	0.255978	2.027156
C	0.720125	1.960522	1.933906
H	0.530914	2.455488	2.896934
H	1.809192	1.830695	1.882574
Si	0.264195	3.187404	0.534795
C	-1.527671	0.508045	3.018776
H	-1.855252	-0.453134	3.433023
H	-1.383174	1.222580	3.836670
C	1.028164	-0.385949	3.470232
H	0.810460	0.147441	4.403079
H	0.852971	-1.456623	3.613756
C	0.380032	4.887501	1.345210
H	-0.382955	5.014968	2.123650
H	1.361321	5.045303	1.810818
H	0.233614	5.685289	0.606491
C	1.492595	3.052814	-0.887791
H	2.503589	3.360775	-0.589104
H	1.167952	3.765620	-1.660776
C	-1.441048	2.887603	-0.181160
H	-2.143656	2.651393	0.625303
H	-1.796560	3.811711	-0.658370
F	3.420201	-2.102737	-2.441526

F	4.554335	-2.266133	0.309912
F	2.380439	-0.196991	3.189689
F	-2.552335	0.998726	2.212470
F	-3.535755	-2.394534	-2.308640
F	-4.804986	-1.858833	0.286147

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.081317	-0.190483	-1.031713
N	0.201099	-0.278669	1.264594
C	2.151915	1.780521	0.792904
H	3.013240	1.163126	1.067426
H	2.465784	2.825208	0.884350
C	-1.926951	-2.264092	0.741331
C	0.186237	-0.330765	-2.768651
O	0.283424	-0.443402	-3.932916
P	-0.783176	-2.220671	-0.688489
P	1.657707	1.387803	-0.935665
Si	-1.104934	-1.196317	2.074119
Si	0.719165	1.299071	1.911963
C	-0.349056	-2.336327	3.358468
H	0.318527	-1.798802	4.041299
H	-1.132020	-2.817422	3.958101
H	0.226735	-3.135523	2.877138
C	1.335170	1.117697	3.679569
H	1.780463	2.053964	4.039410
H	0.531097	0.849221	4.375719
H	2.103188	0.337277	3.729553
H	-2.872909	-1.822632	0.410695
H	-2.121793	-3.283093	1.091191
P	-1.846070	0.944385	-1.208385
C	-3.062467	1.304521	0.142279
H	-3.727198	2.120048	-0.173255
H	-3.698704	0.414034	0.226041
Si	-2.411865	1.678727	1.881745
C	-3.671112	2.810420	2.704221
H	-3.720501	3.778850	2.191049
H	-4.676027	2.370815	2.683312
H	-3.416134	3.003411	3.753443
C	-2.287248	0.050016	2.827035

H	-3.284024	-0.403951	2.915667
H	-1.957805	0.267147	3.853929
C	-0.716865	2.500413	1.850586
H	-0.658207	3.130010	0.956062
H	-0.635023	3.174075	2.714960
H	1.429894	-1.045441	-0.932927
H	1.047631	-0.856886	1.259758
C	3.924674	-1.554089	1.045669
C	4.068185	-2.592994	-0.040043
H	3.279690	-2.425142	-0.783733
H	5.042537	-2.556800	-0.533167
H	3.909823	-3.589454	0.385557
C	5.049773	-0.569471	1.223894
H	6.010475	-1.091736	1.295226
H	5.104338	0.083562	0.342472
H	4.891726	0.040894	2.115565
O	2.918021	-1.504968	1.735695
C	0.515976	-3.426018	-0.140850
H	1.086974	-3.750518	-1.018889
H	1.202343	-2.931903	0.553037
C	-1.590236	-3.183483	-2.038247
H	-2.471710	-2.643148	-2.389430
H	-0.877895	-3.287443	-2.865663
C	-3.076358	0.217778	-2.425122
H	-2.578199	-0.107736	-3.343761
H	-3.879197	0.920675	-2.674187
C	-1.850272	2.634343	-2.021737
H	-1.106055	2.677234	-2.823341
H	-2.832955	2.893599	-2.431338
C	1.495867	3.080693	-1.670108
H	1.366143	2.985872	-2.755982
H	0.617957	3.579459	-1.252745
C	3.247938	0.865346	-1.735387
H	3.143094	0.910688	-2.826161
H	3.446963	-0.170802	-1.452414
F	-0.001399	-4.551412	0.494991
F	-1.983155	-4.453102	-1.633341
F	-3.687559	-0.896799	-1.844383
F	-1.538296	3.620125	-1.081505
F	4.344149	1.638896	-1.364280
F	2.604536	3.886563	-1.433917

A4

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.105266	-0.034544	-0.966944
N	0.383501	-0.188769	1.004796
C	1.593538	2.456868	0.673279
H	2.677897	2.341977	0.770569
H	1.371816	3.516879	0.837841
C	-1.191820	-2.682462	0.771492
C	-0.066548	-0.074318	-2.730986
O	-0.044817	-0.096443	-3.901096
P	-0.440323	-2.287909	-0.827321
P	1.058765	1.941131	-0.995114
Si	-0.379149	-1.439021	1.972496
Si	0.624545	1.324892	1.844110
C	0.808087	-2.437902	3.036239
H	1.440293	-1.806945	3.669485
H	0.237461	-3.111638	3.689244
H	1.471130	-3.053475	2.418225
C	1.598731	1.132437	3.446398
H	1.899721	2.112338	3.838853
H	1.018131	0.632772	4.231740
H	2.504397	0.539989	3.271391
H	-2.268451	-2.496514	0.688376
H	-1.040876	-3.726210	1.063018
P	-2.232460	0.622089	-0.938086
C	-3.204751	0.530017	0.620971
H	-4.098976	1.156871	0.500395
H	-3.574022	-0.501781	0.682050
Si	-2.424862	0.911778	2.323688
C	-3.859305	1.560946	3.361511
H	-4.249313	2.503671	2.957388
H	-4.687525	0.841796	3.392367
H	-3.547448	1.748595	4.396263
C	-1.736187	-0.679937	3.054202
H	-2.532415	-1.417276	3.226517
H	-1.319278	-0.443638	4.044736
C	-1.026640	2.159846	2.238696
H	-1.265268	2.921443	1.488278
H	-0.944857	2.678194	3.204660
H	3.916992	0.461815	0.296509
H	2.266494	-0.765914	1.065424
C	4.191548	-0.560319	0.592471

C	4.513419	-1.367485	-0.664082
H	3.637346	-1.450910	-1.318291
H	5.322291	-0.900879	-1.238382
H	4.818226	-2.384501	-0.391189
C	5.392948	-0.476168	1.523739
H	5.670387	-1.477965	1.871555
H	6.256744	-0.033435	1.015693
H	5.154761	0.134701	2.400667
O	3.128942	-1.160595	1.315556
C	1.211510	-3.121897	-0.726271
H	1.655101	-3.174151	-1.728052
H	1.875357	-2.550760	-0.070545
C	-1.266675	-3.291307	-2.136491
H	-2.297559	-2.952947	-2.258190
H	-0.729842	-3.154033	-3.083297
C	-3.436145	-0.243389	-2.077547
H	-3.004641	-0.381346	-3.074118
H	-4.388135	0.292239	-2.161762
C	-2.670309	2.343239	-1.508491
H	-2.198235	2.561169	-2.473030
H	-3.753612	2.478194	-1.600105
C	0.568496	3.484954	-1.874717
H	0.316209	3.238242	-2.913738
H	-0.299423	3.935436	-1.388935
C	2.635422	1.547214	-1.900371
H	2.494369	1.737790	-2.970376
H	2.866935	0.487149	-1.767629
F	1.113219	-4.410456	-0.218919
F	-1.277304	-4.642678	-1.825749
F	-3.719529	-1.500237	-1.543087
F	-2.219200	3.275765	-0.576533
F	3.720609	2.283012	-1.454795
F	1.603632	4.408548	-1.882675

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.015917	-0.618789	-0.703672
N	-0.140947	0.015428	1.441589
C	2.666605	-0.769268	1.328326
H	2.481773	-1.731436	1.808320

H	3.719750	-0.522412	1.498014
C	-2.812609	0.806129	0.438579
C	-0.000376	-1.436790	-2.257018
O	-0.030877	-2.014624	-3.274128
P	-2.316991	-0.696992	-0.482651
P	2.284489	-0.882088	-0.461070
Si	-1.589708	0.974765	1.876671
Si	1.464952	0.505258	2.028936
C	-2.339244	0.251494	3.433816
H	-1.613550	0.253147	4.255763
H	-3.216778	0.826397	3.754212
H	-2.657987	-0.784298	3.275082
C	1.520123	0.458241	3.906631
H	2.539374	0.622795	4.278169
H	0.880149	1.228671	4.354510
H	1.182210	-0.515861	4.280798
H	-2.731004	1.657813	-0.242193
H	-3.848346	0.745225	0.783094
P	-0.008423	1.444588	-1.690850
C	-0.211280	3.073384	-0.831489
H	0.278457	3.848493	-1.435238
H	-1.282095	3.311812	-0.854574
Si	0.340733	3.281775	0.974204
C	0.728757	5.109679	1.195032
H	1.589701	5.408791	0.584179
H	-0.122005	5.739205	0.905578
H	0.968534	5.339331	2.240637
C	-1.080142	2.766734	2.095952
H	-1.953254	3.410044	1.920475
H	-0.778334	2.931557	3.140366
C	1.845259	2.240407	1.412918
H	2.502871	2.216766	0.537679
H	2.404169	2.760995	2.203770
H	0.280079	-2.137106	0.121338
H	-0.328648	-0.947694	1.790208
C	-0.127276	-3.263379	1.180670
C	-0.803870	-4.138395	0.122354
H	-1.562268	-3.601759	-0.444116
H	-0.067500	-4.526284	-0.589172
H	-1.277534	-4.989936	0.629875
C	1.201736	-3.858572	1.644943
H	0.983435	-4.886904	1.965505
H	1.988197	-3.914254	0.893082
H	1.562813	-3.321242	2.524468

O	-0.799021	-2.671030	2.070841
C	-3.255820	-1.982066	0.503553
H	-3.542235	-2.811652	-0.151084
H	-2.625211	-2.348021	1.317276
C	-3.346145	-0.779839	-2.018472
H	-3.174628	0.087255	-2.654418
H	-3.072496	-1.691087	-2.564813
C	-1.207878	1.770959	-3.097301
H	-1.307174	0.890451	-3.740837
H	-0.897521	2.629168	-3.702583
C	1.496681	1.882886	-2.714416
H	1.908156	0.995274	-3.204351
H	1.261204	2.634165	-3.475715
C	3.757991	0.044539	-1.129879
H	3.721402	0.112007	-2.222390
H	3.825122	1.049907	-0.715275
C	2.816500	-2.556348	-1.081913
H	3.190705	-2.452517	-2.107536
H	1.951930	-3.223145	-1.089506
F	-4.424051	-1.449730	1.042102
F	-4.703106	-0.838165	-1.728465
F	-2.466407	2.081980	-2.581764
F	2.474236	2.437705	-1.892782
F	3.811296	-3.135272	-0.308925
F	4.926095	-0.631324	-0.789516

R^1=R^3=Ph, R^2=NH_2

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.133340	0.420227	-0.211754
N	-0.191435	-1.150974	1.539039
C	-2.682504	-1.777441	0.097627
H	-3.687325	-1.983703	0.482212
H	-2.556710	-2.279886	-0.865740
C	2.213223	0.287574	2.135575
C	-0.234335	1.737250	-1.346330
O	-0.284819	2.619521	-2.120081
P	1.935927	0.993310	0.452845
P	-2.364940	0.022549	-0.163676
Si	1.408050	-1.407019	2.268196

Si	-1.323339	-2.482414	1.202135
C	1.228481	-1.831214	4.095187
H	0.829884	-2.841682	4.244963
H	2.199090	-1.781314	4.604987
H	0.553970	-1.129427	4.601380
C	-2.094694	-3.078253	2.812120
H	-2.859756	-3.841834	2.622846
H	-1.356337	-3.512158	3.496660
H	-2.584455	-2.245123	3.333227
H	3.253793	0.339695	2.473602
H	1.635625	0.937878	2.806246
P	0.380403	-1.003587	-1.869172
C	1.610572	-2.343103	-1.627290
H	1.672251	-2.952698	-2.542063
H	2.586432	-1.852782	-1.520724
Si	1.401637	-3.504452	-0.148646
C	2.240706	-5.124892	-0.626194
H	1.749434	-5.590939	-1.489657
H	3.292101	-4.958735	-0.892870
H	2.219013	-5.850514	0.196331
C	2.275392	-2.809617	1.372129
H	3.295149	-2.525340	1.089271
H	2.379510	-3.638504	2.087590
C	-0.384395	-3.863005	0.338525
H	-0.946074	-4.170881	-0.552380
H	-0.353760	-4.733732	1.010370
H	-0.344770	1.416080	1.023696
H	-0.666058	-0.435665	2.092804
C	3.476645	0.539144	-0.463539
C	3.616109	1.049465	-1.760416
C	4.486993	-0.288760	0.033248
C	4.723518	0.733006	-2.538079
H	2.844263	1.696341	-2.165141
C	5.592510	-0.622090	-0.749761
H	4.430201	-0.680374	1.043344
C	5.712540	-0.112969	-2.038630
H	4.811921	1.143818	-3.539846
H	6.362201	-1.273493	-0.344813
H	6.574517	-0.367706	-2.648954
C	2.309894	2.785082	0.749362
C	3.625500	3.206152	0.983610
C	1.286688	3.735422	0.798157
C	3.910744	4.539884	1.256061
H	4.439223	2.487252	0.945347

C	1.571840	5.073184	1.065665
H	0.262959	3.420488	0.630179
C	2.882481	5.479459	1.295703
H	4.938143	4.845533	1.433984
H	0.764096	5.799473	1.090176
H	3.103501	6.523286	1.500908
C	-3.413392	0.470816	-1.610777
C	-4.107984	-0.460619	-2.387626
C	-3.494808	1.826389	-1.955733
C	-4.855066	-0.050761	-3.492247
H	-4.081161	-1.515888	-2.131961
C	-4.244795	2.236178	-3.051834
H	-2.966379	2.565122	-1.359792
C	-4.924234	1.297304	-3.827236
H	-5.389456	-0.788719	-4.084245
H	-4.297407	3.291686	-3.302699
H	-5.507414	1.617492	-4.685862
C	-3.425260	0.708200	1.201974
C	-2.870180	1.420840	2.264982
C	-4.806470	0.465932	1.207917
C	-3.668205	1.866501	3.319584
H	-1.805472	1.638301	2.248168
C	-5.605025	0.914452	2.253002
H	-5.266087	-0.070055	0.380835
C	-5.034998	1.613486	3.317391
H	-3.216234	2.418312	4.139290
H	-6.674140	0.721516	2.237460
H	-5.658480	1.963251	4.135507
N	1.116031	-0.217486	-3.203588
H	1.261697	-0.791032	-4.029274
H	0.666423	0.657044	-3.452122
N	-0.874181	-1.998621	-2.542206
H	-1.665731	-1.427732	-2.830610
H	-0.567704	-2.542603	-3.347129

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.082146	-0.045048	0.350097
N	0.011730	0.880186	-1.470649
C	-2.931188	0.810213	-1.374165

H	-3.484604	0.283771	-2.159430
H	-3.609327	1.531053	-0.904744
C	2.885190	1.046829	-0.779213
C	-0.138837	-1.175323	1.691841
O	-0.160689	-1.933485	2.588056
P	2.178855	-0.305102	0.209037
P	-2.305059	-0.333866	-0.085956
Si	1.523772	1.496966	-2.037658
Si	-1.393914	1.733313	-2.008880
C	2.055392	0.801900	-3.708755
H	1.306634	0.988173	-4.487959
H	3.003802	1.240670	-4.044882
H	2.195570	-0.284468	-3.636618
C	-1.528114	1.863366	-3.892557
H	-2.487092	2.312862	-4.182180
H	-0.736416	2.491250	-4.320830
H	-1.464048	0.877529	-4.369799
H	3.017503	1.911849	-0.121442
H	3.856492	0.818962	-1.231324
P	-0.075644	1.770083	1.626002
C	0.668164	3.334388	1.002420
H	0.403859	4.125497	1.721874
H	1.755499	3.221510	1.088105
Si	0.265100	4.012993	-0.739301
C	0.407508	5.891577	-0.576896
H	-0.351240	6.297801	0.104310
H	1.392008	6.185731	-0.190287
H	0.275941	6.383011	-1.548969
C	1.483836	3.393874	-2.042441
H	2.493003	3.801158	-1.892028
H	1.134538	3.782296	-3.011148
C	-1.445425	3.498359	-1.310040
H	-2.135812	3.544056	-0.458962
H	-1.810181	4.199561	-2.074070
C	3.268281	-0.557298	1.664525
C	3.191532	-1.772406	2.355925
C	4.120279	0.438664	2.146871
C	3.946278	-1.984549	3.504250
H	2.539277	-2.561903	1.993898
C	4.878243	0.225650	3.296540
H	4.201388	1.389876	1.629811
C	4.792383	-0.984269	3.978861
H	3.873884	-2.934254	4.026435
H	5.539615	1.008672	3.656918

H	5.382277	-1.149179	4.876030
C	2.556588	-1.806214	-0.787119
C	3.826741	-2.027086	-1.333151
C	1.554818	-2.755866	-1.001755
C	4.082960	-3.165033	-2.089451
H	4.624828	-1.309887	-1.159618
C	1.810861	-3.899860	-1.755637
H	0.566833	-2.607075	-0.573863
C	3.073136	-4.103557	-2.303126
H	5.071309	-3.322695	-2.511737
H	1.018075	-4.625226	-1.913114
H	3.275148	-4.993791	-2.892175
C	-3.662890	-0.469810	1.141979
C	-5.004043	-0.429560	0.740399
C	-3.370826	-0.632049	2.499692
C	-6.026671	-0.543221	1.675961
H	-5.249330	-0.310954	-0.311517
C	-4.395436	-0.746662	3.438089
H	-2.337705	-0.679785	2.828088
C	-5.724031	-0.700716	3.027938
H	-7.062436	-0.508688	1.350471
H	-4.151911	-0.874696	4.488813
H	-6.522852	-0.787613	3.758776
C	-2.343413	-1.975410	-0.918828
C	-2.874580	-3.112047	-0.301632
C	-1.724934	-2.110188	-2.168892
C	-2.805956	-4.353343	-0.929822
H	-3.349615	-3.032882	0.671840
C	-1.665075	-3.349764	-2.798126
H	-1.254754	-1.248367	-2.635498
C	-2.207288	-4.475494	-2.181261
H	-3.227343	-5.226593	-0.439981
H	-1.180242	-3.436731	-3.766216
H	-2.158267	-5.443848	-2.671111
N	0.827668	1.615186	3.068066
H	0.749788	2.356418	3.757414
H	0.767762	0.699656	3.498613
N	-1.638368	2.386779	1.975337
H	-2.289822	1.680812	2.301540
H	-1.672671	3.202384	2.581380

A3

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.055402	-0.111803	0.515511
N	-0.048688	-0.448541	-1.766012
C	2.687381	0.263133	-1.450227
H	2.488327	1.220666	-1.944526
H	3.759863	0.069125	-1.549820
C	-2.829712	-1.177026	-1.089055
C	-0.032084	0.408899	2.170509
O	0.010606	0.792973	3.285069
P	-2.312286	-0.054900	0.275360
P	2.117518	0.436729	0.298150
Si	-1.500640	-1.212805	-2.433782
Si	1.561850	-0.976424	-2.301648
C	-2.066258	-0.239578	-3.937485
H	-1.316414	-0.291774	-4.735710
H	-3.013395	-0.621080	-4.339159
H	-2.202774	0.819792	-3.691663
C	1.752765	-0.806996	-4.167098
H	2.786577	-1.012517	-4.473756
H	1.106931	-1.502890	-4.716894
H	1.504251	0.213111	-4.479933
H	-2.866731	-2.172540	-0.631316
H	-3.828979	-0.979383	-1.492475
P	-0.015785	-2.287624	1.131035
C	-0.451525	-3.732826	0.061713
H	-0.119507	-4.647213	0.575925
H	-1.544730	-3.796619	0.015207
Si	0.227626	-3.753458	-1.703515
C	0.523884	-5.548900	-2.197043
H	1.295709	-6.007534	-1.566250
H	-0.391314	-6.144515	-2.089842
H	0.854171	-5.632040	-3.239745
C	-1.063947	-2.990416	-2.855407
H	-1.976238	-3.603414	-2.840580
H	-0.681008	-3.035483	-3.885473
C	1.829813	-2.766038	-1.815242
H	2.321656	-2.840966	-0.836979
H	2.496464	-3.228467	-2.556320
H	-0.160750	1.402480	0.031609
H	-0.106959	0.559023	-1.945995
C	1.905339	4.080569	-2.468690
H	1.775450	5.035166	-2.993374

H	2.184405	4.318117	-1.435530
H	2.702934	3.509847	-2.948848
C	0.607764	3.312993	-2.486555
C	-0.549964	3.925401	-1.750485
H	-1.483774	3.429928	-2.020643
H	-0.381387	3.777507	-0.677852
H	-0.618750	5.003327	-1.932705
O	0.508986	2.236231	-3.053633
C	3.434428	-0.419518	1.271638
C	4.311562	-1.365744	0.736875
C	3.476260	-0.177044	2.652420
C	5.204714	-2.054816	1.555643
H	4.292635	-1.595154	-0.324071
C	4.366806	-0.863642	3.471263
H	2.799569	0.551435	3.091870
C	5.234595	-1.808372	2.924460
H	5.875361	-2.790248	1.119892
H	4.383156	-0.660126	4.538340
H	5.928409	-2.347897	3.562751
C	2.627307	2.180886	0.667951
C	1.722037	3.116166	1.170184
C	3.944307	2.588497	0.419076
C	2.118035	4.432083	1.410742
H	0.698296	2.809963	1.353670
C	4.340377	3.901492	0.648386
H	4.669880	1.870379	0.044626
C	3.425041	4.829404	1.145177
H	1.399092	5.146681	1.802255
H	5.364582	4.200544	0.443561
H	3.732145	5.855608	1.326935
C	-3.522430	-0.450792	1.622166
C	-3.297860	0.056680	2.907347
C	-4.684326	-1.192785	1.396086
C	-4.206884	-0.173814	3.935617
H	-2.400078	0.628593	3.116111
C	-5.593702	-1.428438	2.424893
H	-4.894122	-1.597784	0.411315
C	-5.359116	-0.919323	3.698290
H	-4.011497	0.230233	4.925122
H	-6.490683	-2.008822	2.226322
H	-6.069964	-1.100632	4.499528
C	-3.011422	1.593602	-0.186896
C	-3.822605	1.830500	-1.296998
C	-2.720299	2.665873	0.666497

C	-4.331058	3.106554	-1.550586
H	-4.069911	1.026945	-1.983483
C	-3.246200	3.929631	0.432548
H	-2.058821	2.506364	1.513682
C	-4.052022	4.156718	-0.683683
H	-4.951301	3.272262	-2.427174
H	-3.014568	4.743832	1.113710
H	-4.456253	5.146660	-0.874832
N	-1.176478	-2.589087	2.361189
H	-1.086728	-3.472038	2.856562
H	-1.275629	-1.821707	3.016296
N	1.494680	-2.908204	1.663243
H	2.025602	-2.242305	2.214421
H	1.457089	-3.805666	2.139908

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.081292	-0.297981	-0.449901
N	-0.001119	-0.185616	1.605456
C	-2.833812	0.207971	1.300056
H	-2.826393	1.249294	1.642181
H	-3.858003	-0.162374	1.401601
C	2.883487	-0.734391	1.370245
C	0.085179	0.014377	-2.174391
O	0.057177	0.203009	-3.335196
P	2.356075	-0.052221	-0.232002
P	-2.201050	0.180723	-0.422000
Si	1.387698	-0.624505	2.547703
Si	-1.512905	-0.704662	2.299382
C	1.797702	0.599800	3.922292
H	1.039872	0.568438	4.713467
H	2.768808	0.375343	4.383026
H	1.817348	1.629472	3.548572
C	-1.755723	-0.262104	4.119103
H	-2.796004	-0.459536	4.411537
H	-1.117759	-0.852398	4.788234
H	-1.550074	0.800691	4.283533
H	3.080763	-1.797510	1.188887
H	3.804976	-0.301558	1.774025
P	0.170617	-2.501449	-0.827490

C	0.713110	-3.631257	0.512198
H	0.519305	-4.662527	0.179664
H	1.803210	-3.540759	0.583895
Si	-0.025591	-3.412376	2.255797
C	-0.167723	-5.141266	3.001415
H	-0.841223	-5.776490	2.412005
H	0.806953	-5.643032	3.051008
H	-0.566846	-5.095566	4.022540
C	1.152476	-2.359060	3.288725
H	2.123124	-2.863536	3.397035
H	0.738721	-2.276124	4.304251
C	-1.711467	-2.580597	2.171055
H	-2.178565	-2.872962	1.221745
H	-2.355827	-2.940222	2.985257
H	-1.842765	3.269285	1.292434
H	-0.325100	1.772995	2.173453
C	-1.782570	4.529549	3.019422
H	-1.067634	4.875914	3.775144
H	-2.196173	5.404090	2.505175
H	-2.599002	4.010898	3.533462
C	-1.096571	3.597832	2.032351
C	0.047091	4.282423	1.296092
H	0.799800	4.630605	2.012291
H	0.533033	3.583858	0.607903
H	-0.308321	5.140523	0.713493
O	-0.622808	2.487954	2.773726
C	-3.390496	-0.824911	-1.389700
C	-4.215946	-1.788796	-0.804989
C	-3.390977	-0.691829	-2.784768
C	-5.028818	-2.598129	-1.595494
H	-4.214308	-1.935508	0.270402
C	-4.202102	-1.501754	-3.573666
H	-2.752733	0.049099	-3.258418
C	-5.023930	-2.458628	-2.980315
H	-5.663053	-3.343536	-1.124353
H	-4.192434	-1.382166	-4.653218
H	-5.657261	-3.091312	-3.595388
C	-2.577157	1.874105	-1.036688
C	-1.540280	2.737198	-1.393643
C	-3.894870	2.348341	-1.068022
C	-1.808336	4.050273	-1.776850
H	-0.511516	2.391184	-1.355983
C	-4.164222	3.657635	-1.447904
H	-4.712612	1.688240	-0.789118

C	-3.119611	4.512082	-1.803574
H	-0.987341	4.709624	-2.043161
H	-5.189765	4.015244	-1.466639
H	-3.331510	5.536285	-2.096728
C	3.651152	-0.571918	-1.434987
C	3.435349	-0.402267	-2.807343
C	4.867518	-1.113072	-1.011885
C	4.409821	-0.764321	-3.731316
H	2.495897	0.005529	-3.165285
C	5.841990	-1.482580	-1.936663
H	5.065748	-1.254129	0.045995
C	5.617122	-1.308383	-3.298319
H	4.222955	-0.623868	-4.792240
H	6.780090	-1.904848	-1.587540
H	6.376865	-1.596280	-4.019138
C	2.697876	1.758196	-0.149285
C	3.304590	2.383190	0.942692
C	2.348632	2.540449	-1.259430
C	3.570253	3.751318	0.920548
H	3.576131	1.812404	1.824467
C	2.621399	3.903821	-1.285469
H	1.864471	2.081126	-2.116704
C	3.236017	4.513848	-0.193807
H	4.038458	4.219374	1.781584
H	2.349274	4.489911	-2.158806
H	3.444790	5.579509	-0.209633
N	1.344585	-2.925075	-1.997478
H	1.373813	-3.902124	-2.273917
H	1.352809	-2.321541	-2.811763
N	-1.309140	-3.268064	-1.207054
H	-1.862206	-2.768954	-1.895492
H	-1.250692	-4.254001	-1.446000

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.053049	0.206357	0.314320
N	-0.057275	-0.642125	-1.782868
C	2.741631	0.167690	-1.766351
H	2.588616	1.045226	-2.400588
H	3.792694	-0.115523	-1.882136

C	-2.750690	-1.402569	-0.829793
C	0.110756	1.020269	1.856613
O	0.175281	1.549246	2.904686
P	-2.332991	-0.005176	0.301281
P	2.292441	0.659192	-0.047477
Si	-1.481280	-1.617668	-2.218472
Si	1.544708	-1.177398	-2.324583
C	-2.154828	-1.056392	-3.879118
H	-1.502130	-1.399789	-4.691266
H	-3.154906	-1.468219	-4.064955
H	-2.202270	0.035669	-3.931706
C	1.602372	-1.301555	-4.202962
H	2.630557	-1.439613	-4.561348
H	1.013283	-2.150035	-4.572433
H	1.205167	-0.392285	-4.670518
H	-2.690066	-2.309969	-0.219449
H	-3.778460	-1.343032	-1.205145
P	0.261927	-1.845021	1.371552
C	-0.184104	-3.473381	0.630008
H	0.194226	-4.250516	1.311363
H	-1.275093	-3.568066	0.659861
Si	0.415114	-3.864689	-1.125301
C	0.802023	-5.706649	-1.215055
H	1.636104	-5.971689	-0.553211
H	-0.064883	-6.310839	-0.918964
H	1.079388	-6.003749	-2.234095
C	-0.980367	-3.429144	-2.310096
H	-1.857389	-4.057388	-2.100090
H	-0.671784	-3.665991	-3.338221
C	1.938662	-2.848761	-1.568469
H	2.519605	-2.727789	-0.645478
H	2.560332	-3.411752	-2.278707
H	-0.008304	1.700298	-0.634934
H	-0.296319	0.282618	-2.201207
C	0.769154	3.002285	-2.567364
H	0.489344	3.817325	-3.249647
H	1.515976	3.388249	-1.873968
H	1.190865	2.205284	-3.184157
C	-0.527491	2.533188	-1.910858
C	-1.196936	3.636217	-1.100279
H	-1.697865	4.313111	-1.805965
H	-1.944590	3.240482	-0.419016
H	-0.459664	4.212629	-0.533170
O	-1.220616	1.725229	-2.588919

C	3.663620	-0.020510	0.990417
C	4.554397	-1.010086	0.571335
C	3.768827	0.464034	2.302139
C	5.526766	-1.504458	1.438784
H	4.483528	-1.428963	-0.427384
C	4.737216	-0.030506	3.169989
H	3.084230	1.233670	2.650073
C	5.621008	-1.018889	2.739175
H	6.209899	-2.276018	1.094971
H	4.804127	0.360744	4.181104
H	6.378948	-1.405254	3.414468
C	2.837897	2.422500	0.053547
C	2.040173	3.396589	0.654486
C	4.083780	2.796512	-0.463553
C	2.473737	4.719115	0.732990
H	1.061062	3.129311	1.031969
C	4.512449	4.117755	-0.399019
H	4.727868	2.049804	-0.921445
C	3.706580	5.083945	0.201732
H	1.836896	5.464729	1.200662
H	5.477436	4.393503	-0.814685
H	4.040495	6.116303	0.254669
C	-3.224757	-0.443741	1.864304
C	-2.936733	0.264542	3.037107
C	-4.218857	-1.423303	1.912344
C	-3.610224	-0.008268	4.223581
H	-2.166736	1.028826	3.035514
C	-4.888295	-1.705752	3.100986
H	-4.486076	-1.978779	1.019015
C	-4.584813	-1.002045	4.262226
H	-3.366180	0.553622	5.120994
H	-5.653759	-2.476671	3.115092
H	-5.107421	-1.221137	5.188963
C	-3.510102	1.315076	-0.256400
C	-3.956018	1.384358	-1.578053
C	-3.952230	2.293392	0.642532
C	-4.812831	2.400623	-1.990826
H	-3.625392	0.656077	-2.306403
C	-4.807094	3.311544	0.232315
H	-3.629507	2.273787	1.678017
C	-5.239500	3.370687	-1.089687
H	-5.139530	2.435039	-3.026336
H	-5.134834	4.057686	0.950506
H	-5.907003	4.164159	-1.413703

N	-0.709733	-1.966901	2.768116
H	-0.519956	-2.748555	3.387763
H	-0.820414	-1.106130	3.289712
N	1.856145	-2.300927	1.806042
H	2.386865	-1.556752	2.243890
H	1.914175	-3.142933	2.372844

$R^1=R^2=R^3=NMe_2$

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.230229	-0.703042	-0.539223
N	0.068277	0.082174	1.675302
C	2.856243	-0.458721	0.745028
H	3.763375	-0.841555	1.224242
H	3.130249	0.240079	-0.050076
C	-2.667044	1.031429	0.952318
C	-0.310949	-1.403687	-2.132369
O	-0.338285	-1.892507	-3.200589
P	-2.453756	-0.463133	-0.080913
P	1.712637	-1.689469	0.032351
Si	-1.296591	1.071481	2.247896
Si	1.790032	0.474818	1.992835
C	-1.897075	0.333879	3.868559
H	-1.112136	0.384919	4.633329
H	-2.777070	0.858489	4.259888
H	-2.161775	-0.722043	3.735542
C	2.204743	-0.060265	3.747324
H	3.269291	0.092033	3.965851
H	1.632443	0.510848	4.489416
H	1.979802	-1.123647	3.889081
H	-2.522287	1.871506	0.265554
H	-3.645125	1.170297	1.424175
P	0.435636	1.296304	-1.438493
C	0.085918	2.914075	-0.578483
H	0.430804	3.742166	-1.210833
H	-1.009995	2.986960	-0.610807
Si	0.610797	3.302982	1.201119
C	0.964350	5.153695	1.289752
H	1.807345	5.438601	0.647381
H	0.092269	5.737789	0.969514

H	1.210459	5.459492	2.314133
C	-0.746460	2.852653	2.426862
H	-1.622633	3.503616	2.307170
H	-0.351205	3.031936	3.436956
C	2.095915	2.320086	1.792501
H	2.959838	2.462808	1.132928
H	2.377556	2.735345	2.771042
H	-0.638487	-2.085919	0.028722
H	-0.090444	-0.871885	2.005113
C	-3.064245	-3.032819	0.470834
C	-4.244168	-1.466880	1.807614
H	-2.197954	-3.194452	-0.173858
H	-3.038889	-3.774951	1.279720
H	-3.981164	-3.213464	-0.116124
H	-4.221798	-0.513154	2.336169
H	-5.163327	-1.507717	1.199133
H	-4.322779	-2.253436	2.569103
C	-4.979498	0.319801	-1.036575
C	-3.711297	-1.214926	-2.379775
H	-4.941141	1.061132	-0.236452
H	-5.316303	0.835309	-1.947501
H	-5.748222	-0.427420	-0.778780
H	-2.737034	-1.685431	-2.517554
H	-4.458197	-2.010190	-2.221621
H	-3.971703	-0.696173	-3.313857
C	0.285184	2.776931	-3.769114
C	-1.602846	1.411002	-3.253326
H	1.365048	2.889569	-3.673740
H	0.062266	2.632498	-4.834050
H	-0.192325	3.724855	-3.459464
H	-1.948521	0.562143	-2.671112
H	-2.218496	2.286787	-2.970838
H	-1.783264	1.208099	-4.317455
C	2.935720	2.678927	-1.670688
C	2.704514	0.498881	-2.645067
H	2.494352	3.433050	-1.019564
H	3.926893	2.433690	-1.259610
H	3.106499	3.146885	-2.655421
H	2.181607	-0.455256	-2.559345
H	2.656349	0.830130	-3.695901
H	3.761640	0.326488	-2.395977
C	0.469330	-3.573488	1.713215
C	2.841114	-3.410332	1.837446
H	-0.463326	-3.015233	1.636913

H	0.402617	-4.435512	1.027733
H	0.556029	-3.967209	2.734475
H	3.726273	-2.795013	1.669073
H	2.811051	-3.655947	2.907158
H	2.977781	-4.354271	1.283142
C	1.997131	-3.722786	-1.706324
C	4.077617	-2.618497	-1.161350
H	0.911424	-3.649666	-1.615964
H	2.242191	-3.804641	-2.773547
H	2.321986	-4.653238	-1.209998
H	4.521208	-1.710462	-0.747538
H	4.484466	-3.484871	-0.612333
H	4.411046	-2.702639	-2.205171
N	-3.030842	-1.685730	1.032183
N	-3.678879	-0.273169	-1.274148
N	-0.189857	1.628521	-3.024799
N	2.133536	1.476021	-1.735061
N	1.618920	-2.716753	1.453435
N	2.633300	-2.553238	-1.125950

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.172173	-0.703349	-0.439847
N	0.092820	0.159763	1.435519
C	2.940226	-0.254749	0.832763
H	3.810406	-0.632411	1.381128
H	3.269357	0.469610	0.081637
C	-2.770748	0.780998	1.124193
C	-0.297834	-1.630236	-1.924816
O	-0.353922	-2.232766	-2.931027
P	-2.483686	-0.565387	-0.049217
P	1.961982	-1.537355	0.009001
Si	-1.240190	0.867946	2.250953
Si	1.672879	0.609457	1.957487
C	-1.682464	0.011471	3.875419
H	-0.863067	0.070657	4.602026
H	-2.573620	0.444880	4.348308
H	-1.877467	-1.052443	3.690691
C	2.052905	0.137215	3.751992
H	3.111046	0.311341	3.988326

H	1.462956	0.734578	4.458950
H	1.830866	-0.918500	3.949585
H	-2.801382	1.698982	0.526425
H	-3.707028	0.736477	1.688149
P	0.298949	1.278906	-1.484867
C	-0.199695	2.798857	-0.554175
H	0.002533	3.671819	-1.188632
H	-1.296125	2.723177	-0.539594
Si	0.335291	3.269381	1.222920
C	0.481444	5.155901	1.189461
H	1.283929	5.489999	0.518668
H	-0.450085	5.625529	0.848056
H	0.703063	5.550980	2.188622
C	-0.941191	2.726760	2.500110
H	-1.882979	3.286307	2.425104
H	-0.521323	2.943234	3.493336
C	1.942719	2.484329	1.790672
H	2.776076	2.702736	1.113802
H	2.201237	2.928176	2.762960
C	-2.596077	-3.259285	0.246356
C	-3.996024	-2.044728	1.760494
H	-1.762512	-3.193808	-0.457316
H	-2.342659	-4.013221	1.002999
H	-3.480666	-3.620980	-0.302995
H	-4.130567	-1.120643	2.323944
H	-4.927165	-2.258676	1.209434
H	-3.849752	-2.851365	2.490214
C	-5.042595	0.152149	-0.863790
C	-3.807898	-1.342976	-2.279508
H	-4.972377	0.964912	-0.139014
H	-5.523274	0.553346	-1.765533
H	-5.706812	-0.625535	-0.451091
H	-2.831108	-1.788050	-2.478337
H	-4.505369	-2.159203	-2.029423
H	-4.161742	-0.872584	-3.206752
C	-0.109357	2.838106	-3.716375
C	-1.649113	1.025318	-3.410275
H	0.889870	3.211808	-3.487697
H	-0.170518	2.699335	-4.803561
H	-0.841348	3.616393	-3.438569
H	-1.785581	0.059868	-2.935300
H	-2.489259	1.674792	-3.108448
H	-1.702689	0.885367	-4.498392
C	2.673720	2.817496	-1.669849

C	2.580120	0.669937	-2.740103
H	2.152065	3.528489	-1.030200
H	3.671835	2.655293	-1.237077
H	2.822858	3.291905	-2.654512
H	2.104568	-0.311931	-2.722743
H	2.502709	1.078388	-3.761284
H	3.644529	0.531126	-2.508136
C	0.549073	-3.036295	1.837824
C	2.961710	-3.259141	1.897549
H	-0.290509	-2.666096	1.249065
H	0.412945	-4.116326	1.992304
H	0.489634	-2.534825	2.816055
H	3.872753	-3.130535	1.307224
H	3.095148	-2.729441	2.855749
H	2.858158	-4.330291	2.116926
C	2.575129	-3.451880	-1.771296
C	4.441858	-2.033270	-1.198815
H	1.489999	-3.555052	-1.718725
H	2.866402	-3.482433	-2.829493
H	3.019837	-4.324422	-1.264403
H	4.736151	-1.089877	-0.736465
H	4.981153	-2.850936	-0.689567
H	4.785696	-2.015526	-2.242300
N	-2.834491	-1.972280	0.888470
N	-3.727007	-0.353630	-1.215321
N	-0.357061	1.572148	-3.054036
N	1.971251	1.553472	-1.759142
N	1.805346	-2.793018	1.159894
N	3.004723	-2.203864	-1.168175

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.353788	0.023012	-0.446363
N	0.721570	0.213507	1.669188
C	0.767143	-2.720383	1.138966
H	0.602741	-3.602289	1.769386
H	1.474687	-2.970782	0.340110
C	0.899217	2.970164	0.559103
C	-1.150683	-0.217861	-1.973980
O	-1.682932	-0.403529	-3.006214

P	-0.638476	2.288034	-0.160779
P	-0.738063	-2.060856	0.324270
Si	1.421993	1.828832	1.968802
Si	1.554040	-1.309521	2.111525
C	0.772348	2.426298	3.627303
H	1.128921	1.769311	4.430713
H	1.106908	3.444446	3.860582
H	-0.323262	2.413741	3.648725
C	1.367792	-1.594955	3.963505
H	1.848032	-2.537065	4.257480
H	1.847000	-0.791370	4.537156
H	0.319385	-1.646718	4.279306
H	1.644910	2.915682	-0.239575
H	0.871345	4.010832	0.896987
P	1.672392	-0.212297	-1.522751
C	3.242396	0.583366	-0.910193
H	4.051886	0.356180	-1.615522
H	3.057233	1.657832	-1.046206
Si	3.929651	0.367148	0.840555
C	5.809716	0.431887	0.718908
H	6.204421	-0.400614	0.122737
H	6.143794	1.363414	0.245271
H	6.274971	0.376056	1.710625
C	3.292949	1.733673	1.964035
H	3.686612	2.713061	1.660358
H	3.667394	1.541200	2.979333
C	3.384859	-1.212957	1.695562
H	3.665692	-2.102578	1.120340
H	3.950026	-1.264296	2.637864
H	-1.765972	0.111476	0.214499
H	-0.198673	0.224076	2.111313
C	-5.412086	-0.226211	-0.039902
O	-6.035167	0.629959	0.558367
C	-5.218150	-1.615202	0.523224
H	-5.741577	-1.713144	1.477249
H	-5.594537	-2.366864	-0.181284
H	-4.145474	-1.811100	0.661373
C	-4.755042	0.043465	-1.372765
H	-3.667479	-0.030436	-1.256025
H	-5.049455	-0.706548	-2.115741
H	-5.013659	1.042374	-1.731588
C	-3.131525	2.291705	0.909820
C	-1.725995	4.009883	1.734524
H	-3.165155	1.323824	0.414715

H	-3.658486	2.209175	1.868115
H	-3.675457	3.024593	0.290751
H	-0.722592	4.314037	2.033353
H	-2.141775	4.782956	1.067651
H	-2.341257	3.997416	2.642965
C	-0.750690	4.787187	-1.436727
C	-2.063991	2.997654	-2.363780
H	0.051883	5.049652	-0.745474
H	-0.448530	5.123932	-2.438989
H	-1.649197	5.359628	-1.153588
H	-2.249608	1.924006	-2.334150
H	-3.003017	3.517197	-2.112727
H	-1.798786	3.265256	-3.396796
C	2.819221	0.100708	-4.016546
C	1.057674	1.612047	-3.463428
H	3.244785	-0.888504	-3.847350
H	2.510743	0.151430	-5.068864
H	3.617536	0.851850	-3.872409
H	0.229376	1.802324	-2.786037
H	1.775100	2.448885	-3.362680
H	0.679366	1.620644	-4.494313
C	3.600270	-2.319164	-1.724989
C	1.379244	-2.682460	-2.545213
H	4.257059	-1.691589	-1.123848
H	3.629042	-3.328537	-1.288898
H	4.042215	-2.395775	-2.733590
H	0.332956	-2.401016	-2.423703
H	1.637775	-2.616056	-3.615460
H	1.485264	-3.731904	-2.238724
C	-2.253749	-1.097005	2.494089
C	-2.115016	-3.468227	2.239529
H	-2.181461	-0.138542	1.977590
H	-3.286349	-1.203145	2.853748
H	-1.606256	-1.082501	3.389585
H	-1.964702	-4.286663	1.534151
H	-1.427157	-3.614253	3.091117
H	-3.139805	-3.547891	2.626524
C	-2.487121	-3.211878	-1.378391
C	-0.736262	-4.709185	-0.672254
H	-2.785490	-2.164686	-1.431328
H	-2.408001	-3.590829	-2.406775
H	-3.287514	-3.772770	-0.866778
H	0.211501	-4.791879	-0.138874
H	-1.453910	-5.406197	-0.205361

H	-0.571275	-5.059413	-1.701641
N	-1.743009	2.679278	1.137947
N	-0.986431	3.357397	-1.457439
N	1.666297	0.330115	-3.170013
N	2.232337	-1.841971	-1.722406
N	-1.940633	-2.183924	1.586235
N	-1.216946	-3.346720	-0.695139

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.132946	-0.156916	-0.687515
N	-0.748522	0.255605	1.167526
C	-1.182831	-2.655372	1.247408
H	-2.168888	-3.041781	1.516903
H	-0.449896	-3.442587	1.457212
C	0.141201	3.034912	0.706940
C	0.393854	-0.369717	-2.408650
O	0.511580	-0.492427	-3.570298
P	0.215770	2.178321	-0.899627
P	-0.971835	-2.211337	-0.506728
Si	-0.530332	1.779513	1.969785
Si	-0.710514	-1.106082	2.242623
C	-2.068634	2.543305	2.748422
H	-2.579998	1.849167	3.423080
H	-1.774558	3.426740	3.332477
H	-2.796867	2.863035	1.998662
C	-1.912096	-0.986847	3.697688
H	-1.956372	-1.942338	4.237545
H	-1.615537	-0.220240	4.424337
H	-2.920821	-0.745693	3.343148
H	1.143267	3.354477	1.011164
H	-0.492832	3.927587	0.675088
P	2.362093	-0.386073	-0.150084
C	2.788564	0.702420	1.258382
H	3.872828	0.733400	1.412478
H	2.501033	1.722369	0.987128
Si	1.988910	0.275423	2.947307
C	3.417835	0.207811	4.181413
H	4.115264	-0.603036	3.933783
H	3.986880	1.146235	4.193624

H	3.052969	0.029698	5.200495
C	0.770399	1.644651	3.352890
H	1.270766	2.613118	3.491223
H	0.274827	1.411111	4.306511
C	1.026919	-1.340444	2.968753
H	1.593041	-2.099877	2.417436
H	0.943723	-1.687845	4.009129
H	-4.214398	0.228372	-0.795415
H	-2.789921	0.335289	0.968880
C	-4.541537	0.719690	0.134218
O	-3.738977	0.275167	1.209169
C	-5.971632	0.297451	0.441129
H	-6.313557	0.775922	1.366542
H	-6.650618	0.588350	-0.368351
H	-6.038044	-0.786543	0.578272
C	-4.439455	2.232332	-0.056230
H	-5.029760	2.558386	-0.922223
H	-4.819769	2.752408	0.830883
H	-3.397024	2.528930	-0.215746
C	-2.001904	1.650812	-2.411817
C	-1.568769	3.989662	-1.959952
H	-2.044108	0.676480	-1.917007
H	-3.036446	1.984645	-2.554184
H	-1.546428	1.524571	-3.405906
H	-1.116508	4.689658	-1.252906
H	-1.187051	4.224321	-2.966787
H	-2.650820	4.174321	-1.957879
C	1.652386	4.456287	-1.599468
C	1.911776	2.512722	-2.992500
H	1.283848	4.839117	-0.646125
H	2.722586	4.694344	-1.664740
H	1.140066	4.999945	-2.408672
H	1.993733	1.429023	-2.962700
H	1.237304	2.811490	-3.811889
H	2.906894	2.917584	-3.215932
C	4.498418	1.122888	-1.188563
C	3.677512	-0.758504	-2.462203
H	4.177437	1.962888	-0.569214
H	5.399156	0.671521	-0.736233
H	4.796124	1.535410	-2.161469
H	2.835214	-1.443830	-2.587327
H	3.815995	-0.231570	-3.416383
H	4.581228	-1.363795	-2.277420
C	4.499792	-1.907443	0.705011

C	2.584064	-3.138196	-0.037835
H	4.876699	-0.948982	1.064758
H	4.674838	-2.648168	1.497292
H	5.106047	-2.203094	-0.167238
H	1.514149	-3.091960	-0.226773
H	3.084764	-3.504342	-0.950992
H	2.751471	-3.886149	0.750731
C	-3.746188	-2.469870	-0.427515
C	-2.700373	-1.867605	-2.513333
H	-3.824320	-2.146982	0.611335
H	-4.638128	-2.094880	-0.941193
H	-3.771706	-3.569685	-0.485322
H	-1.809686	-1.442291	-2.980052
H	-2.852726	-2.876896	-2.931659
H	-3.558686	-1.249931	-2.808316
C	0.266610	-3.700766	-2.459007
C	-1.275105	-4.891804	-1.025580
H	0.901101	-2.817201	-2.524898
H	0.915393	-4.586808	-2.485982
H	-0.380220	-3.728801	-3.350418
H	-1.748955	-4.890069	-0.041012
H	-2.062735	-5.002277	-1.788454
H	-0.626517	-5.776168	-1.083830
N	-1.308656	2.615115	-1.570311
N	1.476934	3.015339	-1.698750
N	3.413869	0.188358	-1.396261
N	3.082284	-1.851553	0.394659
N	-2.575294	-1.877629	-1.061246
N	-0.483095	-3.689945	-1.216985

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.276719	0.478066	-0.633854
N	-0.197976	0.425011	1.647861
C	-2.405307	-1.458122	1.158345
H	-3.370374	-1.622445	1.647436
H	-2.053606	-2.418151	0.761466
C	2.282779	1.976237	1.131104
C	-0.537471	0.821726	-2.320894
O	-0.749938	1.112466	-3.440754

P	1.767483	1.596761	-0.600074
P	-2.491119	-0.385609	-0.335005
Si	1.282774	1.035764	2.423221
Si	-1.080948	-0.923999	2.387997
C	0.800928	2.190501	3.828481
H	0.545483	1.628194	4.734767
H	1.611678	2.883152	4.087014
H	-0.082261	2.773107	3.542810
C	-1.847636	-0.335497	4.004415
H	-2.615652	-1.030111	4.367871
H	-1.086713	-0.252556	4.790743
H	-2.305945	0.653484	3.888626
H	3.351233	1.844389	1.321261
H	2.081368	3.042640	1.263882
P	0.816359	-1.726135	-0.823684
C	2.195341	-1.905049	0.376727
H	2.797766	-2.785044	0.129212
H	2.837458	-1.038255	0.186516
Si	1.871979	-2.024657	2.248556
C	3.015516	-3.369110	2.921395
H	2.797353	-4.365182	2.517931
H	4.063737	-3.141197	2.689011
H	2.928415	-3.432096	4.013246
C	2.311284	-0.397405	3.067910
H	3.378362	-0.172503	2.941217
H	2.141385	-0.512898	4.147650
C	0.087425	-2.361387	2.730954
H	-0.291670	-3.264799	2.241670
H	0.084593	-2.557527	3.813244
H	-0.782655	2.102583	-0.217884
H	-0.861765	1.230330	1.700493
C	-1.519499	3.228715	0.722725
O	-1.898196	2.628194	1.765473
C	-2.539746	3.613983	-0.334915
H	-3.170461	4.414975	0.077273
H	-2.063858	3.981914	-1.248919
H	-3.159530	2.752684	-0.556194
C	-0.407034	4.261050	0.870087
H	0.140749	4.442343	-0.054569
H	-0.888396	5.198367	1.184134
H	0.291060	3.976000	1.658087
C	0.939348	3.579805	-2.352585
C	3.059865	3.924901	-1.242212
H	-0.056295	3.170175	-2.193952

H	0.855804	4.675464	-2.352531
H	1.295979	3.271567	-3.348264
H	3.637407	3.691469	-0.343743
H	3.699720	3.732767	-2.118968
H	2.840872	5.001149	-1.220546
C	4.519385	0.897757	-0.768843
C	3.109058	0.743279	-2.712105
H	4.576441	0.696799	0.304334
H	5.123508	0.126376	-1.263889
H	5.001645	1.869511	-0.965115
H	2.078403	0.618611	-3.049329
H	3.518149	1.656691	-3.176811
H	3.688509	-0.111155	-3.080811
C	2.825392	-2.736015	-2.524423
C	0.865798	-1.822952	-3.551446
H	3.542204	-2.604355	-1.712582
H	2.618790	-3.812817	-2.642906
H	3.320925	-2.400299	-3.445459
H	-0.086264	-1.327114	-3.371074
H	1.418371	-1.230384	-4.295657
H	0.657753	-2.807646	-3.999683
C	0.747025	-4.430632	-0.094875
C	-0.940257	-3.636190	-1.543828
H	1.327968	-4.261777	0.810730
H	0.031742	-5.230709	0.133097
H	1.427485	-4.809004	-0.876149
H	-1.466268	-2.761354	-1.915456
H	-0.441789	-4.148265	-2.384253
H	-1.691163	-4.325091	-1.133343
C	-4.468700	0.755571	1.307674
C	-4.647641	1.042896	-1.095114
H	-3.755908	0.632803	2.122179
H	-4.900041	1.757573	1.424722
H	-5.283728	0.018483	1.428889
H	-4.046182	1.210579	-1.995400
H	-5.417933	0.289941	-1.333712
H	-5.166644	1.984276	-0.873275
C	-3.115633	-1.236524	-2.906843
C	-4.297725	-2.327007	-1.133414
H	-2.315912	-0.544778	-3.160279
H	-2.929821	-2.185492	-3.434391
H	-4.057936	-0.824640	-3.303024
H	-4.363275	-2.491143	-0.057206
H	-5.261834	-1.917528	-1.475358

H	-4.167063	-3.307948	-1.614275
N	1.818905	3.174703	-1.274623
N	3.158886	0.792931	-1.259457
N	1.631286	-1.939942	-2.323924
N	0.000270	-3.247943	-0.501891
N	-3.809986	0.669054	0.025588
N	-3.185304	-1.463674	-1.478012

R^1=R^2=R^3=OMe

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.264221	-1.016769	-0.297654
N	0.021372	0.964207	-1.430140
C	-2.669282	1.315675	-0.301413
H	-3.544177	1.707297	-0.832398
H	-2.812848	1.482703	0.770078
C	2.436883	-0.446789	-2.073803
C	-0.680547	-2.643524	0.219179
O	-0.976710	-3.733425	0.504418
P	1.809726	-1.483962	-0.693856
P	-2.375802	-0.483295	-0.555932
Si	1.741902	1.273887	-1.767996
Si	-1.088114	2.216024	-0.814895
C	1.921780	2.337521	-3.309196
H	1.631214	3.378254	-3.122798
H	2.962522	2.347309	-3.657176
H	1.301842	1.959001	-4.131198
C	-1.499537	3.434588	-2.188269
H	-2.253767	4.159090	-1.855809
H	-0.620341	4.002361	-2.514860
H	-1.904330	2.914914	-3.065942
H	3.526638	-0.469426	-2.186501
H	1.996318	-0.825737	-3.004703
P	-0.109943	-0.300547	1.751452
C	1.253786	0.831464	2.217628
H	1.216807	1.068815	3.288577
H	2.178757	0.267336	2.044557
Si	1.409117	2.421097	1.208734
C	2.225335	3.705574	2.322793
H	1.597242	3.931923	3.193808

H	3.191457	3.345591	2.698316
H	2.404500	4.648560	1.791657
C	2.519706	2.126751	-0.289499
H	3.393314	1.551205	0.044843
H	2.901171	3.102285	-0.623504
C	-0.255885	3.096266	0.623597
H	-0.949029	3.121700	1.474619
H	-0.091312	4.143375	0.330069
H	-0.256215	-1.591913	-1.797478
H	-0.381975	0.522256	-2.258795
O	0.008304	-1.429387	2.964559
O	-1.426205	0.480113	2.391166
O	-3.508833	-1.254822	0.347045
O	-2.968979	-0.686924	-2.089451
O	2.981944	-1.266262	0.452807
O	2.265590	-3.015648	-1.109079
C	4.356778	-1.505309	0.194666
H	4.846403	-1.636419	1.163536
H	4.502255	-2.409019	-0.403761
H	4.818009	-0.649394	-0.314715
C	1.585590	-3.718017	-2.133995
H	0.529628	-3.866846	-1.892085
H	1.657966	-3.195094	-3.096597
H	2.078946	-4.689333	-2.226103
C	1.095326	-2.333597	2.982012
H	2.035508	-1.826449	3.234718
H	0.875580	-3.076444	3.753253
H	1.220220	-2.845698	2.022657
C	-1.445370	0.974422	3.719476
H	-1.048350	0.241699	4.428219
H	-0.878624	1.911024	3.805517
H	-2.489950	1.180634	3.968984
C	-4.544571	-0.606042	1.059406
H	-5.237638	-1.384798	1.387871
H	-4.143477	-0.095357	1.942027
H	-5.094632	0.113770	0.441025
C	-4.349934	-0.540735	-2.366424
H	-4.945763	-1.261067	-1.795136
H	-4.713140	0.474365	-2.155446
H	-4.486404	-0.738367	-3.432439

A2

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.138888	-1.036541	-0.128987
N	-0.125480	0.563317	-1.362465
C	-2.994929	0.704473	-0.629476
H	-3.810767	0.751122	-1.358722
H	-3.340507	1.147388	0.310356
C	2.811292	0.081340	-1.365528
C	-0.217004	-2.644209	0.615518
O	-0.263979	-3.704171	1.091854
P	2.033143	-1.301911	-0.465440
P	-2.351847	-0.965011	-0.307216
Si	1.374452	1.219483	-1.913716
Si	-1.454810	1.667182	-1.222410
C	1.499240	1.394126	-3.787769
H	0.728713	2.061448	-4.191371
H	2.475897	1.796034	-4.088166
H	1.372791	0.417169	-4.271594
C	-1.897064	2.536516	-2.841088
H	-2.825456	3.112713	-2.732726
H	-1.116162	3.239947	-3.155917
H	-2.042370	1.812207	-3.651883
H	3.465017	0.645657	-0.690260
H	3.414656	-0.223427	-2.227588
P	0.072472	0.016075	1.743103
C	1.166605	1.496327	1.716902
H	1.264188	1.922125	2.723649
H	2.168965	1.134589	1.451720
Si	0.734318	2.962804	0.556728
C	1.219634	4.508809	1.530278
H	0.632990	4.608601	2.452593
H	2.280355	4.488955	1.811942
H	1.053925	5.415704	0.935752
C	1.696384	2.885479	-1.061986
H	2.771554	3.056019	-0.918973
H	1.330840	3.714834	-1.686497
C	-1.078429	3.010267	0.073821
H	-1.713448	2.877178	0.956917
H	-1.297708	4.005336	-0.339315
O	0.591079	-0.833841	3.052340
O	-1.352933	0.656248	2.285791
O	-3.282915	-1.627461	0.861723
O	-2.716625	-1.788814	-1.684335

O	2.980563	-1.531913	0.859365
O	2.266969	-2.612016	-1.423201
C	4.385648	-1.711150	0.786576
H	4.787461	-1.524253	1.785566
H	4.632268	-2.738848	0.498929
H	4.856306	-1.012254	0.083202
C	3.472440	-2.973085	-2.080124
H	4.235409	-2.188617	-2.041317
H	3.873674	-3.881490	-1.619399
H	3.240732	-3.180528	-3.129042
C	1.502214	-0.373498	4.029961
H	1.148119	0.525777	4.549517
H	1.602885	-1.177627	4.763405
H	2.486698	-0.172426	3.593029
C	-1.467147	1.279391	3.550887
H	-1.318495	0.554418	4.359303
H	-0.758879	2.109892	3.670361
H	-2.481366	1.680950	3.622093
C	-4.680455	-1.426139	0.995104
H	-5.230446	-2.253891	0.534495
H	-4.906962	-1.403442	2.064493
H	-5.011311	-0.482379	0.546978
C	-4.037376	-1.987569	-2.157018
H	-4.481953	-2.873046	-1.688800
H	-4.686290	-1.121999	-1.975039
H	-3.976309	-2.154110	-3.235549

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.318675	-0.183336	-0.844109
N	-0.544634	-0.005524	1.436636
C	0.403154	-2.789910	1.134984
H	-0.035573	-3.657531	1.640404
H	1.445776	-3.019229	0.895340
C	-1.405636	2.607188	0.568277
C	-0.561769	-0.431870	-2.569062
O	-0.803875	-0.609847	-3.693283
P	-0.689494	1.950388	-0.985893
P	-0.447512	-2.325850	-0.428390
Si	-0.527609	1.695041	1.960161

Si	0.415112	-1.262402	2.250406
C	-1.483084	1.917987	3.562321
H	-0.962060	1.470951	4.417550
H	-1.623776	2.983853	3.783986
H	-2.472615	1.455582	3.483082
C	-0.386399	-1.699619	3.895925
H	0.110665	-2.556337	4.368547
H	-0.353500	-0.865566	4.607015
H	-1.441536	-1.963496	3.749725
H	-1.342773	3.693826	0.693630
H	-2.458022	2.308616	0.631532
P	1.846801	-0.167200	-1.034602
C	2.879241	1.028101	-0.102988
H	3.951899	0.901861	-0.292442
H	2.596843	2.021736	-0.471327
Si	2.603725	1.059493	1.768317
C	4.224099	1.647134	2.537191
H	5.031685	0.924047	2.365802
H	4.541600	2.606008	2.108650
H	4.128037	1.784508	3.621348
C	1.240254	2.285863	2.191800
H	1.395235	3.200902	1.605144
H	1.360396	2.568352	3.247432
C	2.165547	-0.620132	2.507074
H	2.876773	-1.365810	2.128563
H	2.341582	-0.544004	3.590393
H	-1.906840	-0.110394	-0.783134
H	-1.531139	-0.280745	1.391246
C	-4.290668	-0.028136	0.519748
C	-4.641439	1.048456	-0.479389
H	-3.833934	1.074720	-1.222837
H	-5.576311	0.832866	-1.005998
H	-4.707394	2.022227	0.012549
C	-4.666922	-1.436795	0.149988
H	-5.740565	-1.501455	-0.062532
H	-4.119682	-1.718134	-0.756662
H	-4.396887	-2.124484	0.952594
O	-3.706653	0.232621	1.559547
O	0.602403	2.984845	-1.196541
O	-1.725877	2.423219	-2.177420
O	2.624015	-1.596296	-0.638940
O	2.362312	0.042742	-2.594003
O	-1.967712	-2.921824	-0.153228
O	0.112216	-3.376391	-1.565252

C	0.922926	-4.499541	-1.289873
H	0.924139	-5.119037	-2.191079
H	1.952245	-4.189800	-1.074545
H	0.548213	-5.100836	-0.452248
C	-2.219634	-4.308077	-0.050514
H	-1.965986	-4.827453	-0.981688
H	-1.672972	-4.773408	0.781540
H	-3.290598	-4.427702	0.136081
C	3.477249	0.812905	-2.990691
H	4.412024	0.492465	-2.513744
H	3.580038	0.678924	-4.070949
H	3.320151	1.878510	-2.785219
C	3.971244	-1.854103	-0.970626
H	4.109763	-1.907401	-2.056636
H	4.658847	-1.104876	-0.554860
H	4.232384	-2.824377	-0.537478
C	0.471661	4.372911	-1.425736
H	1.438259	4.834059	-1.201452
H	0.226802	4.572384	-2.475293
H	-0.287173	4.839904	-0.784515
C	-2.563632	3.563025	-2.144318
H	-2.832661	3.855305	-1.123424
H	-2.088037	4.414988	-2.643423
H	-3.479893	3.312760	-2.687191

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.348892	0.078521	-0.760549
N	0.432826	0.089323	1.295508
C	0.082962	2.988199	0.914775
H	0.657652	3.794345	1.379615
H	-0.890699	3.387219	0.612976
C	0.737192	-2.783159	0.894627
C	0.818081	0.092495	-2.473574
O	1.151068	0.120132	-3.585951
P	0.260818	-2.165808	-0.745131
P	0.812246	2.260660	-0.580575
Si	0.143548	-1.428456	2.087146
Si	-0.214483	1.503531	2.072534
C	1.132672	-1.661874	3.674795

H	0.776729	-1.032960	4.498587
H	1.080881	-2.705183	4.013267
H	2.185762	-1.414691	3.494465
C	0.599079	1.876962	3.736704
H	0.375150	2.900914	4.063082
H	0.241020	1.203174	4.524075
H	1.689327	1.767831	3.685872
H	0.368229	-3.778904	1.162349
H	1.830269	-2.797508	0.963421
P	-1.768697	0.355512	-1.190736
C	-2.991504	-0.463507	-0.105351
H	-4.008048	-0.134143	-0.354512
H	-2.942611	-1.534646	-0.330627
Si	-2.795549	-0.311206	1.784156
C	-4.547695	-0.517326	2.462022
H	-5.201967	0.305229	2.145585
H	-5.003328	-1.454958	2.118404
H	-4.548347	-0.533323	3.559159
C	-1.701784	-1.695665	2.439436
H	-2.032523	-2.656408	2.020703
H	-1.855179	-1.762599	3.526575
C	-2.089323	1.339016	2.347945
H	-2.620359	2.157245	1.843684
H	-2.309486	1.440735	3.420972
H	2.767140	-1.037215	-0.438820
H	2.403931	0.079292	1.300069
C	3.695187	-0.787977	0.106027
O	3.365828	-0.118183	1.312343
C	4.433238	-2.080963	0.442247
H	3.853890	-2.707323	1.128787
H	4.647897	-2.659938	-0.463644
H	5.385373	-1.850663	0.935509
C	4.538166	0.097314	-0.806420
H	5.452143	0.410151	-0.286288
H	4.828829	-0.447288	-1.713059
H	3.975219	0.985619	-1.100462
O	-1.208621	-2.862019	-1.009116
O	1.265441	-2.883371	-1.825092
O	2.434217	2.467663	-0.396758
O	0.484109	3.274973	-1.818717
O	-2.265419	-0.031506	-2.709464
O	-2.214910	1.938463	-1.037308
C	1.836749	-4.174804	-1.679541
H	1.179020	-4.943262	-2.100147

H	2.776241	-4.174233	-2.237091
H	2.048291	-4.416520	-0.632319
C	-1.408351	-4.264692	-1.082214
H	-1.161761	-4.633265	-2.083490
H	-0.818935	-4.812438	-0.337525
H	-2.468446	-4.449078	-0.888749
C	-3.529800	-0.573387	-3.046405
H	-4.364641	0.052365	-2.708540
H	-3.560418	-0.633204	-4.137107
H	-3.650455	-1.581993	-2.635446
C	-3.475214	2.441378	-1.433019
H	-3.624508	2.326708	-2.512255
H	-4.303457	1.961319	-0.895109
H	-3.481178	3.507788	-1.193134
C	0.852942	4.641919	-1.724835
H	1.942298	4.754790	-1.686158
H	0.477903	5.135927	-2.623685
H	0.403725	5.120402	-0.844870
C	3.081918	3.136049	0.669210
H	4.153604	2.986721	0.522270
H	2.869225	4.212555	0.661961
H	2.808955	2.714440	1.641706

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.290761	0.548742	-0.681473
N	0.112177	0.437359	1.552225
C	-2.430018	1.675219	0.861070
H	-2.008751	2.665931	1.061884
H	-3.515757	1.703425	1.002221
C	2.641983	-1.092770	1.014915
C	0.578230	1.037165	-2.353587
O	0.794682	1.437561	-3.422619
P	2.443473	0.092382	-0.363737
P	-1.848995	1.093302	-0.766099
Si	1.229322	-0.771365	2.235476
Si	-1.578441	0.559363	2.117107
C	1.943914	-0.102772	3.837792
H	1.165803	0.088358	4.586106
H	2.667626	-0.800735	4.277249

H	2.462436	0.847179	3.655783
C	-1.629616	1.357790	3.814154
H	-2.660639	1.601553	4.100717
H	-1.221360	0.696820	4.588768
H	-1.047679	2.285641	3.808267
H	2.512212	-2.102847	0.615208
H	3.617483	-1.039883	1.511829
P	-0.148697	-1.541148	-1.228772
C	-1.309572	-2.619916	-0.292563
H	-2.327446	-2.334865	-0.580465
H	-1.177847	-3.666427	-0.594288
Si	-1.346080	-2.570154	1.600449
C	-2.144864	-4.197201	2.122789
H	-3.119104	-4.335854	1.637222
H	-1.516317	-5.056684	1.856695
H	-2.308380	-4.231347	3.206990
C	0.304643	-2.389734	2.487497
H	0.974082	-3.222964	2.237267
H	0.071910	-2.498972	3.557921
C	-2.403672	-1.129737	2.176605
H	-3.337027	-1.100942	1.599706
H	-2.684820	-1.326666	3.221169
H	0.488619	2.188227	-0.332021
H	0.468091	1.403752	1.698139
C	-0.375018	4.352549	-0.406707
H	-0.194652	5.414593	-0.189349
H	-0.190502	4.178094	-1.469717
H	-1.421777	4.146348	-0.184884
C	0.568082	3.535530	0.477556
C	2.025658	3.875458	0.196990
H	2.167339	4.934558	0.456633
H	2.681245	3.266149	0.814147
H	2.287757	3.733894	-0.855054
O	0.229708	3.261036	1.661930
O	3.274568	-0.522050	-1.639990
O	3.437072	1.310024	0.121737
O	1.153036	-2.579824	-1.304862
O	-0.719273	-1.630122	-2.772976
O	-2.919967	-0.139065	-1.070941
O	-2.277580	2.225284	-1.870838
C	4.191680	-1.593529	-1.541949
H	4.720468	-1.645499	-2.497201
H	4.928146	-1.451637	-0.741586
H	3.666408	-2.539700	-1.376431

C	4.842612	1.179298	0.190877
H	5.153631	0.379122	0.876113
H	5.271809	0.995733	-0.800480
H	5.230757	2.127721	0.571765
C	1.137180	-3.746353	-2.102629
H	0.988777	-3.501624	-3.159657
H	2.110292	-4.231598	-1.986870
H	0.364157	-4.459872	-1.785883
C	-1.760787	-2.470787	-3.224217
H	-1.780380	-2.382899	-4.313781
H	-1.604643	-3.524605	-2.963630
H	-2.727865	-2.139847	-2.828577
C	-4.307481	0.059925	-1.259061
H	-4.512887	0.405735	-2.278152
H	-4.798810	-0.906620	-1.112282
H	-4.732907	0.773554	-0.542560
C	-3.365693	3.125777	-1.755462
H	-4.252246	2.729796	-2.262920
H	-3.617880	3.341525	-0.711355
H	-3.069121	4.058220	-2.242672

$R^1=R^2=R^3=Me$

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.333884	0.119575	-0.229108
N	-0.742676	-0.261147	-1.231688
C	0.049121	-3.034984	-0.568233
H	0.067376	-3.809327	-1.345798
H	-0.071524	-3.558027	0.388822
C	-0.734128	2.728299	-1.023395
C	2.992448	0.369721	0.244318
O	4.118985	0.541490	0.528905
P	1.030710	2.301063	-0.635198
P	1.646888	-2.084184	-0.522765
Si	-1.756012	1.189577	-1.415166
Si	-1.407187	-1.850219	-0.789886
C	-2.374888	1.278383	-3.189118
H	-2.963742	0.393580	-3.459072
H	-3.003963	2.162642	-3.349434
H	-1.533589	1.341750	-3.891730

C	-2.530917	-2.478657	-2.165789
H	-2.880367	-3.497524	-1.955035
H	-3.420022	-1.846758	-2.284502
H	-2.007168	-2.501743	-3.129636
H	-1.164646	3.201807	-0.131430
H	-0.790655	3.473720	-1.826949
C	2.384865	-2.568183	-2.139302
H	3.352692	-2.068580	-2.248653
H	2.520902	-3.652641	-2.233035
H	1.742318	-2.212440	-2.951208
C	2.699387	-3.104656	0.595199
H	2.729289	-4.154633	0.281835
H	3.718978	-2.703664	0.583537
H	2.329527	-3.052744	1.622552
C	1.912457	2.950772	-2.116196
H	1.746607	4.024654	-2.264876
H	2.984649	2.761204	-1.999648
H	1.578564	2.403235	-3.002416
C	1.457396	3.644467	0.560714
H	2.502996	3.542350	0.871595
H	1.316653	4.638132	0.119087
H	0.826347	3.575037	1.452389
P	0.552031	0.125112	1.888668
C	-1.128019	0.848739	2.215286
H	-1.305870	0.856633	3.300359
H	-1.076257	1.903880	1.910639
Si	-2.661136	0.094304	1.383996
C	0.442118	-1.427167	2.902805
H	0.005036	-2.255368	2.340100
H	1.458014	-1.718589	3.190855
H	-0.138181	-1.279508	3.821955
C	1.548708	1.084236	3.114872
H	1.598763	2.140388	2.840644
H	1.135651	1.002913	4.127723
H	2.572891	0.696491	3.118832
C	-4.062108	0.158325	2.643865
H	-3.840220	-0.467497	3.517595
H	-4.227876	1.181280	3.004420
H	-5.004960	-0.198379	2.211207
C	-3.150655	1.053381	-0.165656
H	-3.504497	2.061089	0.089824
H	-4.007795	0.528720	-0.613041
C	-2.417123	-1.676708	0.792201
H	-2.009104	-2.304382	1.592225

H	-3.420798	-2.075484	0.582561
H	1.780760	0.160401	-1.789830
H	-0.132727	-0.342841	-2.049401

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.207495	0.079646	-0.132353
N	-0.568005	-0.117034	-1.123691
C	-0.038569	-3.017434	-0.899913
H	0.010271	-3.631289	-1.807564
H	-0.249737	-3.692145	-0.061820
C	-0.678126	2.821340	-0.774569
C	2.910597	0.251644	0.254755
O	4.053795	0.367963	0.495713
P	1.054695	2.302320	-0.535211
P	1.532843	-2.124625	-0.595979
Si	-1.616052	1.249133	-1.305642
Si	-1.359260	-1.649488	-0.974941
C	-2.214738	1.538885	-3.074519
H	-2.742298	0.669346	-3.482673
H	-2.898992	2.396249	-3.124217
H	-1.368151	1.750835	-3.740593
C	-2.541566	-2.051348	-2.398280
H	-2.897270	-3.087536	-2.322364
H	-3.429697	-1.406572	-2.397516
H	-2.048697	-1.938926	-3.371933
H	-1.068571	3.154298	0.195451
H	-0.781064	3.658786	-1.475873
C	2.334423	-2.140256	-2.252295
H	3.326296	-1.680438	-2.183214
H	2.437865	-3.154472	-2.655778
H	1.728326	-1.541296	-2.940603
C	2.598490	-3.292919	0.338682
H	2.714028	-4.243490	-0.194157
H	3.586334	-2.845085	0.491110
H	2.161016	-3.493781	1.321390
C	1.808598	2.583781	-2.191430
H	1.628964	3.599942	-2.561542
H	2.888982	2.411896	-2.133978
H	1.392521	1.865202	-2.905872

C	1.831954	3.648090	0.446553
H	2.879220	3.403440	0.653592
H	1.787319	4.604742	-0.086220
H	1.311325	3.763812	1.402434
P	0.560360	0.059658	1.994833
C	-1.155832	0.673954	2.305693
H	-1.363574	0.557127	3.379136
H	-1.130745	1.757965	2.124182
Si	-2.659000	-0.012389	1.340024
C	0.557960	-1.551525	2.893961
H	0.042039	-2.320109	2.312263
H	1.595177	-1.872756	3.038631
H	0.077980	-1.472431	3.876585
C	1.506177	1.055047	3.225524
H	1.505599	2.110700	2.938623
H	1.085719	0.965718	4.234229
H	2.547487	0.716318	3.243427
C	-4.080133	-0.030021	2.587106
H	-3.883330	-0.729965	3.409448
H	-4.242004	0.962045	3.028142
H	-5.019195	-0.336812	2.109883
C	-3.097611	1.087575	-0.127359
H	-3.448646	2.078791	0.190679
H	-3.946001	0.609929	-0.641393
C	-2.385976	-1.731557	0.629686
H	-1.929172	-2.396255	1.373418
H	-3.373014	-2.162804	0.405243

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.205059	1.227493	-0.076492
N	-0.301339	-1.053628	0.369142
C	-1.314730	-1.020978	-2.297432
H	-2.315252	-1.176038	-1.877481
H	-1.328531	-1.380967	-3.333144
C	0.829639	-0.027461	2.887017
C	-0.407933	2.944635	-0.282763
O	-0.575743	4.101837	-0.407174
P	-0.247263	1.297546	2.174141
P	-0.907417	0.779743	-2.169000

Si	0.546628	-1.580230	1.839868
Si	-0.120536	-1.924312	-1.162153
C	-0.543134	-2.777737	2.794207
H	-0.810890	-3.646592	2.181363
H	-0.035574	-3.143214	3.695847
H	-1.477373	-2.297230	3.107498
C	-0.631821	-3.728073	-0.978106
H	-0.681348	-4.230120	-1.952880
H	0.070545	-4.295945	-0.354964
H	-1.623272	-3.796119	-0.515000
H	1.870850	0.306199	2.793500
H	0.633989	-0.205409	3.952930
P	2.038546	1.457873	-0.311959
C	3.315502	0.153708	0.076225
H	4.255246	0.421574	-0.426739
H	3.528028	0.217465	1.152640
Si	2.898450	-1.657026	-0.273199
C	4.501186	-2.563131	-0.683149
H	4.957626	-2.169602	-1.600215
H	5.238035	-2.461454	0.123520
H	4.324411	-3.635136	-0.836171
C	2.148228	-2.394300	1.294465
H	2.886898	-2.339535	2.106234
H	1.956572	-3.464266	1.127022
C	1.677786	-1.847738	-1.703040
H	1.837930	-1.023379	-2.408195
H	1.909426	-2.773408	-2.248369
H	-1.805766	1.093871	0.081958
H	-1.304810	-1.000530	0.565160
C	-4.848082	-1.488214	-1.064801
H	-5.914429	-1.680778	-0.895144
H	-4.786222	-0.676624	-1.800952
H	-4.372543	-2.387608	-1.461470
C	-4.198345	-1.057874	0.225769
C	-4.718775	0.203819	0.864356
H	-4.758579	0.089364	1.951048
H	-3.995975	1.000473	0.641701
H	-5.700174	0.495383	0.480457
O	-3.275216	-1.687302	0.717282
C	2.660364	1.979524	-1.974473
H	2.562006	1.169714	-2.702490
H	2.064975	2.828414	-2.326552
H	3.714541	2.279624	-1.935393
C	-0.011279	1.005184	-3.778554

H	-0.664307	0.767275	-4.627080
H	0.327700	2.040635	-3.883303
H	0.864534	0.352318	-3.835020
C	-2.482543	1.604849	-2.659363
H	-2.299415	2.675093	-2.808473
H	-2.895021	1.187181	-3.585602
H	-3.209666	1.505169	-1.849630
C	2.794586	2.839680	0.662901
H	2.229336	3.764002	0.505991
H	2.766796	2.598711	1.729958
H	3.841072	3.010020	0.382963
C	0.151491	2.787878	3.182012
H	1.167626	3.137937	2.986185
H	-0.535804	3.594091	2.902535
H	0.044903	2.591481	4.255138
C	-1.866287	0.868662	2.945545
H	-1.783900	0.714768	4.028654
H	-2.568079	1.686537	2.752613
H	-2.279309	-0.031623	2.480948

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.007557	-1.133904	0.028886
N	-0.419530	0.869303	-0.249914
C	-1.201537	0.800744	2.542013
H	-2.277668	0.890670	2.356117
H	-1.015213	1.124539	3.572700
C	0.532936	0.336213	-2.983640
C	-0.261771	-2.870608	0.125096
O	-0.451923	-4.026618	0.170526
P	-0.071381	-1.229513	-2.258461
P	-0.670605	-0.934442	2.249598
Si	0.156019	1.677475	-1.682288
Si	-0.270058	1.780881	1.218590
C	-1.087555	2.863814	-2.459452
H	-1.360230	3.677196	-1.777553
H	-0.664083	3.318427	-3.365051
H	-2.014029	2.348427	-2.736403
C	-1.034831	3.506821	1.114606
H	-1.144614	3.951953	2.112121

H	-0.430062	4.198785	0.515420
H	-2.030602	3.453205	0.657827
H	1.616574	0.246638	-3.129598
H	0.084779	0.548406	-3.962314
P	2.226284	-1.332467	0.237881
C	3.206488	0.127644	-0.325870
H	4.254025	-0.030602	-0.033248
H	3.199047	0.108920	-1.424390
Si	2.675232	1.894249	0.170221
C	4.270265	2.848969	0.505621
H	4.792382	2.451020	1.385458
H	4.962914	2.796075	-0.343880
H	4.063797	3.909322	0.697581
C	1.745364	2.640111	-1.287974
H	2.394102	2.689611	-2.173986
H	1.483977	3.680724	-1.044066
C	1.558809	1.963623	1.692589
H	1.854229	1.182690	2.405820
H	1.713786	2.923567	2.206241
H	-3.369800	-0.263667	0.651807
H	-2.282996	1.038263	-0.593801
C	-4.706389	1.379237	1.035880
H	-5.377051	2.043243	0.478131
H	-5.296443	0.846068	1.791155
H	-3.971231	2.006966	1.551121
C	-4.020544	0.410319	0.075158
C	-5.035240	-0.436665	-0.683668
H	-5.663688	0.203731	-1.313693
H	-4.529183	-1.159826	-1.331085
H	-5.686038	-0.987082	0.005705
O	-3.229823	1.128923	-0.853175
C	3.037789	-1.652328	1.863859
H	2.875882	-0.823002	2.556156
H	2.634002	-2.564911	2.312799
H	4.118555	-1.778786	1.733026
C	0.334893	-1.275074	3.755180
H	-0.296496	-1.201858	4.648128
H	0.765653	-2.279350	3.712510
H	1.146461	-0.549347	3.852520
C	-2.139675	-1.971618	2.659608
H	-1.823953	-3.013182	2.784581
H	-2.619045	-1.632459	3.584831
H	-2.872590	-1.945251	1.848265
C	3.041111	-2.682971	-0.719068

H	2.575183	-3.643882	-0.476639
H	2.918857	-2.510319	-1.790551
H	4.114073	-2.741692	-0.503620
C	0.603102	-2.563254	-3.334034
H	1.684880	-2.462860	-3.454982
H	0.395705	-3.542476	-2.889850
H	0.148060	-2.520139	-4.329737
C	-1.841435	-1.280980	-2.751576
H	-1.959682	-1.204830	-3.838938
H	-2.274112	-2.230583	-2.416406
H	-2.390365	-0.462406	-2.274350

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.811383	0.328948	0.682478
N	0.167765	-0.582206	-1.147245
C	-0.363128	2.128035	-2.084754
H	-1.254993	1.803588	-2.624041
H	0.005523	3.039363	-2.571617
C	0.557142	-2.713060	0.871232
C	-1.865865	0.872978	1.968580
O	-2.603864	1.214514	2.813081
P	-1.062050	-1.922153	1.272842
P	-0.790828	2.399521	-0.309836
Si	1.046262	-2.104191	-0.856080
Si	0.885913	0.720093	-2.114357
C	0.526901	-3.364863	-2.146421
H	0.798344	-3.027994	-3.154346
H	1.011297	-4.334653	-1.976593
H	-0.557962	-3.518915	-2.135475
C	1.165108	0.136786	-3.882377
H	1.469072	0.963504	-4.536788
H	1.949216	-0.628814	-3.937533
H	0.246469	-0.296553	-4.296592
H	1.304541	-2.379772	1.599498
H	0.512709	-3.808497	0.925677
P	1.058353	0.585277	2.013589
C	2.792510	0.064262	1.548977
H	3.489279	0.724040	2.084793
H	2.961426	-0.934099	1.976432

Si	3.344764	-0.056750	-0.258116
C	5.217841	0.159249	-0.270865
H	5.507244	1.167171	0.052575
H	5.703501	-0.557309	0.403413
H	5.632810	0.002570	-1.274334
C	2.889174	-1.757587	-0.924750
H	3.423369	-2.538062	-0.365164
H	3.236732	-1.829533	-1.965767
C	2.533171	1.236656	-1.359559
H	2.425054	2.166609	-0.788938
H	3.220187	1.467955	-2.186080
H	-2.140029	0.331024	-0.437526
H	-0.742827	-0.843824	-1.571211
C	-3.502632	0.710255	-2.526463
H	-4.456301	0.423393	-2.992197
H	-3.652387	1.677793	-2.045963
H	-2.765653	0.791022	-3.328317
C	-3.131387	-0.422928	-1.572916
C	-4.219388	-0.676153	-0.532067
H	-5.022339	-1.257679	-1.007877
H	-3.845834	-1.227081	0.326370
H	-4.640205	0.268537	-0.173763
O	-2.442607	-1.355002	-2.056247
C	1.417939	2.322075	2.526154
H	1.841971	2.888599	1.695372
H	0.492269	2.810669	2.845944
H	2.135202	2.343936	3.354394
C	0.206859	3.939631	-0.014523
H	-0.127083	4.720538	-0.708470
H	0.066346	4.307796	1.005435
H	1.275159	3.780556	-0.182296
C	-2.432117	3.240957	-0.257627
H	-2.481799	3.839300	0.659636
H	-2.582706	3.909301	-1.112842
H	-3.233208	2.502601	-0.211690
C	1.042148	-0.139607	3.717465
H	0.134215	0.169602	4.245884
H	1.071127	-1.231867	3.676248
H	1.915025	0.196912	4.288947
C	-1.458725	-2.424599	3.003210
H	-0.874688	-1.884193	3.747316
H	-2.514151	-2.190565	3.184207
H	-1.314356	-3.501628	3.146343
C	-2.182977	-3.136261	0.436618

H	-1.773893	-4.148527	0.535689
H	-3.168023	-3.128712	0.913419
H	-2.312383	-2.875230	-0.616754

R^1=NH_2, R^2=R^3=Ph

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.006401	-0.270914	-1.073553
N	0.431777	-2.191279	0.215495
C	1.690339	-0.083703	1.826765
H	2.604373	-0.051465	2.429104
H	0.997888	0.650837	2.253027
C	-1.012887	-3.296848	-2.037031
C	0.063815	0.971173	-2.283193
O	0.157727	1.708466	-3.196279
P	-1.300496	-1.512688	-2.355318
P	1.892381	0.381577	0.058811
Si	-0.640409	-3.547579	-0.211852
Si	0.865241	-1.784503	1.890733
C	0.279862	-5.174428	0.014990
H	0.485087	-5.384450	1.071614
H	-0.305319	-6.014836	-0.379603
H	1.240500	-5.164330	-0.514764
C	2.082167	-3.052515	2.564869
H	2.505036	-2.726562	3.523730
H	1.601328	-4.023939	2.731750
H	2.914604	-3.211070	1.868404
H	-1.833224	-3.931043	-2.397410
H	-0.111129	-3.567424	-2.599627
P	-1.667196	0.629235	0.201311
C	-2.885014	-0.538849	0.935440
H	-3.685383	0.000708	1.456517
H	-3.343328	-1.029822	0.066947
Si	-2.321267	-1.993328	2.004357
C	-3.694526	-2.292243	3.263431
H	-3.782961	-1.454833	3.967431
H	-4.666906	-2.414956	2.770259
H	-3.505048	-3.198401	3.852081
C	-2.155407	-3.506321	0.894919
H	-3.058673	-3.581223	0.274557

H	-2.137937	-4.402260	1.531907
C	-0.697536	-1.749854	2.928903
H	-0.733533	-0.814837	3.502147
H	-0.637232	-2.560511	3.669948
H	0.988449	-1.057476	-2.058313
H	1.282773	-2.297262	-0.342017
C	-2.799836	1.739835	-0.775978
C	-4.167993	1.494067	-0.936426
C	-2.259017	2.866461	-1.409222
C	-4.965080	2.335782	-1.713066
H	-4.633315	0.638500	-0.458760
C	-3.052794	3.714358	-2.172503
H	-1.200289	3.081795	-1.319593
C	-4.411356	3.450279	-2.332650
H	-6.023805	2.118025	-1.825273
H	-2.604192	4.580698	-2.650196
H	-5.030861	4.107338	-2.936332
C	-1.336068	1.775409	1.627550
C	-0.410447	2.807672	1.435353
C	-1.929864	1.654835	2.888327
C	-0.088787	3.691225	2.460209
H	0.088147	2.908384	0.476980
C	-1.600327	2.528211	3.923940
H	-2.659114	0.875638	3.083416
C	-0.679858	3.550331	3.713651
H	0.638934	4.476762	2.279104
H	-2.070772	2.408364	4.896021
H	-0.423387	4.231601	4.519912
C	2.575901	2.094449	0.103880
C	3.088596	2.676028	1.266617
C	2.595729	2.835591	-1.083323
C	3.603882	3.969997	1.245509
H	3.077504	2.128748	2.203952
C	3.111216	4.128477	-1.105299
H	2.195393	2.407411	-1.996352
C	3.615682	4.700420	0.060088
H	3.996259	4.407705	2.159321
H	3.115146	4.688453	-2.036142
H	4.017139	5.709664	0.044493
C	3.442033	-0.518230	-0.429476
C	3.703068	-0.690448	-1.794478
C	4.383913	-0.989390	0.491031
C	4.867357	-1.318974	-2.224363
H	2.973890	-0.344783	-2.520494

C	5.542272	-1.636289	0.063196
H	4.228484	-0.858942	1.557063
C	5.787150	-1.802739	-1.296127
H	5.050082	-1.441506	-3.288197
H	6.254594	-2.004652	0.796260
H	6.690276	-2.304550	-1.631778
N	-0.966576	-1.378123	-4.033767
H	-1.743150	-1.604879	-4.647008
H	-0.582203	-0.471441	-4.277015
N	-3.025966	-1.518029	-2.228344
H	-3.405291	-0.577667	-2.311850
H	-3.502675	-2.127095	-2.890441

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.145342	-0.395004	-0.960431
N	0.542898	-1.865834	0.383707
C	1.718585	0.346823	1.945465
H	2.676246	0.432854	2.470990
H	1.000490	1.035467	2.406073
C	-1.065022	-3.556510	-1.448196
C	0.295386	0.635839	-2.367732
O	0.451385	1.237772	-3.366747
P	-0.804019	-1.960501	-2.272823
P	1.823039	0.745673	0.174053
Si	-0.106887	-3.458635	0.195339
Si	0.998359	-1.414507	1.992391
C	1.205921	-4.812906	0.152046
H	1.790234	-4.865152	1.077432
H	0.755691	-5.800530	-0.013928
H	1.908373	-4.618518	-0.668744
C	2.292923	-2.545316	2.777288
H	2.633111	-2.137533	3.738357
H	1.899194	-3.550039	2.974169
H	3.169532	-2.649610	2.126185
H	-2.133741	-3.673391	-1.241412
H	-0.747792	-4.401677	-2.070685
P	-1.787867	0.360297	-0.037735
C	-2.719614	-1.005405	0.791484
H	-3.676301	-0.616676	1.161152

H	-2.992601	-1.679505	-0.032110
Si	-2.002891	-2.100718	2.199117
C	-3.462302	-2.354587	3.375804
H	-3.782365	-1.413979	3.842928
H	-4.331213	-2.777498	2.855340
H	-3.193225	-3.046413	4.183681
C	-1.395752	-3.765795	1.555581
H	-2.212819	-4.400904	1.189594
H	-0.951976	-4.290701	2.414946
C	-0.531093	-1.382404	3.119345
H	-0.725793	-0.369730	3.488959
H	-0.363037	-2.014068	4.004030
C	-3.132797	1.154405	-1.042768
C	-4.386492	1.431156	-0.483676
C	-2.898066	1.545124	-2.362224
C	-5.383700	2.047665	-1.230967
H	-4.587262	1.186107	0.555615
C	-3.894091	2.165816	-3.115769
H	-1.924282	1.378535	-2.807203
C	-5.142420	2.411296	-2.554709
H	-6.349064	2.250356	-0.776062
H	-3.687304	2.459462	-4.141110
H	-5.920799	2.893788	-3.138908
C	-1.664999	1.667198	1.258053
C	-0.958611	2.828914	0.927744
C	-2.265482	1.584964	2.517085
C	-0.836426	3.873089	1.838870
H	-0.493798	2.913438	-0.051026
C	-2.135357	2.624236	3.436488
H	-2.840694	0.708066	2.796967
C	-1.417755	3.768883	3.100895
H	-0.277061	4.761959	1.563102
H	-2.600410	2.537429	4.414401
H	-1.316466	4.577908	3.818660
C	2.269652	2.525633	0.075986
C	2.539102	3.287736	1.215935
C	2.352907	3.138762	-1.180014
C	2.881989	4.633970	1.105462
H	2.473728	2.835819	2.200669
C	2.690800	4.483712	-1.290480
H	2.148332	2.565977	-2.079024
C	2.955616	5.235689	-0.147178
H	3.088171	5.211052	2.002623
H	2.747312	4.945439	-2.271937

H	3.217402	6.286317	-0.234512
C	3.417679	-0.035317	-0.323441
C	4.634307	0.392555	0.219467
C	3.419973	-1.093887	-1.236214
C	5.826176	-0.231681	-0.132710
H	4.652277	1.223151	0.921077
C	4.613547	-1.719443	-1.590417
H	2.486905	-1.451826	-1.663567
C	5.817102	-1.291795	-1.037849
H	6.762859	0.110424	0.298222
H	4.598178	-2.543119	-2.298512
H	6.747637	-1.781375	-1.311140
N	-2.308524	-1.696748	-3.024530
H	-2.448850	-0.758317	-3.380710
H	-2.618956	-2.396275	-3.692441
N	0.401902	-2.406460	-3.403931
H	0.182608	-3.176712	-4.029972
H	0.781408	-1.622272	-3.924329

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.166618	-0.547136	-0.765251
N	0.693965	-1.899835	1.109240
C	2.299702	0.348910	1.641067
H	3.103183	-0.277662	1.237393
H	2.768791	1.091955	2.292969
C	-1.168365	-3.624688	-0.358911
C	0.050428	0.270401	-2.298758
O	0.029110	0.788044	-3.354004
P	-0.183288	-2.624379	-1.550819
P	1.447396	1.075730	0.170556
Si	-0.323259	-3.346276	1.312072
Si	1.125502	-0.854123	2.469855
C	0.761903	-4.823819	1.730528
H	1.284261	-4.671469	2.682753
H	0.168368	-5.742479	1.820303
H	1.525769	-4.992302	0.962230
C	2.027883	-1.813795	3.815087
H	2.414266	-1.138978	4.589641
H	1.370964	-2.538468	4.311974

H	2.880576	-2.361740	3.396891
H	-2.199009	-3.250659	-0.367401
H	-1.197987	-4.691319	-0.624560
P	-2.005136	0.003540	-0.217011
C	-2.880803	-0.675613	1.284305
H	-3.697371	0.001413	1.561335
H	-3.368612	-1.599006	0.944819
Si	-1.970709	-1.154858	2.868515
C	-3.184247	-0.933317	4.294921
H	-3.433439	0.124650	4.445868
H	-4.121478	-1.473473	4.112578
H	-2.762509	-1.309824	5.235360
C	-1.508434	-2.977473	2.718526
H	-2.428740	-3.564480	2.592370
H	-1.052004	-3.318419	3.659225
C	-0.437623	-0.101830	3.172728
H	-0.610446	0.886515	2.730950
H	-0.305888	0.052304	4.252329
H	1.678806	-0.912654	-1.116313
H	1.573619	-2.155217	0.653906
C	5.444769	-0.995443	-0.037557
H	6.456185	-1.299916	-0.333428
H	5.278246	0.003836	-0.458949
H	5.376470	-0.957852	1.051735
C	4.438183	-1.953427	-0.611334
C	4.411962	-2.121255	-2.109371
H	4.414706	-3.186336	-2.362049
H	3.468578	-1.702320	-2.479309
H	5.246704	-1.619263	-2.604438
O	3.656942	-2.568907	0.100992
C	0.925118	2.735828	0.808115
C	0.911852	3.096962	2.158035
C	0.564744	3.701228	-0.140447
C	0.570237	4.391567	2.550038
H	1.178753	2.377355	2.925364
C	0.240515	4.995068	0.246038
H	0.551150	3.439695	-1.195822
C	0.245449	5.347119	1.595052
H	0.571071	4.650288	3.605624
H	-0.028136	5.729488	-0.507351
H	-0.009383	6.359395	1.896144
C	2.927861	1.663761	-0.789462
C	3.195847	1.210882	-2.081645
C	3.844655	2.536968	-0.187561

C	4.351137	1.609076	-2.754507
H	2.505334	0.528491	-2.559739
C	5.004217	2.925761	-0.849663
H	3.650125	2.922555	0.809873
C	5.262514	2.460532	-2.138992
H	4.535288	1.245651	-3.761809
H	5.704998	3.597154	-0.361242
H	6.166069	2.765904	-2.659225
C	-2.366937	1.813999	-0.037628
C	-2.472364	2.585377	-1.202003
C	-2.575274	2.441429	1.192149
C	-2.825862	3.928083	-1.140882
H	-2.302693	2.125073	-2.171091
C	-2.914767	3.791772	1.257444
H	-2.488822	1.881952	2.118977
C	-3.057961	4.535199	0.091206
H	-2.922651	4.499148	-2.060178
H	-3.068872	4.259931	2.225505
H	-3.333459	5.584792	0.142906
C	-3.366089	-0.318662	-1.459150
C	-4.718592	-0.182355	-1.110258
C	-3.064593	-0.621254	-2.785649
C	-5.726149	-0.361942	-2.050483
H	-4.997858	0.083243	-0.095602
C	-4.070167	-0.799097	-3.735197
H	-2.033060	-0.721429	-3.084862
C	-5.404862	-0.673729	-3.371135
H	-6.765556	-0.248825	-1.754303
H	-3.801804	-1.036454	-4.760917
H	-6.190940	-0.810755	-4.108627
N	-0.966624	-2.969069	-3.030739
H	-0.590458	-2.392476	-3.778998
H	-0.890570	-3.944493	-3.309104
N	1.259273	-3.555875	-1.643524
H	1.168586	-4.550252	-1.456004
H	2.059330	-3.166596	-1.152117

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.215445	-0.435411	-0.686818

N	1.134631	-1.456774	0.859769
C	1.916726	1.107799	1.871519
H	2.986227	0.956547	1.677853
H	1.833613	1.901372	2.620232
C	0.144633	-3.842016	-0.566215
C	0.048949	0.399728	-2.225802
O	-0.001394	0.945454	-3.261114
P	0.164413	-2.443026	-1.742269
P	1.114854	1.534196	0.264690
Si	0.879151	-3.166571	1.054000
Si	1.189377	-0.564042	2.346840
C	2.477762	-4.104175	1.400073
H	2.964538	-3.759444	2.319923
H	2.297620	-5.182073	1.503892
H	3.184173	-3.953229	0.574780
C	2.257479	-1.286672	3.732931
H	2.298394	-0.565302	4.560314
H	1.845104	-2.216961	4.141300
H	3.290313	-1.487787	3.429620
H	-0.892614	-4.159239	-0.412536
H	0.697714	-4.710352	-0.947300
P	-2.022528	-0.446697	-0.213906
C	-2.478156	-1.757507	0.994500
H	-3.547147	-1.685487	1.228225
H	-2.354697	-2.701561	0.450380
Si	-1.528574	-1.965634	2.636299
C	-2.830174	-2.314921	3.958515
H	-3.513359	-1.465698	4.089493
H	-3.436109	-3.194671	3.707503
H	-2.357791	-2.506077	4.930216
C	-0.378496	-3.449573	2.449266
H	-0.968614	-4.356619	2.256736
H	0.143332	-3.622531	3.401248
C	-0.545607	-0.420024	3.076957
H	-1.074147	0.451502	2.670271
H	-0.504210	-0.290912	4.167059
H	4.531063	0.237287	-0.107178
H	2.823313	-1.379999	-0.023307
C	5.278535	-1.453155	0.988151
H	5.503224	-2.514575	0.833248
H	6.194010	-0.944257	1.311627
H	4.545220	-1.377202	1.797101
C	4.731211	-0.829383	-0.290610
C	5.711567	-0.942630	-1.445924

H	5.944815	-1.995959	-1.642696
H	5.279697	-0.511970	-2.354569
H	6.644079	-0.413856	-1.221708
O	3.536677	-1.473338	-0.699867
C	0.179596	3.074223	0.625572
C	-0.393330	3.308813	1.878360
C	0.031574	4.041640	-0.375298
C	-1.070798	4.497624	2.135073
H	-0.311416	2.567991	2.667916
C	-0.639239	5.232195	-0.115783
H	0.465320	3.876045	-1.357751
C	-1.186710	5.466802	1.143367
H	-1.511488	4.662088	3.113914
H	-0.728628	5.980085	-0.898641
H	-1.707622	6.397856	1.347609
C	2.539545	2.237413	-0.675602
C	3.007236	1.651444	-1.852649
C	3.223552	3.346138	-0.156208
C	4.122868	2.174829	-2.508191
H	2.521123	0.770564	-2.256278
C	4.338925	3.861654	-0.802920
H	2.874967	3.813290	0.761156
C	4.789737	3.277196	-1.986747
H	4.470642	1.710954	-3.426513
H	4.854808	4.721875	-0.385982
H	5.659463	3.681760	-2.496482
C	-2.872017	1.053657	0.452035
C	-2.858160	2.214656	-0.330814
C	-3.578567	1.076147	1.657066
C	-3.570867	3.342739	0.053187
H	-2.282142	2.240722	-1.250897
C	-4.269795	2.218260	2.059908
H	-3.609299	0.201036	2.297809
C	-4.280964	3.349004	1.252011
H	-3.554148	4.227425	-0.575428
H	-4.808852	2.213272	3.003159
H	-4.829491	4.235628	1.556797
C	-3.206850	-0.811565	-1.605122
C	-4.205084	-1.786104	-1.511699
C	-3.108933	-0.088101	-2.800658
C	-5.068193	-2.036109	-2.575793
H	-4.322855	-2.373745	-0.609009
C	-3.970562	-0.334892	-3.865665
H	-2.344177	0.668828	-2.920655

C	-4.953916	-1.314710	-3.758918
H	-5.831412	-2.802935	-2.476190
H	-3.865638	0.237956	-4.782800
H	-5.625118	-1.512975	-4.589634
N	-1.067728	-2.861111	-2.832876
H	-1.373847	-2.081119	-3.406046
H	-0.872860	-3.669598	-3.416818
N	1.640243	-2.603447	-2.590619
H	1.946984	-3.564695	-2.722281
H	2.398216	-2.077777	-2.149194

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.095096	-0.775051	-0.707260
N	-0.415096	-2.015643	1.195866
C	2.236109	-0.992225	1.678609
H	2.624219	-1.941616	1.303974
H	2.991297	-0.589606	2.360645
C	-3.101850	-2.194302	-0.014568
C	0.190837	-0.278124	-2.350737
O	0.358455	-0.064121	-3.494897
P	-1.874101	-2.108656	-1.376375
P	1.927413	0.061118	0.196287
Si	-2.092385	-2.533143	1.548403
Si	0.593814	-1.362256	2.500769
C	-2.078616	-4.368761	1.937406
H	-1.517258	-4.573253	2.857048
H	-3.095462	-4.758029	2.072587
H	-1.600846	-4.934483	1.129541
C	0.833874	-2.639775	3.861446
H	1.570890	-2.299152	4.599679
H	-0.098357	-2.843527	4.402658
H	1.194220	-3.588096	3.444286
H	-3.646069	-1.247325	0.046852
H	-3.845089	-2.982605	-0.198508
P	-1.544474	1.035263	-0.216033
C	-2.580161	1.046135	1.331299
H	-2.875377	2.080361	1.543841
H	-3.512620	0.530482	1.073949
Si	-2.066115	0.246478	2.969951

C	-2.865509	1.268506	4.335162
H	-2.449102	2.283065	4.372596
H	-3.948309	1.359597	4.184376
H	-2.706004	0.808832	5.318395
C	-2.733147	-1.513495	2.987327
H	-3.831318	-1.499464	2.954826
H	-2.454725	-1.994009	3.935837
C	-0.205664	0.183554	3.200875
H	0.224001	1.078735	2.737939
H	0.029297	0.243115	4.272649
H	1.101436	-2.034504	-0.939536
H	0.073460	-2.833570	0.787685
C	3.048214	-3.570461	-0.538958
H	3.537232	-4.464840	-0.949988
H	3.602025	-2.700931	-0.890991
H	3.101561	-3.651085	0.549093
C	1.604986	-3.622499	-1.018192
C	1.502168	-3.674398	-2.538748
H	1.818160	-4.677936	-2.859105
H	0.484646	-3.505760	-2.888046
H	2.172130	-2.941261	-2.995679
O	0.793007	-4.255296	-0.284539
C	2.397597	1.748605	0.815422
C	2.587599	2.070764	2.161861
C	2.684713	2.726648	-0.144703
C	3.053334	3.330099	2.539459
H	2.390954	1.341108	2.939932
C	3.160234	3.976955	0.227907
H	2.551331	2.502548	-1.199555
C	3.348894	4.284316	1.574073
H	3.197806	3.553677	3.592949
H	3.379573	4.716611	-0.536241
H	3.722782	5.261838	1.865119
C	3.479568	-0.192569	-0.782763
C	3.455485	-0.429512	-2.156903
C	4.719534	-0.151835	-0.132681
C	4.639018	-0.638534	-2.864697
H	2.512035	-0.472628	-2.682539
C	5.899809	-0.372023	-0.832795
H	4.767173	0.056148	0.932773
C	5.862440	-0.619426	-2.204662
H	4.595871	-0.825339	-3.934033
H	6.851208	-0.346015	-0.309020
H	6.784394	-0.791814	-2.752687

C	-0.772282	2.721021	-0.115266
C	-0.390694	3.362081	-1.299750
C	-0.615968	3.413505	1.087766
C	0.067416	4.674268	-1.288029
H	-0.476561	2.845168	-2.250135
C	-0.138257	4.722142	1.104796
H	-0.873652	2.944968	2.032024
C	0.183837	5.365007	-0.084720
H	0.332399	5.157829	-2.224096
H	-0.022378	5.236968	2.054051
H	0.541545	6.390578	-0.073228
C	-2.864817	1.514189	-1.451973
C	-4.101080	2.046225	-1.067701
C	-2.596147	1.430443	-2.822389
C	-5.035908	2.460815	-2.013965
H	-4.355882	2.160130	-0.020704
C	-3.519600	1.856039	-3.771187
H	-1.653560	1.025740	-3.166402
C	-4.750245	2.367656	-3.371367
H	-5.987736	2.866056	-1.681586
H	-3.276842	1.775638	-4.827211
H	-5.477181	2.694229	-4.109503
N	-2.835127	-1.635924	-2.699265
H	-2.274166	-1.326924	-3.486595
H	-3.480428	-2.355404	-3.014679
N	-1.576329	-3.765157	-1.643555
H	-2.369263	-4.372136	-1.452594
H	-0.733201	-4.110600	-1.162817

$R^1=R^2=R^3=Et$

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.120743	-1.115109	0.354906
N	-0.075589	0.108802	-1.633360
C	-2.965839	0.306593	-0.915473
H	-3.786990	0.088397	-1.606881
H	-3.368921	1.014062	-0.179763
C	2.847119	-0.136409	-0.940291
C	-0.227659	-2.225696	1.688047
O	-0.313060	-3.002955	2.567519

P	2.066085	-1.521101	0.003792
P	-2.360623	-1.185268	0.008938
Si	1.564678	0.625507	-2.101330
Si	-1.512372	1.152063	-1.780178
C	1.896878	0.039862	-3.857417
H	1.146213	0.419853	-4.561072
H	2.881786	0.372893	-4.207810
H	1.882839	-1.056261	-3.916335
C	-1.909630	1.399915	-3.605955
H	-2.836766	1.972360	-3.736175
H	-1.109803	1.946906	-4.121306
H	-2.038266	0.439562	-4.121237
H	3.151208	0.636125	-0.226639
H	3.750802	-0.430471	-1.487666
P	0.110989	0.730723	1.700548
C	1.077627	2.223117	1.143523
H	1.070686	2.977191	1.940602
H	2.123315	1.899977	1.061694
Si	0.618439	3.111688	-0.467761
C	0.930179	4.952532	-0.203979
H	0.274344	5.364758	0.573240
H	1.966347	5.139342	0.105008
H	0.751841	5.521690	-1.124522
C	1.648635	2.488894	-1.919731
H	2.700583	2.786491	-1.813411
H	1.271749	2.981869	-2.827669
C	-1.167596	2.824507	-0.985151
H	-1.849775	2.987801	-0.142511
H	-1.414007	3.597946	-1.727272
C	2.382319	-2.945319	-1.149343
C	3.826356	-3.285444	-1.513169
H	1.798800	-2.736249	-2.054091
H	1.888870	-3.806428	-0.683213
H	3.852384	-4.142017	-2.197287
H	4.332726	-2.454655	-2.017611
H	4.419413	-3.555336	-0.632355
C	3.252115	-1.948555	1.386463
C	4.617352	-1.263355	1.378187
H	3.379439	-3.037958	1.357734
H	2.737473	-1.741341	2.328706
H	5.241270	-1.641420	2.196609
H	5.156804	-1.432945	0.440330
H	4.523794	-0.179801	1.513138
C	1.047763	0.336156	3.263668

C	1.094197	1.342125	4.411451
H	2.070488	0.125427	2.929849
H	0.645818	-0.617030	3.625394
H	1.755590	0.972441	5.204259
H	1.480882	2.316915	4.094066
H	0.106665	1.493595	4.859353
C	-1.434172	1.541342	2.389045
C	-1.415452	3.003189	2.839248
H	-1.749850	0.896322	3.220110
H	-2.204815	1.427741	1.621505
H	-2.390988	3.277918	3.258449
H	-0.661513	3.204640	3.604088
H	-1.222259	3.681884	2.001418
C	-3.508138	-1.319524	1.461198
C	-5.013825	-1.396438	1.218677
H	-3.275379	-0.463032	2.101894
H	-3.167185	-2.202351	2.016595
H	-5.555229	-1.333526	2.170241
H	-5.365941	-0.575102	0.583379
H	-5.299989	-2.339970	0.743788
C	-2.926532	-2.607250	-1.065147
C	-4.158965	-2.450291	-1.956583
H	-3.050531	-3.450895	-0.372891
H	-2.062022	-2.869199	-1.681300
H	-4.429719	-3.418870	-2.393360
H	-5.035299	-2.072420	-1.422931
H	-3.960276	-1.768495	-2.791360
H	-0.201968	-2.363928	-0.655649
H	-0.266049	-0.809273	-2.041430

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.049932	-0.804035	0.613885
N	-0.025058	-0.274419	-1.375992
C	-2.969873	-0.236243	-1.080261
H	-3.639413	-0.801044	-1.737251
H	-3.558283	0.581371	-0.645386
C	2.895337	-0.155666	-0.905561
C	-0.093866	-1.663941	2.141641
O	-0.123070	-2.248624	3.160737

P	2.167428	-1.231213	0.375603
P	-2.263272	-1.225383	0.289869
Si	1.462528	0.202009	-2.114118
Si	-1.452548	0.491689	-1.972949
C	1.850656	-0.723645	-3.716504
H	1.045548	-0.621492	-4.453804
H	2.774956	-0.354148	-4.179940
H	1.982214	-1.796697	-3.524829
C	-1.712194	0.285575	-3.837149
H	-2.686030	0.690291	-4.143103
H	-0.946334	0.812591	-4.420458
H	-1.682063	-0.771249	-4.130661
H	3.192352	0.785455	-0.427476
H	3.786058	-0.569642	-1.392574
P	-0.000192	1.224292	1.573811
C	0.832136	2.559205	0.602380
H	0.766404	3.499588	1.165056
H	1.899659	2.300021	0.588243
Si	0.323738	2.936683	-1.202111
C	0.470398	4.813895	-1.379027
H	-0.232434	5.338220	-0.718705
H	1.480884	5.163187	-1.130766
H	0.255383	5.130228	-2.407273
C	1.474623	2.075523	-2.421853
H	2.497975	2.471016	-2.366691
H	1.107186	2.302034	-3.434406
C	-1.416821	2.366755	-1.627748
H	-2.124709	2.641491	-0.835685
H	-1.741524	2.906857	-2.529609
C	2.205842	-2.917726	-0.398692
C	3.560163	-3.508725	-0.786122
H	1.551747	-2.852236	-1.276991
H	1.695241	-3.583333	0.309239
H	3.422864	-4.469422	-1.295931
H	4.115275	-2.852981	-1.465557
H	4.184213	-3.692353	0.094873
C	3.386230	-1.375875	1.769482
C	4.847231	-1.068215	1.441679
H	3.284409	-2.393954	2.167077
H	3.039021	-0.712442	2.568583
H	5.474379	-1.213175	2.328745
H	5.238383	-1.712242	0.648371
H	4.971966	-0.030540	1.114175
C	0.918642	1.319045	3.186099

C	0.866116	2.594864	4.023883
H	1.960527	1.096807	2.923592
H	0.572142	0.467257	3.782992
H	1.551824	2.512126	4.875514
H	1.163869	3.479776	3.450690
H	-0.135478	2.769373	4.430080
C	-1.660582	1.963776	1.984991
C	-1.811361	3.483460	2.068889
H	-1.964497	1.491054	2.928693
H	-2.353348	1.584656	1.226688
H	-2.833374	3.741749	2.370720
H	-1.127997	3.939724	2.789570
H	-1.631803	3.956132	1.097370
C	-3.556453	-1.266911	1.607750
C	-4.909992	-1.862350	1.225476
H	-3.680550	-0.230896	1.945411
H	-3.120261	-1.810648	2.454805
H	-5.627235	-1.749513	2.046610
H	-5.332980	-1.366781	0.344226
H	-4.828963	-2.932334	1.006934
C	-2.200928	-2.984248	-0.324581
C	-3.135045	-3.393825	-1.461999
H	-2.362081	-3.614813	0.559290
H	-1.164045	-3.160728	-0.635377
H	-3.038603	-4.468094	-1.657327
H	-4.186265	-3.188612	-1.236746
H	-2.881015	-2.869986	-2.389458

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.170278	0.201927	-0.963459
N	0.584120	0.042270	1.318293
C	-0.435035	2.808316	1.191473
H	0.153402	3.617235	1.641056
H	-1.473366	3.157442	1.182037
C	1.589854	-2.549222	0.431513
C	0.212830	0.494323	-2.676270
O	0.309246	0.717396	-3.828491
P	1.004566	-1.893127	-1.208735
P	0.136806	2.418668	-0.535290

Si	0.791390	-1.629318	1.868807
Si	-0.338402	1.239515	2.242065
C	1.985334	-1.687902	3.327723
H	1.509284	-1.380529	4.266371
H	2.384066	-2.699892	3.477619
H	2.826880	-1.009577	3.144527
C	0.547107	1.643665	3.855682
H	0.086003	2.505258	4.355779
H	0.522839	0.803838	4.560541
H	1.600405	1.887108	3.670163
H	1.457870	-3.635429	0.515358
H	2.669298	-2.362691	0.499380
P	-2.090288	-0.170931	-0.938175
C	-2.853439	-1.367585	0.250205
H	-3.945815	-1.369471	0.158938
H	-2.523322	-2.366548	-0.048526
Si	-2.387641	-1.229460	2.072866
C	-3.842347	-1.903829	3.068960
H	-4.751489	-1.313038	2.899274
H	-4.066324	-2.941975	2.792493
H	-3.634197	-1.887347	4.146151
C	-0.878550	-2.311769	2.403954
H	-1.053030	-3.295672	1.947282
H	-0.823120	-2.491703	3.487541
C	-2.044750	0.540872	2.624729
H	-2.819865	1.200605	2.213344
H	-2.175579	0.574312	3.716296
C	2.585652	-1.867221	-2.200032
C	3.394630	-3.154174	-2.350641
H	3.186828	-1.093594	-1.714794
H	2.326944	-1.457175	-3.183995
H	4.383096	-2.932327	-2.771009
H	3.551179	-3.655376	-1.387134
H	2.915988	-3.870566	-3.025777
C	0.276190	-3.437507	-1.973767
C	-0.985448	-4.020588	-1.345232
H	1.056660	-4.206016	-1.954394
H	0.092458	-3.208356	-3.032087
H	-1.175526	-5.025843	-1.739224
H	-0.895827	-4.109062	-0.255696
H	-1.867571	-3.416774	-1.567721
C	-2.647168	-0.841016	-2.584849
C	-4.074809	-1.352052	-2.759278
H	-1.929535	-1.631005	-2.831584

H	-2.444731	-0.037955	-3.304026
H	-4.194165	-1.810948	-3.748271
H	-4.334695	-2.111249	-2.013224
H	-4.809856	-0.543847	-2.688243
C	-3.254942	1.293225	-0.752591
C	-4.670457	1.093483	-0.209254
H	-3.306145	1.756410	-1.745993
H	-2.742650	2.020700	-0.117057
H	-5.212629	2.046878	-0.224100
H	-5.252581	0.375650	-0.794308
H	-4.661853	0.741901	0.828428
C	-0.793189	3.565303	-1.679414
C	-1.539138	4.750658	-1.070892
H	-1.487698	2.942707	-2.250544
H	-0.050431	3.918404	-2.406486
H	-1.931078	5.401622	-1.861374
H	-2.394455	4.419487	-0.471077
H	-0.897444	5.358745	-0.424939
C	1.815681	3.205138	-0.526673
C	1.923749	4.713469	-0.315506
H	2.267123	2.922197	-1.484888
H	2.384242	2.664455	0.239503
H	2.977389	5.017419	-0.289122
H	1.443630	5.273824	-1.125322
H	1.470273	5.035090	0.628861
H	1.760545	0.440750	-0.945386
H	1.523320	0.412220	1.142613
C	4.417102	0.369026	0.648673
O	3.620213	0.765114	1.482964
C	4.796918	1.210463	-0.542633
H	5.748644	0.901615	-0.984212
H	4.004443	1.089217	-1.293046
H	4.833369	2.267817	-0.268199
C	5.062434	-0.990699	0.753132
H	4.955285	-1.536512	-0.191632
H	6.139061	-0.864480	0.924504
H	4.632598	-1.567816	1.574561

A4

Coordinates (Angstroms)		
X	Y	Z

Mn	0.050642	0.096190	-0.895576
N	0.658014	-0.137420	1.064275
C	0.349113	2.822216	1.112592
H	1.191008	3.438429	1.448794
H	-0.560133	3.413457	1.264959
C	0.712463	-3.016848	0.417311
C	0.098130	0.317348	-2.634673
O	0.161999	0.472141	-3.797087
P	0.369039	-2.183489	-1.188083
P	0.526078	2.320884	-0.646667
Si	0.577475	-1.713439	1.794705
Si	0.207039	1.193445	2.091769
C	1.967655	-2.051917	3.034545
H	1.761494	-1.599179	4.011394
H	2.090959	-3.130936	3.197054
H	2.924010	-1.645417	2.688692
C	1.293320	1.349419	3.631199
H	1.136212	2.319250	4.121732
H	1.072096	0.573326	4.373949
H	2.355116	1.269123	3.369482
H	-0.008460	-3.824508	0.590699
H	1.701708	-3.488398	0.415534
P	-2.202353	0.194020	-0.803860
C	-2.928743	-0.879979	0.501237
H	-4.023715	-0.815050	0.480429
H	-2.676701	-1.913124	0.235851
Si	-2.353764	-0.660395	2.308328
C	-3.898796	-0.926680	3.364089
H	-4.663051	-0.163625	3.167950
H	-4.353335	-1.906404	3.168650
H	-3.659493	-0.883888	4.434081
C	-1.069258	-1.970620	2.713368
H	-1.473792	-2.974012	2.521939
H	-0.876430	-1.923370	3.795579
C	-1.594369	1.018551	2.689888
H	-2.222256	1.828319	2.297916
H	-1.605305	1.138403	3.783868
C	1.971651	-2.273990	-2.128350
C	2.712013	-3.606349	-2.216356
H	2.622270	-1.512012	-1.686918
H	1.736012	-1.907264	-3.134873
H	3.649494	-3.474957	-2.768660
H	2.971201	-4.003779	-1.229555
H	2.129369	-4.369430	-2.742821

C	-0.625475	-3.413613	-2.163516
C	-1.964198	-3.855437	-1.574543
H	0.003286	-4.299867	-2.306704
H	-0.778013	-2.970102	-3.155948
H	-2.395884	-4.653162	-2.189308
H	-1.853411	-4.254056	-0.559713
H	-2.694106	-3.043028	-1.539833
C	-3.037543	-0.334168	-2.375027
C	-4.548450	-0.549099	-2.398215
H	-2.518238	-1.244476	-2.692160
H	-2.753292	0.426899	-3.112675
H	-4.856834	-0.958913	-3.367106
H	-4.876022	-1.253430	-1.625652
H	-5.093371	0.389200	-2.255085
C	-3.028100	1.840022	-0.482161
C	-4.375984	1.861837	0.240077
H	-3.127082	2.324825	-1.461208
H	-2.315727	2.448443	0.083707
H	-4.754948	2.889272	0.293243
H	-5.134325	1.255781	-0.263409
H	-4.289927	1.494401	1.267630
C	-0.300715	3.583007	-1.738025
C	-0.686793	4.912444	-1.093937
H	-1.183471	3.106724	-2.173746
H	0.386807	3.750939	-2.576380
H	-1.058980	5.611390	-1.851782
H	-1.482851	4.781024	-0.352529
H	0.161312	5.385151	-0.588226
C	2.321095	2.638942	-0.964604
C	2.783534	4.095066	-0.931025
H	2.554307	2.187872	-1.937450
H	2.854262	2.059160	-0.203024
H	3.867707	4.151346	-1.082230
H	2.312716	4.695369	-1.717229
H	2.564593	4.568494	0.032567
H	3.771496	0.038331	-0.845257
H	2.581577	0.140336	1.058384
C	4.297351	-0.118741	0.112377
O	3.523152	0.410836	1.171339
C	5.599612	0.667004	0.068833
H	6.123923	0.575242	1.027019
H	6.258225	0.296423	-0.724434
H	5.402569	1.729029	-0.111743
C	4.540697	-1.615180	0.295375

H	5.089736	-2.035332	-0.555996
H	5.119755	-1.797048	1.208054
H	3.591333	-2.152965	0.387117

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.568762	0.002942	-0.812861
N	0.478907	-0.139232	1.442754
C	0.446992	2.816558	1.167184
H	1.247241	3.351962	1.692579
H	-0.376083	3.531801	1.060155
C	0.216398	-3.051285	0.696783
C	0.999387	0.149051	-2.499191
O	1.348984	0.257363	-3.614581
P	0.374037	-2.289321	-0.992147
P	1.065816	2.230875	-0.484914
Si	0.013885	-1.742082	2.060113
Si	-0.118307	1.347459	2.215509
C	1.124370	-2.162432	3.526933
H	0.735452	-1.718899	4.451432
H	1.202332	-3.244628	3.689191
H	2.134760	-1.764847	3.378561
C	0.641935	1.492164	3.931548
H	0.441145	2.474785	4.377518
H	0.249820	0.733203	4.619922
H	1.729417	1.362175	3.877094
H	-0.655843	-3.717626	0.716688
H	1.074528	-3.697167	0.912690
P	-1.702343	0.394486	-1.126283
C	-2.849487	-0.572102	-0.049909
H	-3.886096	-0.457967	-0.389996
H	-2.596617	-1.625487	-0.186897
Si	-2.801259	-0.307317	1.826749
C	-4.577635	-0.397675	2.456279
H	-5.193748	0.420117	2.062314
H	-5.053088	-1.341189	2.159787
H	-4.612021	-0.340032	3.551322
C	-1.786207	-1.683178	2.610287
H	-2.261993	-2.656515	2.429894
H	-1.811242	-1.528704	3.698968

C	-1.997538	1.304404	2.366463
H	-2.444164	2.164508	1.854732
H	-2.238335	1.432840	3.432127
C	1.904345	-3.007830	-1.787855
C	2.345647	-4.415590	-1.396171
H	2.707016	-2.288108	-1.628004
H	1.690996	-2.973298	-2.864299
H	3.200754	-4.724637	-2.008843
H	2.662589	-4.469289	-0.349472
H	1.556158	-5.161874	-1.539719
C	-0.782895	-3.366127	-2.018176
C	-2.259289	-3.550689	-1.677190
H	-0.315956	-4.357799	-2.015832
H	-0.688853	-2.994914	-3.046788
H	-2.663882	-4.386619	-2.259637
H	-2.418047	-3.794284	-0.619741
H	-2.862456	-2.672590	-1.917986
C	-2.185302	-0.078518	-2.859194
C	-3.652481	-0.069182	-3.279954
H	-1.749367	-1.065439	-3.034115
H	-1.608990	0.601998	-3.498679
H	-3.756673	-0.489580	-4.287241
H	-4.280772	-0.668853	-2.611464
H	-4.062541	0.945213	-3.309500
C	-2.492900	2.094008	-1.027906
C	-3.973724	2.215538	-0.662532
H	-2.329727	2.559273	-2.006808
H	-1.908428	2.685982	-0.319044
H	-4.286865	3.263898	-0.735682
H	-4.622206	1.631353	-1.320672
H	-4.171913	1.891700	0.363790
C	0.447304	3.427685	-1.782226
C	-0.103339	4.779999	-1.332630
H	-0.296714	2.903589	-2.386628
H	1.304713	3.579220	-2.450075
H	-0.286580	5.421457	-2.202784
H	-1.057415	4.673783	-0.805145
H	0.585384	5.309011	-0.667208
C	2.834719	2.754178	-0.403161
C	3.146991	4.242514	-0.261510
H	3.294739	2.362012	-1.317767
H	3.252460	2.187380	0.434617
H	4.225650	4.385513	-0.126214
H	2.852606	4.814295	-1.148283

H	2.651319	4.689549	0.607993
H	2.242051	-0.425880	-0.438109
H	1.512723	-0.065624	1.528164
C	3.591608	-0.498787	0.579539
O	3.305938	0.246155	1.552112
C	4.637307	-0.084612	-0.451380
H	5.610442	-0.453755	-0.095000
H	4.441883	-0.534183	-1.428959
H	4.708881	0.995260	-0.558184
C	3.645572	-2.001168	0.849704
H	3.956894	-2.581298	-0.020614
H	4.399170	-2.144088	1.635130
H	2.700972	-2.388757	1.225281

R^1=R^3=Ph, R^2=H

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.122848	-0.470557	-0.195287
N	0.203461	1.322617	1.303833
C	2.572409	1.775430	-0.421745
H	3.598953	2.100146	-0.216871
H	2.319897	2.090069	-1.440045
C	-2.249592	-0.007228	2.075555
C	0.192381	-1.898703	-1.202538
O	0.216149	-2.843070	-1.894599
P	-1.942714	-0.929350	0.507732
P	2.342667	-0.050714	-0.315853
Si	-1.401514	1.669618	1.991199
Si	1.323973	2.590669	0.742519
C	-1.207641	2.351255	3.735341
H	-0.743982	3.345325	3.727651
H	-2.181382	2.449091	4.231934
H	-0.582098	1.698618	4.357008
C	2.238860	3.316058	2.214857
H	2.963960	4.074093	1.893538
H	1.556889	3.787962	2.932184
H	2.795051	2.533672	2.747016
H	-3.301288	0.031032	2.381123
H	-1.723108	-0.585876	2.846130
P	-0.381306	0.771625	-2.000189

C	-1.594330	2.174810	-2.007819
H	-1.574711	2.666701	-2.987991
H	-2.594312	1.734277	-1.901659
Si	-1.433980	3.483590	-0.653554
C	-2.288952	5.037193	-1.293194
H	-1.800451	5.422907	-2.196441
H	-3.337161	4.832273	-1.544378
H	-2.277793	5.836097	-0.541721
C	-2.295828	2.928129	0.925253
H	-3.299550	2.567584	0.671444
H	-2.441278	3.828402	1.540084
C	0.345286	3.902794	-0.183796
H	0.912775	4.208689	-1.073347
H	0.283477	4.797606	0.454205
H	0.382513	-1.330484	1.137839
H	0.688525	0.704484	1.956903
C	-3.391758	-0.534527	-0.568581
C	-3.354117	-1.061749	-1.867479
C	-4.473464	0.275104	-0.213983
C	-4.355707	-0.773839	-2.786933
H	-2.523606	-1.699074	-2.161903
C	-5.474892	0.576191	-1.138199
H	-4.549400	0.685275	0.788191
C	-5.417069	0.056236	-2.426991
H	-4.305001	-1.194247	-3.787145
H	-6.302684	1.215919	-0.844701
H	-6.194956	0.292120	-3.147266
C	-2.390846	-2.655818	0.995992
C	-3.724209	-3.003705	1.246274
C	-1.400348	-3.626000	1.166462
C	-4.058170	-4.288553	1.660870
H	-4.512308	-2.267796	1.109592
C	-1.734757	-4.915307	1.576947
H	-0.364572	-3.362881	0.981073
C	-3.062291	-5.249594	1.826061
H	-5.097900	-4.540758	1.850294
H	-0.952922	-5.660046	1.697497
H	-3.322468	-6.255707	2.143305
C	3.330494	-0.737771	-1.703502
C	3.905504	0.044730	-2.707199
C	3.473769	-2.129880	-1.767711
C	4.605483	-0.550501	-3.756216
H	3.819177	1.126709	-2.677626
C	4.176947	-2.722785	-2.809372

H	3.027947	-2.753280	-0.996968
C	4.743008	-1.933473	-3.809604
H	5.045759	0.072192	-4.530135
H	4.278407	-3.803613	-2.844739
H	5.286720	-2.396940	-4.627831
C	3.476424	-0.410224	1.108541
C	2.988159	-0.950604	2.298645
C	4.839081	-0.091356	1.024854
C	3.835020	-1.151847	3.389403
H	1.938946	-1.229793	2.354669
C	5.685901	-0.296343	2.107409
H	5.245029	0.311373	0.099705
C	5.182874	-0.823410	3.297362
H	3.437035	-1.574515	4.307811
H	6.740399	-0.049068	2.023127
H	5.844470	-0.983631	4.144029
H	-0.878751	0.060188	-3.117510
H	0.646950	1.429086	-2.733364

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.097141	-0.031743	0.339016
N	0.006633	1.005154	-1.407742
C	-2.932873	1.010459	-1.303866
H	-3.411031	0.507868	-2.151507
H	-3.670700	1.684137	-0.854769
C	2.915413	0.960143	-0.842315
C	-0.199515	-1.316071	1.547835
O	-0.267734	-2.185296	2.326865
P	2.145013	-0.344228	0.178960
P	-2.341475	-0.189454	-0.041726
Si	1.521956	1.627018	-1.961889
Si	-1.372206	1.977168	-1.787285
C	1.943197	1.144552	-3.735602
H	1.180442	1.482868	-4.446890
H	2.904855	1.569037	-4.051538
H	2.015474	0.052548	-3.821304
C	-1.526193	2.442279	-3.614542
H	-2.482149	2.949963	-3.798931
H	-0.731275	3.119741	-3.949452

H	-1.497590	1.551496	-4.254459
H	3.244207	1.781074	-0.196965
H	3.793494	0.603227	-1.391137
P	0.024531	1.629613	1.820146
C	0.922693	3.169438	1.326843
H	0.826154	3.899489	2.140646
H	1.989143	2.916740	1.275563
Si	0.424034	4.030912	-0.309159
C	0.609851	5.881525	0.018345
H	-0.088485	6.226761	0.791108
H	1.625931	6.127076	0.353142
H	0.412647	6.464200	-0.890099
C	1.550282	3.514052	-1.733418
H	2.577660	3.873462	-1.583676
H	1.179293	4.018751	-2.638253
C	-1.344009	3.588570	-0.778593
H	-1.948176	3.476784	0.133177
H	-1.797173	4.408080	-1.354016
C	3.159719	-0.524193	1.699357
C	3.170381	-1.755781	2.366055
C	3.820269	0.559832	2.284557
C	3.829517	-1.899137	3.582135
H	2.660678	-2.611064	1.931830
C	4.477959	0.417269	3.504703
H	3.834071	1.528259	1.792803
C	4.484488	-0.811892	4.156850
H	3.828655	-2.863108	4.082489
H	4.986854	1.270839	3.943539
H	4.996900	-0.923451	5.107958
C	2.552020	-1.878959	-0.747955
C	3.877184	-2.217587	-1.048896
C	1.523953	-2.721150	-1.175919
C	4.165443	-3.371722	-1.767634
H	4.688845	-1.578378	-0.709577
C	1.811033	-3.877374	-1.899771
H	0.489641	-2.483088	-0.943015
C	3.130269	-4.203299	-2.196140
H	5.197564	-3.625188	-1.992137
H	0.998564	-4.520926	-2.224472
H	3.355772	-5.106370	-2.756397
C	-3.647681	-0.245909	1.237936
C	-5.003113	-0.293664	0.886648
C	-3.296530	-0.246477	2.589625
C	-5.984837	-0.344189	1.869361

H	-5.289194	-0.300844	-0.162221
C	-4.280621	-0.296664	3.575594
H	-2.248889	-0.217484	2.872612
C	-5.623888	-0.344324	3.216893
H	-7.032836	-0.384933	1.586671
H	-3.994876	-0.298158	4.623428
H	-6.391336	-0.382512	3.984550
C	-2.488096	-1.815263	-0.888957
C	-3.042787	-2.936512	-0.264947
C	-1.903835	-1.961884	-2.154066
C	-3.029007	-4.175337	-0.901222
H	-3.489906	-2.846645	0.720750
C	-1.896420	-3.199747	-2.790128
H	-1.422124	-1.110533	-2.628803
C	-2.460031	-4.310520	-2.165107
H	-3.466781	-5.037560	-0.406362
H	-1.438316	-3.297186	-3.770309
H	-2.452283	-5.277837	-2.659202
H	0.605102	1.406762	3.092196
H	-1.174268	2.212863	2.300881

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.052956	-0.077206	0.563043
N	-0.073058	-0.565295	-1.691218
C	2.678079	0.126028	-1.415865
H	2.470782	1.066722	-1.939583
H	3.748067	-0.073398	-1.531863
C	-2.860999	-1.213439	-0.968377
C	-0.091382	0.578854	2.176027
O	-0.127723	1.068510	3.243972
P	-2.295218	-0.066771	0.365249
P	2.132312	0.373591	0.328682
Si	-1.537580	-1.352431	-2.308731
Si	1.528171	-1.133070	-2.206976
C	-2.080575	-0.471451	-3.875956
H	-1.343585	-0.606820	-4.676459
H	-3.046664	-0.841190	-4.241610
H	-2.171054	0.607078	-3.701002
C	1.709530	-1.056177	-4.078548

H	2.740836	-1.274397	-4.384338
H	1.059229	-1.778166	-4.587955
H	1.456037	-0.053004	-4.439219
H	-2.949362	-2.190710	-0.479814
H	-3.858326	-0.980400	-1.358408
P	0.195954	-2.199829	1.277536
C	-0.437475	-3.702643	0.387654
H	-0.141625	-4.602047	0.941996
H	-1.534073	-3.673954	0.409391
Si	0.157262	-3.864487	-1.407297
C	0.423278	-5.694418	-1.769288
H	1.192531	-6.120508	-1.113250
H	-0.499778	-6.266808	-1.614488
H	0.743286	-5.855399	-2.806117
C	-1.130363	-3.164092	-2.597867
H	-2.053730	-3.756671	-2.536741
H	-0.748048	-3.295837	-3.620759
C	1.772068	-2.909674	-1.640520
H	2.346606	-2.954883	-0.706316
H	2.378548	-3.422149	-2.400595
H	-0.158871	1.405531	-0.010545
H	-0.125608	0.433900	-1.917244
C	1.921734	3.878527	-2.481504
H	1.826423	4.844083	-2.992960
H	2.235194	4.089898	-1.452615
H	2.680147	3.275403	-2.985140
C	0.589450	3.171612	-2.477520
C	-0.532753	3.845438	-1.738263
H	-1.488343	3.381727	-1.986991
H	-0.358680	3.715052	-0.663974
H	-0.559866	4.920779	-1.945847
O	0.437712	2.095886	-3.035717
C	3.338073	-0.607043	1.323519
C	4.238740	-1.532275	0.791836
C	3.262393	-0.475734	2.717416
C	5.044811	-2.306829	1.627930
H	4.320996	-1.669635	-0.282060
C	4.069528	-1.239934	3.551068
H	2.558502	0.228585	3.153837
C	4.963902	-2.162500	3.008145
H	5.737383	-3.022957	1.194102
H	3.996559	-1.118437	4.628090
H	5.591190	-2.764862	3.658906
C	2.762323	2.075180	0.678752

C	1.909689	3.073610	1.152402
C	4.104156	2.393465	0.435700
C	2.385154	4.366415	1.372479
H	0.866757	2.838448	1.331495
C	4.578401	3.683932	0.644013
H	4.786930	1.624437	0.082212
C	3.716899	4.675749	1.113140
H	1.708207	5.131321	1.742857
H	5.620935	3.915970	0.445346
H	4.086643	5.683809	1.279091
C	-3.455336	-0.530337	1.728624
C	-2.961879	-1.012242	2.941537
C	-4.842952	-0.440999	1.555343
C	-3.831786	-1.411178	3.956368
H	-1.891222	-1.065105	3.101046
C	-5.712343	-0.838303	2.564029
H	-5.248004	-0.047476	0.626251
C	-5.206938	-1.328461	3.768519
H	-3.428942	-1.782616	4.894382
H	-6.785582	-0.761022	2.414133
H	-5.886303	-1.638007	4.557692
C	-3.030723	1.560818	-0.096030
C	-3.733973	1.811578	-1.274647
C	-2.842593	2.613737	0.809463
C	-4.243232	3.084522	-1.543750
H	-3.891778	1.022634	-2.003528
C	-3.359138	3.876234	0.550405
H	-2.280494	2.438474	1.723298
C	-4.061442	4.117287	-0.631744
H	-4.782419	3.261700	-2.470332
H	-3.211025	4.676649	1.269949
H	-4.462418	5.105708	-0.837176
H	1.509764	-2.680569	1.518208
H	-0.279971	-2.515381	2.574166

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.066969	-0.071321	0.436275
N	-0.112529	-0.438645	-1.594143
C	2.762926	-0.088532	-1.441333

H	2.757025	0.886876	-1.940912
H	3.772759	-0.495133	-1.553132
C	-2.983870	-0.893333	-1.119525
C	-0.036871	0.630575	2.050410
O	-0.002885	1.080594	3.132209
P	-2.360649	0.029892	0.328211
P	2.243476	0.194425	0.290572
Si	-1.549791	-1.042607	-2.361927
Si	1.366735	-1.102040	-2.220797
C	-2.009450	-0.108759	-3.934608
H	-1.270758	-0.279942	-4.726643
H	-2.985421	-0.434862	-4.317809
H	-2.046082	0.973756	-3.767357
C	1.546296	-0.932063	-4.092688
H	2.571823	-1.167280	-4.406477
H	0.876792	-1.596252	-4.652761
H	1.329813	0.100784	-4.390621
H	-3.230145	-1.899162	-0.760980
H	-3.904196	-0.480931	-1.546224
P	-0.002969	-2.175265	1.230543
C	-0.787660	-3.520722	0.241892
H	-0.636817	-4.469113	0.772655
H	-1.870031	-3.341773	0.239879
Si	-0.177935	-3.728638	-1.559704
C	-0.106267	-5.585796	-1.883932
H	0.611565	-6.081474	-1.218403
H	-1.084724	-6.058952	-1.731977
H	0.201730	-5.791816	-2.916590
C	-1.370330	-2.891453	-2.752056
H	-2.353195	-3.381905	-2.737738
H	-0.975097	-3.024430	-3.770016
C	1.521579	-2.942114	-1.778610
H	2.103370	-3.089141	-0.859031
H	2.067215	-3.464145	-2.577660
H	1.171567	2.358297	-1.185678
H	-0.033157	1.284408	-2.480827
C	2.041185	3.591785	-2.701451
H	1.729862	4.237450	-3.531740
H	2.614713	4.195301	-1.988540
H	2.701310	2.818164	-3.109058
C	0.825394	2.968619	-2.029469
C	-0.122547	4.024769	-1.473327
H	-0.555163	4.616493	-2.288460
H	-0.940201	3.550307	-0.924881

H	0.401945	4.705048	-0.791271
O	0.158340	2.125015	-2.951304
C	3.246332	-0.943173	1.325306
C	4.027486	-1.979203	0.810341
C	3.143972	-0.803310	2.716313
C	4.688675	-2.861497	1.665552
H	4.125087	-2.118373	-0.261463
C	3.806697	-1.678857	3.567629
H	2.537519	-0.005665	3.137371
C	4.579422	-2.714965	3.043668
H	5.290156	-3.663615	1.247449
H	3.717109	-1.553459	4.642694
H	5.094231	-3.402137	3.708693
C	3.003306	1.813751	0.728541
C	2.210967	2.895235	1.119238
C	4.386783	1.993690	0.612457
C	2.788065	4.136481	1.383125
H	1.134938	2.776902	1.203403
C	4.963481	3.231067	0.873749
H	5.017663	1.159338	0.315307
C	4.163266	4.306639	1.258769
H	2.158106	4.968789	1.683301
H	6.037564	3.358929	0.775656
H	4.614229	5.273902	1.460476
C	-3.487797	-0.469136	1.693368
C	-2.990014	-0.729907	2.971650
C	-4.863832	-0.599172	1.464791
C	-3.846435	-1.119449	4.000702
H	-1.930979	-0.619978	3.172638
C	-5.718141	-0.990455	2.488876
H	-5.271990	-0.391417	0.479199
C	-5.209355	-1.253889	3.760577
H	-3.442213	-1.316581	4.989330
H	-6.782576	-1.089343	2.296762
H	-5.877201	-1.560810	4.560317
C	-2.878345	1.771872	0.049701
C	-3.397337	2.235428	-1.161326
C	-2.707230	2.681207	1.102894
C	-3.751892	3.574798	-1.313399
H	-3.521522	1.562626	-2.003214
C	-3.065982	4.015599	0.951944
H	-2.297020	2.341139	2.050148
C	-3.591283	4.466634	-0.258522
H	-4.147372	3.919649	-2.264224

H	-2.931337	4.706437	1.779124
H	-3.864627	5.510605	-0.379655
H	1.252937	-2.775373	1.475397
H	-0.552069	-2.447445	2.505035

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.052375	0.277751	0.246641
N	-0.013240	-0.705231	-1.807540
C	2.839041	-0.115487	-1.639413
H	2.782396	0.730498	-2.332387
H	3.872908	-0.474025	-1.679478
C	-2.821851	-1.192258	-0.985005
C	0.024631	1.290495	1.668933
O	-0.005502	2.000884	2.602130
P	-2.259502	0.053602	0.262074
P	2.316401	0.515911	0.010285
Si	-1.484891	-1.606187	-2.250817
Si	1.573361	-1.401446	-2.188548
C	-2.035535	-1.140625	-3.981141
H	-1.294222	-1.445559	-4.729555
H	-2.985520	-1.626568	-4.237296
H	-2.160334	-0.055531	-4.053987
C	1.760584	-1.690166	-4.039633
H	2.792789	-1.966428	-4.290740
H	1.110074	-2.497032	-4.398900
H	1.512107	-0.785047	-4.607283
H	-3.037031	-2.116495	-0.438325
H	-3.759955	-0.898300	-1.466646
P	0.257942	-1.663480	1.425509
C	-0.460657	-3.281059	0.883055
H	-0.217139	-4.041157	1.635279
H	-1.553664	-3.189945	0.879380
Si	0.143521	-3.884786	-0.816419
C	0.388796	-5.749042	-0.708463
H	1.163218	-6.003458	0.025868
H	-0.535753	-6.255079	-0.403981
H	0.695441	-6.169370	-1.673992
C	-1.116783	-3.449412	-2.140743
H	-2.056876	-3.992051	-1.970055

H	-0.730992	-3.803287	-3.108198
C	1.767938	-3.038757	-1.279783
H	2.375228	-2.913583	-0.374485
H	2.336480	-3.714377	-1.934936
H	0.004617	1.682754	-0.732616
H	-0.172789	0.204832	-2.277573
C	0.922346	2.729614	-2.689064
H	0.775450	3.514966	-3.443956
H	1.678962	3.076695	-1.983777
H	1.275100	1.840652	-3.218352
C	-0.441468	2.461436	-2.054488
C	-0.999166	3.673191	-1.317635
H	-1.418724	4.357059	-2.068073
H	-1.789069	3.396628	-0.623791
H	-0.211863	4.203162	-0.772587
O	-1.207365	1.688151	-2.688407
C	3.395469	-0.365803	1.220120
C	4.275318	-1.400146	0.898906
C	3.259542	0.002934	2.566098
C	4.997534	-2.057623	1.896299
H	4.404052	-1.717884	-0.130880
C	3.981574	-0.646600	3.559399
H	2.571880	0.799046	2.840775
C	4.852090	-1.684730	3.227119
H	5.674884	-2.862593	1.625161
H	3.860627	-0.346782	4.596350
H	5.412128	-2.197667	4.003587
C	3.114289	2.174517	0.113797
C	2.373889	3.301106	0.473990
C	4.480509	2.318854	-0.154289
C	2.984449	4.551183	0.561283
H	1.312025	3.201601	0.666824
C	5.090097	3.565623	-0.073642
H	5.075054	1.447914	-0.420191
C	4.341276	4.686017	0.285888
H	2.393821	5.418879	0.841261
H	6.150905	3.664611	-0.285730
H	4.817865	5.659802	0.353024
C	-3.109753	-0.560169	1.794858
C	-2.562239	-0.333674	3.060987
C	-4.351397	-1.205900	1.717463
C	-3.220237	-0.760705	4.213564
H	-1.618755	0.189269	3.159942
C	-5.008095	-1.637050	2.864904

H	-4.823622	-1.364265	0.752194
C	-4.440285	-1.420768	4.119039
H	-2.771085	-0.576008	5.185192
H	-5.968692	-2.137087	2.779125
H	-4.951029	-1.758893	5.016026
C	-3.333135	1.518751	-0.043236
C	-3.913142	1.787579	-1.283778
C	-3.505501	2.440569	0.996667
C	-4.658004	2.948069	-1.478171
H	-3.754461	1.118501	-2.120620
C	-4.244429	3.602489	0.800837
H	-3.048741	2.259551	1.965853
C	-4.824760	3.859018	-0.439887
H	-5.098036	3.144150	-2.451828
H	-4.362704	4.309696	1.616802
H	-5.398165	4.768198	-0.596913
H	1.557352	-2.133354	1.719617
H	-0.188016	-1.651513	2.765818

R^1=H, R^2=R^3=Ph

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.050768	-0.212472	-1.229941
N	0.706084	-2.152906	-0.078823
C	1.526019	-0.017979	1.761029
H	2.388689	0.084233	2.427432
H	0.711762	0.576131	2.189132
C	-0.489948	-3.261258	-2.490830
C	-0.057650	1.162691	-2.305990
O	-0.063567	2.024537	-3.098137
P	-1.071092	-1.511747	-2.630111
P	1.772917	0.604264	0.047216
Si	-0.093806	-3.621228	-0.683975
Si	0.945459	-1.811492	1.651024
C	1.092345	-5.078590	-0.596207
H	1.333332	-5.345922	0.439523
H	0.660736	-5.966759	-1.074956
H	2.036292	-4.853724	-1.108187
C	2.267976	-2.947801	2.356579
H	2.496801	-2.687124	3.397907

H	1.945722	-3.996297	2.346455
H	3.200551	-2.879525	1.782890
H	-1.190650	-3.979473	-2.931001
H	0.451171	-3.327269	-3.050928
P	-1.824190	0.289835	-0.025674
C	-2.879359	-1.150746	0.441479
H	-3.831772	-0.818485	0.872602
H	-3.139424	-1.643507	-0.502908
Si	-2.158142	-2.546226	1.503491
C	-3.551198	-3.150866	2.619406
H	-3.871330	-2.368729	3.319390
H	-4.429657	-3.451718	2.034926
H	-3.237960	-4.016951	3.215468
C	-1.618071	-3.948456	0.364037
H	-2.457988	-4.234016	-0.284401
H	-1.410139	-4.826437	0.993200
C	-0.679501	-2.060355	2.559881
H	-0.916681	-1.156044	3.134541
H	-0.539247	-2.864698	3.296777
H	1.139910	-0.774372	-2.271740
H	1.597781	-2.070460	-0.572849
C	-3.022809	1.293288	-1.031201
C	-4.191853	0.754922	-1.577567
C	-2.720680	2.631442	-1.315153
C	-5.032295	1.527724	-2.378488
H	-4.467866	-0.276272	-1.386013
C	-3.561755	3.406804	-2.103924
H	-1.811725	3.078743	-0.926663
C	-4.723254	2.856929	-2.642289
H	-5.933155	1.083717	-2.793369
H	-3.303646	4.442647	-2.304844
H	-5.378025	3.460453	-3.264344
C	-1.844391	1.293611	1.536293
C	-1.012756	2.417867	1.592786
C	-2.622780	0.995594	2.659927
C	-0.962737	3.224072	2.725637
H	-0.376821	2.654710	0.745270
C	-2.564549	1.790176	3.803694
H	-3.287501	0.137638	2.660138
C	-1.735978	2.908112	3.839993
H	-0.304645	4.088153	2.737662
H	-3.172532	1.533587	4.666918
H	-1.692677	3.527403	4.731404
C	2.171515	2.391384	0.253778

C	2.402480	2.984168	1.498505
C	2.246005	3.186864	-0.895304
C	2.690848	4.343933	1.593755
H	2.343663	2.392567	2.406937
C	2.537298	4.544403	-0.800761
H	2.067832	2.745470	-1.870449
C	2.756417	5.127953	0.444849
H	2.861444	4.791016	2.569303
H	2.587062	5.146497	-1.703421
H	2.976721	6.188895	0.520597
C	3.479996	-0.024821	-0.345140
C	3.819718	-0.300884	-1.673397
C	4.467905	-0.176083	0.636629
C	5.101460	-0.732016	-2.008787
H	3.060911	-0.190794	-2.441659
C	5.745355	-0.619368	0.306245
H	4.254092	0.057089	1.674985
C	6.065583	-0.901307	-1.019801
H	5.342229	-0.938884	-3.047852
H	6.493103	-0.737301	1.085594
H	7.062805	-1.245429	-1.279480
H	-0.954124	-1.266047	-4.014410
H	-2.478095	-1.745349	-2.651168

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.082599	-0.488186	-1.105942
N	0.086514	-2.146452	0.105694
C	1.760815	-0.415658	1.843483
H	2.737822	-0.585093	2.309163
H	1.208731	0.312018	2.450234
C	-1.981871	-3.113939	-1.774894
C	0.423947	0.671765	-2.385779
O	0.659676	1.386015	-3.284006
P	-1.054242	-1.775481	-2.593853
P	1.878797	0.263200	0.157566
Si	-1.005842	-3.461939	-0.172677
Si	0.687229	-1.979942	1.723541
C	-0.144819	-5.125942	-0.409076
H	0.410860	-5.433587	0.484122

H	-0.866426	-5.920217	-0.639848
H	0.575106	-5.076432	-1.236620
C	1.724167	-3.449099	2.303874
H	2.182408	-3.244720	3.280266
H	1.124369	-4.361052	2.413377
H	2.531298	-3.664427	1.592615
H	-2.972574	-2.722847	-1.516107
H	-2.123073	-3.995516	-2.408154
P	-1.653020	0.588561	-0.149445
C	-2.828951	-0.486129	0.803006
H	-3.551912	0.176207	1.297464
H	-3.411017	-0.995615	0.021438
Si	-2.391844	-1.871095	2.058875
C	-3.826046	-1.818759	3.288058
H	-3.853496	-0.867669	3.835620
H	-4.793458	-1.935536	2.782969
H	-3.741978	-2.623012	4.029436
C	-2.299980	-3.549699	1.209174
H	-3.268364	-3.876643	0.808404
H	-2.011566	-4.284077	1.975627
C	-0.746445	-1.731596	2.950650
H	-0.630562	-0.791139	3.500877
H	-0.736659	-2.532868	3.704654
C	-2.885763	1.518932	-1.173897
C	-3.912386	2.255649	-0.566726
C	-2.822121	1.490992	-2.567283
C	-4.854298	2.930807	-1.333512
H	-3.968215	2.317629	0.517349
C	-3.764678	2.168630	-3.340688
H	-2.020839	0.951786	-3.057399
C	-4.784554	2.885564	-2.726028
H	-5.641934	3.497779	-0.845313
H	-3.692610	2.137322	-4.424168
H	-5.518489	3.416041	-3.326032
C	-1.220914	1.923287	1.041218
C	-0.648107	3.090499	0.519854
C	-1.404643	1.826765	2.421361
C	-0.268039	4.131591	1.356800
H	-0.494894	3.181803	-0.552523
C	-1.006531	2.863593	3.265960
H	-1.868258	0.946170	2.853077
C	-0.438157	4.016769	2.735723
H	0.182150	5.023871	0.932949
H	-1.152601	2.768214	4.338277

H	-0.128530	4.824331	3.392850
C	2.451776	1.994728	0.358315
C	2.842311	2.503819	1.599287
C	2.510412	2.832990	-0.761849
C	3.269913	3.823768	1.723365
H	2.812552	1.874106	2.482494
C	2.939067	4.150337	-0.639117
H	2.217282	2.459198	-1.737013
C	3.317017	4.651084	0.605581
H	3.564394	4.204162	2.697289
H	2.975179	4.787279	-1.518259
H	3.648312	5.681146	0.702129
C	3.380504	-0.562018	-0.532275
C	4.644799	0.035952	-0.515750
C	3.246971	-1.840264	-1.091162
C	5.748136	-0.625608	-1.048938
H	4.773891	1.025690	-0.088667
C	4.352414	-2.502050	-1.619230
H	2.273595	-2.324605	-1.093844
C	5.605173	-1.894889	-1.603455
H	6.722136	-0.144870	-1.031096
H	4.230801	-3.492961	-2.047855
H	6.466712	-2.406604	-2.022845
H	-1.888335	-1.328920	-3.643508
H	-0.151135	-2.508414	-3.399336

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.187409	-0.488891	-0.928541
N	0.715098	-2.101953	0.688083
C	2.381520	0.020279	1.548384
H	3.197741	-0.534633	1.071564
H	2.832056	0.667245	2.307072
C	-1.234021	-3.584595	-0.913276
C	0.068101	0.586583	-2.296162
O	0.045252	1.291731	-3.235389
P	-0.345695	-2.389148	-2.011461
P	1.527885	0.943236	0.194403
Si	-0.310145	-3.553317	0.739115
Si	1.197230	-1.283801	2.185155

C	0.782588	-5.076412	0.852830
H	1.368845	-5.076960	1.779174
H	0.190578	-5.999900	0.827798
H	1.493587	-5.107889	0.018557
C	2.084140	-2.459507	3.356548
H	2.492946	-1.920300	4.220837
H	1.414788	-3.236421	3.747166
H	2.917664	-2.953943	2.844768
H	-2.257331	-3.207471	-0.797387
H	-1.296427	-4.591614	-1.340960
P	-1.959966	-0.016407	-0.279986
C	-2.824393	-0.887894	1.127544
H	-3.631503	-0.249143	1.505409
H	-3.325641	-1.756016	0.679437
Si	-1.891867	-1.584804	2.617300
C	-3.080424	-1.535902	4.079628
H	-3.330471	-0.502325	4.351042
H	-4.019581	-2.055481	3.852538
H	-2.643075	-2.013715	4.965062
C	-1.447853	-3.376631	2.220562
H	-2.372123	-3.946510	2.052023
H	-0.962162	-3.830231	3.096507
C	-0.335508	-0.606674	3.023972
H	-0.498242	0.439091	2.737122
H	-0.174477	-0.613512	4.110905
H	1.668797	-0.862702	-1.398755
H	1.585337	-2.343094	0.201769
C	5.287788	-1.408795	-0.675923
H	6.219106	-1.791118	-1.110668
H	5.071827	-0.452588	-1.167287
H	5.425439	-1.249855	0.395461
C	4.163176	-2.378859	-0.933000
C	3.846205	-2.679151	-2.374406
H	4.757920	-2.880891	-2.947316
H	3.160540	-3.526199	-2.444916
H	3.362761	-1.796295	-2.810046
O	3.532357	-2.884739	-0.018056
C	0.999802	2.506809	1.031577
C	0.992681	2.705572	2.414162
C	0.608700	3.568446	0.205263
C	0.623776	3.936571	2.957569
H	1.284515	1.907056	3.089054
C	0.254256	4.798290	0.743324
H	0.592376	3.430891	-0.873215

C	0.263480	4.988523	2.124418
H	0.629933	4.071184	4.035920
H	-0.040696	5.608082	0.082724
H	-0.015894	5.949895	2.546046
C	2.999344	1.649424	-0.693744
C	3.251007	1.390223	-2.042071
C	3.919197	2.430806	0.017895
C	4.391101	1.899885	-2.664772
H	2.559770	0.775286	-2.604891
C	5.063871	2.927167	-0.595074
H	3.736102	2.660426	1.064463
C	5.302987	2.663488	-1.943113
H	4.563898	1.694466	-3.717663
H	5.766083	3.526218	-0.022007
H	6.192641	3.057242	-2.426624
C	-2.362243	1.748903	0.112504
C	-2.513716	2.654422	-0.944800
C	-2.536801	2.217904	1.416656
C	-2.875866	3.975345	-0.706752
H	-2.366510	2.320403	-1.967859
C	-2.888223	3.544023	1.658189
H	-2.410822	1.550050	2.263699
C	-3.073849	4.423467	0.597179
H	-3.004491	4.656333	-1.543569
H	-3.017297	3.886887	2.680842
H	-3.356071	5.455525	0.785048
C	-3.297850	-0.243939	-1.572970
C	-4.655839	-0.240260	-1.220306
C	-2.981557	-0.369055	-2.927883
C	-5.651727	-0.385677	-2.179365
H	-4.949553	-0.110779	-0.183578
C	-3.976342	-0.512433	-3.895120
H	-1.947625	-0.337702	-3.244091
C	-5.315403	-0.528755	-3.524322
H	-6.695192	-0.380488	-1.876121
H	-3.696537	-0.607956	-4.940612
H	-6.092446	-0.641544	-4.275064
H	-1.080703	-2.509850	-3.214000
H	0.728809	-3.216975	-2.418054

A4

Coordinates (Angstroms)

	X	Y	Z
Mn	0.133006	-0.672082	-0.784800
N	0.364871	-2.051098	0.767912
C	2.382538	-0.222984	1.706333
H	3.171491	-0.864063	1.296543
H	2.838870	0.382081	2.495722
C	-1.774600	-3.476382	-0.619156
C	0.302710	0.226461	-2.288389
O	0.411505	0.796952	-3.305855
P	-0.795804	-2.498881	-1.814741
P	1.728578	0.753076	0.299993
Si	-0.757675	-3.360811	0.988775
Si	0.980196	-1.366691	2.233288
C	0.072904	-5.037167	1.224559
H	0.779284	-5.029823	2.062628
H	-0.672443	-5.818385	1.423226
H	0.635989	-5.326720	0.329094
C	1.700265	-2.624191	3.445562
H	2.199500	-2.111982	4.278614
H	0.938077	-3.282060	3.880706
H	2.447258	-3.258923	2.953222
H	-2.751621	-2.991177	-0.511406
H	-1.944488	-4.506368	-0.949257
P	-1.903758	0.271865	-0.315467
C	-2.842084	-0.406094	1.135886
H	-3.571877	0.349966	1.449056
H	-3.440902	-1.232120	0.731779
Si	-2.061261	-1.135934	2.714296
C	-3.303235	-0.769860	4.088157
H	-3.409923	0.308563	4.261985
H	-4.296964	-1.167740	3.846664
H	-2.986753	-1.227129	5.033868
C	-1.898748	-2.994405	2.455089
H	-2.887026	-3.450145	2.302082
H	-1.486078	-3.452881	3.365689
C	-0.382344	-0.397021	3.120340
H	-0.382240	0.650888	2.795103
H	-0.218071	-0.393366	4.206745
H	2.614009	-1.524000	-1.057508
H	1.749920	-3.072953	-0.031493
C	4.554239	-2.367933	-0.693224
H	5.110580	-3.289355	-0.904290
H	5.093370	-1.524432	-1.139037

H	4.538347	-2.233364	0.393623
C	3.135973	-2.477871	-1.246015
C	3.141774	-2.713235	-2.752314
H	3.551187	-3.704954	-2.977337
H	2.128663	-2.656399	-3.164045
H	3.759070	-1.964584	-3.262331
O	2.432666	-3.511993	-0.588695
C	1.357778	2.413646	0.994799
C	1.338205	2.701384	2.360979
C	1.159539	3.457049	0.082149
C	1.141386	4.008420	2.806404
H	1.484756	1.916195	3.095354
C	0.979510	4.759935	0.526048
H	1.162268	3.249344	-0.984882
C	0.973803	5.040688	1.891465
H	1.132328	4.215151	3.872931
H	0.835145	5.557032	-0.196719
H	0.831318	6.060369	2.237707
C	3.283214	1.184790	-0.609825
C	3.485055	0.858930	-1.951081
C	4.320897	1.816737	0.089568
C	4.694211	1.152133	-2.581836
H	2.706187	0.362366	-2.515407
C	5.528137	2.104593	-0.534536
H	4.181779	2.088942	1.132729
C	5.718764	1.771834	-1.875621
H	4.830085	0.890962	-3.627370
H	6.322274	2.591402	0.024309
H	6.662231	1.995887	-2.364817
C	-2.025048	2.092500	-0.034041
C	-2.025926	2.946379	-1.143286
C	-2.150016	2.650806	1.240112
C	-2.200926	4.316445	-0.984861
H	-1.915185	2.537007	-2.143571
C	-2.316531	4.024249	1.400220
H	-2.130645	2.019254	2.123397
C	-2.359154	4.858839	0.288179
H	-2.218623	4.960525	-1.859519
H	-2.414539	4.440250	2.398576
H	-2.501566	5.928189	0.413984
C	-3.228922	0.139430	-1.620425
C	-4.586153	0.260146	-1.288227
C	-2.899375	-0.024820	-2.968860
C	-5.574299	0.189260	-2.263819

H	-4.884588	0.418528	-0.257284
C	-3.886741	-0.092367	-3.950690
H	-1.862232	-0.092979	-3.268653
C	-5.228383	0.007488	-3.601237
H	-6.618385	0.283633	-1.978968
H	-3.599740	-0.222655	-4.990250
H	-5.999732	-0.047773	-4.363851
H	-1.552076	-2.513711	-3.005845
H	0.185712	-3.436085	-2.196728

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.065188	-0.708498	-0.847960
N	-0.142570	-2.262836	0.839958
C	2.271082	-0.925500	1.682982
H	2.865496	-1.741648	1.262600
H	2.882341	-0.462939	2.464337
C	-2.623920	-2.848904	-0.626237
C	0.403210	0.177936	-2.314160
O	0.650857	0.718524	-3.325188
P	-1.413793	-2.160157	-1.837919
P	1.875741	0.205042	0.280700
Si	-1.692629	-3.134691	0.996777
Si	0.655156	-1.650348	2.299267
C	-1.363308	-4.965002	1.227587
H	-0.831397	-5.160093	2.166432
H	-2.299731	-5.536398	1.249212
H	-0.743758	-5.341219	0.406311
C	0.991640	-3.033786	3.529448
H	1.624016	-2.680771	4.354054
H	0.066911	-3.423034	3.973030
H	1.510859	-3.871902	3.048880
H	-3.418177	-2.105643	-0.490183
H	-3.094317	-3.765108	-0.999124
P	-1.684557	0.717049	-0.272689
C	-2.808887	0.349191	1.166371
H	-3.282694	1.282865	1.490985
H	-3.624695	-0.258352	0.755165
Si	-2.264650	-0.579797	2.724585
C	-3.310541	0.093942	4.139032

H	-3.104519	1.156829	4.318453
H	-4.382275	-0.005270	3.926271
H	-3.108741	-0.444191	5.073519
C	-2.623705	-2.407892	2.458072
H	-3.702492	-2.556904	2.312533
H	-2.355428	-2.965206	3.367092
C	-0.438233	-0.349779	3.094797
H	-0.149620	0.652219	2.755852
H	-0.276912	-0.373590	4.181396
H	1.316057	-1.827190	-1.267466
H	0.467761	-2.937185	0.340242
C	3.191257	-3.252757	-0.880154
H	3.780214	-4.090436	-1.279295
H	3.738839	-2.329937	-1.076619
H	3.091722	-3.416218	0.195926
C	1.818512	-3.317749	-1.544389
C	1.884138	-3.161276	-3.061708
H	2.289417	-4.093091	-3.480051
H	0.897433	-2.997421	-3.498256
H	2.543627	-2.338959	-3.353280
O	0.978579	-4.103642	-1.029022
C	1.965502	1.885695	1.048483
C	2.036908	2.130358	2.421493
C	2.059437	2.974284	0.172063
C	2.213989	3.425912	2.908143
H	1.971321	1.315998	3.135307
C	2.251814	4.261721	0.654119
H	1.999674	2.808222	-0.900567
C	2.334289	4.492508	2.026485
H	2.273663	3.592698	3.980120
H	2.329513	5.088785	-0.044944
H	2.485186	5.500081	2.403293
C	3.511422	0.300111	-0.585597
C	3.638760	0.068212	-1.954789
C	4.663310	0.606316	0.151027
C	4.885141	0.136083	-2.576800
H	2.765727	-0.184815	-2.540831
C	5.908324	0.664840	-0.463679
H	4.586525	0.811127	1.215827
C	6.022695	0.430405	-1.833548
H	4.961827	-0.048042	-3.644683
H	6.790797	0.899563	0.124949
H	6.994417	0.480194	-2.316418
C	-1.306116	2.506415	0.011478

C	-1.043591	3.314551	-1.101307
C	-1.312731	3.097588	1.276644
C	-0.847972	4.683165	-0.957834
H	-1.013917	2.876300	-2.094605
C	-1.105955	4.467672	1.423212
H	-1.489127	2.499779	2.166174
C	-0.890119	5.267122	0.305870
H	-0.664347	5.293349	-1.837671
H	-1.114899	4.908353	2.415735
H	-0.740175	6.336728	0.420835
C	-3.003072	1.000986	-1.574080
C	-4.274677	1.481624	-1.228074
C	-2.731010	0.812990	-2.932450
C	-5.241202	1.731178	-2.196613
H	-4.523908	1.678721	-0.191090
C	-3.694686	1.065788	-3.907393
H	-1.753924	0.473120	-3.247353
C	-4.957339	1.518508	-3.543359
H	-6.217887	2.100108	-1.895865
H	-3.450346	0.905789	-4.953687
H	-5.711879	1.711404	-4.300480
H	-2.249461	-1.844141	-2.930022
H	-0.873234	-3.355320	-2.340069

$R^1=R^2=R^3=F$

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-1.270147	-0.236376	-0.279062
N	0.636017	0.596834	-1.188253
C	-0.436828	2.941892	0.191237
H	-0.535859	3.949833	-0.226467
H	-0.480007	3.011942	1.283641
C	0.639682	-2.091751	-2.201857
C	-2.930991	-0.742202	0.085965
O	-4.029414	-1.051055	0.267324
P	-0.667780	-2.154665	-0.957526
P	-1.780533	1.848718	-0.328586
Si	1.789648	-0.704777	-1.630923
Si	1.174475	2.077358	-0.320891
C	2.878608	-0.145447	-3.050835

H	3.626008	0.587669	-2.726340
H	3.419871	-0.998601	-3.478192
H	2.289423	0.308988	-3.856452
C	2.122469	3.183191	-1.499234
H	2.383392	4.131949	-1.014214
H	3.055224	2.718625	-1.839154
H	1.523791	3.421233	-2.387128
H	1.140092	-3.057392	-2.329372
H	0.188626	-1.801219	-3.158245
P	-0.671572	-0.371673	1.757804
C	0.915612	-1.037545	2.304640
H	0.990727	-0.939950	3.394776
H	0.907197	-2.109170	2.070899
Si	2.448552	-0.277495	1.486773
C	3.888853	-0.526859	2.667444
H	3.719682	-0.007900	3.618640
H	4.036743	-1.590643	2.889936
H	4.824424	-0.143727	2.241743
C	2.807314	-1.175659	-0.132706
H	2.720294	-2.255880	0.043920
H	3.862517	-0.992536	-0.381142
C	2.223461	1.566630	1.147375
H	1.835680	2.046622	2.055306
H	3.228031	1.985948	0.990140
H	-1.696836	-0.361449	-1.813896
H	0.182371	0.877926	-2.061035
F	-1.651728	-1.231841	2.711688
F	-0.678015	0.957487	2.703201
F	-0.020718	-3.288996	0.015253
F	-1.761963	-3.135616	-1.601272
F	-3.067166	2.454480	0.413598
F	-2.077385	2.506410	-1.775644

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-1.214317	-0.119696	-0.195799
N	0.519760	0.116793	-1.087512
C	-0.076725	2.989987	-0.886889
H	-0.182519	3.557566	-1.817534
H	0.099382	3.696050	-0.068283

C	0.700049	-2.812303	-0.737992
C	-2.951591	-0.334522	0.163046
O	-4.076974	-0.472281	0.390758
P	-0.974442	-2.260898	-0.459474
P	-1.542082	2.015279	-0.554776
Si	1.617271	-1.230284	-1.307741
Si	1.306248	1.676991	-0.953524
C	2.143269	-1.489551	-3.090130
H	2.683492	-0.626186	-3.493444
H	2.795626	-2.366468	-3.185919
H	1.262979	-1.654168	-3.723553
C	2.456282	2.084451	-2.383785
H	2.779677	3.131326	-2.318876
H	3.364061	1.468594	-2.380705
H	1.956677	1.948054	-3.349988
H	1.120806	-3.147926	0.217016
H	0.756681	-3.643396	-1.448363
P	-0.591683	-0.042977	1.820327
C	1.050034	-0.663408	2.256082
H	1.186399	-0.494457	3.332493
H	1.031263	-1.752385	2.116112
Si	2.596406	0.041367	1.354265
C	3.955122	0.048461	2.654046
H	3.716389	0.736610	3.474282
H	4.103101	-0.948548	3.087519
H	4.910922	0.367173	2.220634
C	3.075874	-1.031542	-0.121286
H	3.453090	-2.014745	0.189611
H	3.915828	-0.524695	-0.619906
C	2.274486	1.762663	0.672502
H	1.739590	2.367610	1.414983
H	3.241240	2.257190	0.500979
F	-1.475112	-0.710369	2.987596
F	-0.489426	1.426932	2.490114
F	-1.601049	-3.327935	0.560119
F	-1.713029	-2.774872	-1.791550
F	-2.442825	2.928273	0.402885
F	-2.391441	2.209793	-1.906082

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.531427	-1.022023	0.016006
N	0.072317	1.180561	0.166139
C	0.845798	1.036949	-2.552002
H	1.788992	1.522713	-2.274621
H	0.675706	1.163119	-3.625553
C	-0.521358	0.302487	2.898020
C	1.264771	-2.632175	-0.010866
O	1.801839	-3.656895	-0.013232
P	0.618754	-0.891500	2.147093
P	0.901035	-0.697751	-2.063580
Si	-0.778073	1.707252	1.647725
Si	-0.477688	1.778829	-1.426274
C	0.022154	3.272179	2.288257
H	-0.043868	4.082094	1.552433
H	-0.460605	3.614876	3.211412
H	1.084531	3.109506	2.503623
C	-0.438105	3.650571	-1.505417
H	-0.636239	4.000376	-2.526238
H	-1.194935	4.103823	-0.853473
H	0.544926	4.030980	-1.206415
H	-1.468109	-0.222538	3.074644
H	-0.156350	0.659001	3.867866
P	-1.440828	-1.821993	-0.061579
C	-2.979513	-0.995689	0.427898
H	-3.821472	-1.612243	0.088957
H	-3.018681	-0.991589	1.525153
Si	-3.203206	0.795658	-0.168418
C	-5.034713	1.072121	-0.476786
H	-5.393616	0.443217	-1.300539
H	-5.630083	0.830114	0.412105
H	-5.240478	2.116718	-0.740655
C	-2.587703	1.926992	1.212818
H	-3.200099	1.766423	2.110914
H	-2.754764	2.971956	0.914393
C	-2.211139	1.136908	-1.740402
H	-2.187176	0.231096	-2.359418
H	-2.748122	1.895299	-2.327177
H	2.022054	-0.480305	-0.054251
H	1.050459	1.481923	0.254404
C	3.750954	1.603313	-0.042632
C	4.280389	1.087134	1.265515
H	4.305448	-0.007910	1.244617
H	5.310669	1.436369	1.405941

H	3.660577	1.421977	2.097261
C	4.453356	1.136211	-1.290876
H	5.518526	0.955175	-1.120220
H	3.999351	0.182674	-1.589107
H	4.317971	1.855936	-2.101960
O	2.783746	2.350300	-0.102322
F	2.286488	-1.234200	-2.689292
F	-0.024231	-1.321969	-3.231635
F	-1.953446	-2.387118	-1.490029
F	-1.650516	-3.218435	0.730622
F	1.988919	-0.437189	2.872820
F	0.393965	-2.198760	3.059135

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.603527	-0.788410	0.112547
N	-0.036682	1.087482	-0.174446
C	0.428100	0.578004	-2.955965
H	1.306641	1.233844	-3.008003
H	0.051830	0.385332	-3.964742
C	-0.083993	1.208923	2.745009
C	1.697023	-2.183889	0.360701
O	2.437152	-3.056741	0.517975
P	0.547400	-0.404007	2.269267
P	0.905158	-0.908872	-2.089056
Si	-0.723561	2.016098	1.137200
Si	-0.778358	1.394858	-1.731972
C	-0.131187	3.800697	1.168988
H	-0.611593	4.418532	0.403063
H	-0.337008	4.263535	2.142411
H	0.951767	3.846883	0.997971
C	-0.914424	3.213106	-2.191640
H	-1.160292	3.306153	-3.257302
H	-1.702995	3.731569	-1.633365
H	0.030378	3.742554	-2.023427
H	-0.845208	1.116312	3.527267
H	0.734220	1.812778	3.155922
P	-1.184967	-1.956187	0.211680
C	-2.691127	-1.170094	0.810820
H	-3.507850	-1.898117	0.723592

H	-2.555579	-0.978560	1.883120
Si	-3.220134	0.474097	-0.024591
C	-5.099467	0.442315	-0.070413
H	-5.467669	-0.371044	-0.707613
H	-5.522128	0.299989	0.931933
H	-5.500941	1.382292	-0.468468
C	-2.610633	1.906991	1.043565
H	-3.053091	1.837291	2.046628
H	-3.000995	2.839380	0.608794
C	-2.502900	0.625303	-1.765646
H	-2.490446	-0.363128	-2.243117
H	-3.169901	1.252222	-2.373610
H	2.976780	0.153101	0.156489
H	1.705391	1.797577	-0.521112
C	3.454219	1.141904	-0.004742
O	2.627386	1.950029	-0.820403
C	3.664654	1.787841	1.361272
H	2.703152	1.948055	1.861811
H	4.282289	1.157963	2.011161
H	4.152789	2.762266	1.245618
C	4.758920	0.901049	-0.744803
H	5.265711	1.853876	-0.937784
H	5.427890	0.264874	-0.155454
H	4.567280	0.410433	-1.703524
F	0.171199	-2.052554	-2.934164
F	2.398954	-1.222542	-2.584153
F	-1.168373	-3.305126	1.085474
F	-1.763566	-2.628221	-1.131697
F	-0.284684	-1.395172	3.226956
F	1.946649	-0.521054	3.046300

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.876249	-0.603118	-0.074198
N	0.197340	1.259220	0.120885
C	-0.414811	0.938855	2.849921
H	-1.160204	1.729367	2.687566
H	-0.181957	0.858259	3.915514
C	0.047368	1.240648	-2.754306
C	-2.167307	-1.824540	-0.251985

O	-3.044290	-2.565206	-0.367591
P	-0.690993	-0.315136	-2.250086
P	-1.030692	-0.582337	2.143426
Si	1.084106	1.860513	-1.287462
Si	1.011212	1.402804	1.684420
C	1.066837	3.732195	-1.374070
H	1.749152	4.194010	-0.652629
H	1.361011	4.075368	-2.374101
H	0.055421	4.102917	-1.171240
C	1.565783	3.149918	2.076708
H	1.795136	3.243153	3.145693
H	2.470685	3.433149	1.526045
H	0.779543	3.875457	1.840079
H	0.579044	1.148382	-3.706938
H	-0.752144	1.980986	-2.886375
P	0.680024	-2.106083	-0.144615
C	2.364278	-1.771992	-0.686620
H	2.983331	-2.646456	-0.450650
H	2.342029	-1.681066	-1.779024
Si	3.171926	-0.189920	0.007951
C	5.015523	-0.529382	0.120925
H	5.228217	-1.316631	0.854360
H	5.423881	-0.851924	-0.844444
H	5.563550	0.369196	0.430197
C	2.843721	1.194220	-1.233090
H	3.160494	0.852672	-2.228209
H	3.504640	2.038159	-0.986299
C	2.484601	0.234780	1.720276
H	2.238915	-0.699541	2.242335
H	3.286258	0.705456	2.306470
H	-2.226232	0.555838	-0.038505
H	-0.743759	1.953757	0.184669
C	-3.826732	1.413767	1.127816
H	-4.537380	2.248758	1.117899
H	-4.384054	0.479852	0.996561
H	-3.346304	1.400432	2.107737
C	-2.803421	1.628141	0.008184
C	-3.504491	1.687785	-1.352896
H	-4.220443	2.518239	-1.347987
H	-2.784444	1.879121	-2.151291
H	-4.044104	0.760751	-1.575349
F	-0.231199	-1.648245	3.035129
F	-2.461228	-0.839787	2.820975
F	0.232956	-1.345312	-3.081300

F	-1.987421	-0.471846	-3.179592
F	1.013079	-2.946774	1.184941
F	0.316934	-3.383665	-1.053553
O	-1.919225	2.594685	0.230402

$R^1=R^2=R^3=NH_2$

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.309861	0.126224	-0.351777
N	-0.741342	-0.534850	-1.206037
C	0.131534	-3.021547	0.150657
H	0.126044	-4.029561	-0.283605
H	0.110298	-3.107886	1.241582
C	-0.569111	2.217215	-2.127419
C	2.964584	0.459287	0.026545
O	4.101078	0.668406	0.260392
P	0.856091	2.195008	-0.974903
P	1.617391	-2.062538	-0.320789
Si	-1.767912	0.874863	-1.577311
Si	-1.364313	-2.001015	-0.402203
C	-2.940754	0.462261	-2.994228
H	-3.720027	-0.245598	-2.686907
H	-3.444991	1.367463	-3.356211
H	-2.405515	0.020103	-3.843601
C	-2.381636	-3.011032	-1.621864
H	-2.712467	-3.952831	-1.165315
H	-3.276394	-2.475817	-1.960860
H	-1.786921	-3.263790	-2.508747
H	-1.044384	3.203636	-2.205991
H	-0.180047	1.949043	-3.117046
P	0.710455	0.379084	1.780718
C	-0.927554	0.965278	2.380624
H	-1.014533	0.764048	3.458539
H	-0.939523	2.054496	2.253254
Si	-2.477434	0.337498	1.505726
C	-3.920286	0.630326	2.688258
H	-3.799607	0.057554	3.616350
H	-3.998876	1.690438	2.960726
H	-4.875515	0.333266	2.237696
C	-2.762047	1.349673	-0.057919

H	-2.562295	2.402736	0.180003
H	-3.828273	1.280881	-0.316796
C	-2.416822	-1.494032	1.070574
H	-2.083690	-2.053029	1.954656
H	-3.451891	-1.810178	0.873827
H	1.737949	0.078744	-1.913152
H	-0.239863	-0.801039	-2.056917
N	1.646389	1.648157	2.507381
H	1.528859	1.737588	3.514336
H	2.634239	1.556952	2.288364
N	0.840311	-1.017664	2.770423
H	1.626900	-1.607189	2.500631
H	0.821487	-0.868039	3.775807
N	0.314669	3.328474	0.194827
H	0.840848	3.222861	1.062477
H	0.273751	4.301988	-0.095294
N	2.084075	2.967167	-1.892458
H	2.070657	3.982475	-1.874502
H	3.007008	2.623308	-1.650439
N	1.864118	-2.734089	-1.875962
H	2.484345	-2.163356	-2.439991
H	2.108941	-3.719436	-1.927831
N	2.781448	-2.679975	0.787760
H	2.960518	-3.679641	0.729650
H	3.658868	-2.170289	0.731341

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.192339	0.147554	-0.345836
N	-0.585252	-0.423769	-1.112594
C	0.237594	-3.088211	-0.115439
H	0.270551	-4.002216	-0.719888
H	0.167693	-3.364661	0.941248
C	-0.737740	2.347075	-1.989320
C	2.885550	0.548506	-0.154888
O	4.026168	0.808233	-0.021289
P	0.701758	2.300687	-0.882128
P	1.690266	-2.033560	-0.346132
Si	-1.738917	0.801566	-1.520992
Si	-1.224684	-1.939682	-0.566890

C	-2.827266	0.403913	-3.017409
H	-3.612087	-0.327435	-2.794577
H	-3.326304	1.316913	-3.369483
H	-2.229386	0.009658	-3.848057
C	-2.277820	-2.863233	-1.837962
H	-2.469589	-3.889682	-1.497578
H	-3.252972	-2.391892	-2.004675
H	-1.764550	-2.921263	-2.805576
H	-1.301340	3.285802	-1.931572
H	-0.379255	2.214571	-3.017218
P	0.740492	0.354544	1.814809
C	-0.938963	0.861302	2.337197
H	-1.033804	0.677321	3.418034
H	-1.007444	1.944798	2.187548
Si	-2.470801	0.132559	1.471268
C	-3.863984	0.304734	2.741630
H	-3.677842	-0.316890	3.626947
H	-3.972758	1.342769	3.081436
H	-4.827502	-0.006296	2.318456
C	-2.877210	1.174025	-0.045988
H	-2.810595	2.236253	0.226302
H	-3.923316	0.987363	-0.329519
C	-2.279557	-1.679855	0.996813
H	-1.835300	-2.216626	1.845262
H	-3.282073	-2.106820	0.845022
N	1.632472	1.626052	2.578124
H	1.489959	1.710872	3.582082
H	2.626494	1.559722	2.378830
N	0.883202	-1.079773	2.719820
H	1.665235	-1.672177	2.443917
H	0.772614	-1.017398	3.726780
N	0.213307	3.338988	0.379314
H	0.773100	3.203994	1.221482
H	0.108385	4.322219	0.146022
N	1.917021	3.050884	-1.827543
H	1.728926	4.008458	-2.112586
H	2.843517	2.980740	-1.419148
N	2.201894	-2.485969	-1.903828
H	2.860783	-1.841663	-2.326173
H	2.471927	-3.452492	-2.058108
N	2.794889	-2.608222	0.846162
H	3.028251	-3.596471	0.784835
H	3.648404	-2.056341	0.866557

A3

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.496105	-1.062283	-0.221637
N	-0.152811	1.089131	0.548096
C	0.384117	-0.494718	3.007967
H	-0.084306	-0.289404	3.978380
H	1.321417	-1.034416	3.178344
C	-0.841159	1.607564	-2.221788
C	-1.072430	-2.621065	-0.696676
O	-1.509455	-3.671219	-1.011201
P	-0.694332	-0.217017	-2.252769
P	-0.678466	-1.526941	1.929754
Si	0.181705	2.241836	-0.774811
Si	0.789946	1.096272	2.057944
C	-0.377532	3.977918	-0.314039
H	0.259758	4.420934	0.460970
H	-0.335428	4.640358	-1.188795
H	-1.408484	3.962863	0.053607
C	0.295879	2.575663	3.112263
H	0.774844	2.530576	4.098745
H	0.581622	3.526700	2.647963
H	-0.790068	2.595865	3.266810
H	-0.568642	2.073416	-3.177136
H	-1.885072	1.853337	-2.005284
P	1.647520	-1.679884	-0.428301
C	3.034269	-0.591194	-0.944109
H	3.987324	-1.117044	-0.785411
H	2.929536	-0.428826	-2.023109
Si	3.124758	1.126926	-0.168335
C	4.919588	1.695933	-0.314565
H	5.586330	1.057642	0.279300
H	5.265744	1.661444	-1.355361
H	5.045632	2.725612	0.043120
C	2.021232	2.284493	-1.157301
H	2.167232	2.066404	-2.223450
H	2.369395	3.314711	-0.996046
C	2.626090	1.170694	1.648473
H	3.136501	0.347204	2.164720
H	3.027114	2.103190	2.072508
H	-2.038278	-0.602253	-0.183439

H	-1.150486	1.183669	0.767596
C	-3.969421	1.452202	0.166358
C	-4.419253	1.413019	-1.271332
H	-3.867313	0.605207	-1.777097
H	-5.489177	1.195962	-1.356546
H	-4.189918	2.357916	-1.770967
C	-4.704325	0.549104	1.123115
H	-5.718112	0.942150	1.276015
H	-4.804454	-0.453242	0.691626
H	-4.178111	0.502089	2.077444
N	-0.196754	-3.116552	2.418936
H	-0.359308	-3.336775	3.399060
H	-0.632871	-3.826496	1.836543
N	-2.205235	-1.192996	2.628908
H	-2.957798	-1.476798	2.011526
H	-2.358598	-1.533495	3.574906
N	-2.136714	-0.673723	-3.076671
H	-2.125125	-0.531991	-4.083117
H	-2.396414	-1.631687	-2.864229
N	0.608050	-0.394775	-3.356337
H	1.035014	-1.317339	-3.272009
H	0.426525	-0.156059	-4.327486
N	2.394799	-2.346023	0.963392
H	1.747167	-2.897799	1.526715
H	3.276702	-2.830074	0.818708
N	1.796497	-2.822166	-1.728437
H	2.714752	-3.254306	-1.806196
H	1.086648	-3.546578	-1.671756
O	-3.066340	2.181671	0.540069

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.475333	-0.911025	0.208861
N	0.069943	0.973986	-0.468661
C	-0.257801	-0.457010	-3.056095
H	0.271585	-0.185286	-3.976816
H	-1.162905	-1.012577	-3.320928
C	0.599411	1.740234	2.282551
C	1.324893	-2.355203	0.713777
O	1.912176	-3.319613	1.044270

P	0.569428	-0.073124	2.328935
P	0.748556	-1.471887	-1.944459
Si	-0.356997	2.191477	0.708776
Si	-0.746959	1.063813	-2.000844
C	0.158094	3.942079	0.220402
H	-0.504428	4.385108	-0.532223
H	0.129630	4.598455	1.100844
H	1.180893	3.952344	-0.171802
C	-0.313731	2.596116	-3.017331
H	-0.710792	2.505039	-4.037195
H	-0.727310	3.516501	-2.590436
H	0.773451	2.724111	-3.088573
H	0.215882	2.208702	3.196336
H	1.632564	2.062877	2.113377
P	-1.554384	-1.810620	0.440948
C	-2.978323	-0.751043	0.881461
H	-3.898483	-1.330826	0.715128
H	-2.915294	-0.548232	1.956358
Si	-3.180106	0.949132	0.049382
C	-5.032204	1.323400	0.141134
H	-5.615957	0.622058	-0.469070
H	-5.408545	1.262350	1.170420
H	-5.246235	2.334416	-0.228161
C	-2.222633	2.216413	1.053989
H	-2.408008	2.036027	2.121397
H	-2.616099	3.218192	0.829726
C	-2.632450	1.009021	-1.751926
H	-3.056834	0.145949	-2.281545
H	-3.085670	1.904140	-2.203893
H	3.274606	-0.014071	0.100472
H	1.951912	1.545845	-0.506953
C	3.772866	0.962586	-0.038236
O	2.797162	1.967632	-0.236994
C	4.548859	1.278736	1.233910
H	3.886150	1.255665	2.103582
H	5.348994	0.546630	1.396454
H	5.002651	2.274213	1.158220
C	4.695971	0.894052	-1.253647
H	5.229856	1.845246	-1.366691
H	5.440806	0.093839	-1.152261
H	4.111168	0.720143	-2.161429
N	2.317917	-1.081337	-2.472525
H	3.058313	-1.419414	-1.868177
H	2.539804	-1.243212	-3.450457

N	0.368910	-3.090242	-2.407759
H	0.545176	-3.309375	-3.385527
H	0.845372	-3.767047	-1.817040
N	-1.639498	-2.915710	1.769112
H	-2.535119	-3.386017	1.879562
H	-0.894507	-3.605620	1.734923
N	-2.203364	-2.524089	-0.958921
H	-1.532408	-3.037256	-1.529226
H	-3.099731	-2.992791	-0.877031
N	2.032534	-0.453618	3.127113
H	2.150963	-0.072730	4.061401
H	2.271762	-1.439194	3.105517
N	-0.761107	-0.379622	3.348970
H	-1.088378	-1.342614	3.269094
H	-0.665057	-0.089419	4.317880

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.858877	-0.661597	-0.233888
N	-0.201012	1.222146	0.476113
C	0.012183	1.735586	-2.441195
H	0.893778	2.377788	-2.485402
H	-0.590724	1.933211	-3.336479
C	-0.225732	-0.454611	2.946656
C	1.972036	-1.921567	-0.670723
O	2.752702	-2.753054	-0.957897
P	1.240617	-0.971165	1.973573
P	0.558218	-0.010463	-2.354240
Si	-1.051185	0.978991	2.032438
Si	-0.976604	2.098071	-0.876738
C	-0.901394	2.551323	3.052945
H	-1.379707	3.407733	2.563008
H	-1.370331	2.427606	4.037582
H	0.152725	2.808928	3.213771
C	-0.932612	3.944953	-0.511565
H	-1.188596	4.530133	-1.404103
H	-1.647196	4.216475	0.275082
H	0.062736	4.261902	-0.176578
H	-0.937726	-1.285488	2.963902
H	0.033844	-0.194668	3.981338

P	-0.911807	-2.056783	-0.278386
C	-2.620574	-1.536708	-0.716082
H	-2.649115	-1.421716	-1.805974
H	-3.310677	-2.352898	-0.457767
Si	-3.322882	0.085161	-0.041732
C	-5.199904	-0.074193	-0.156409
H	-5.518503	-0.295396	-1.182840
H	-5.572176	-0.880864	0.487749
H	-5.699457	0.852110	0.153301
C	-2.851168	0.534371	1.721990
H	-3.137518	-0.266132	2.415692
H	-3.473028	1.405170	1.980257
C	-2.749816	1.520981	-1.112137
H	-2.897071	1.266372	-2.169521
H	-3.413685	2.371371	-0.898169
H	2.104664	0.439310	-0.394622
H	0.695809	1.692005	0.686025
C	3.134354	2.497236	-1.180024
H	4.062589	3.086573	-1.185472
H	3.105373	1.884613	-2.084615
H	2.298968	3.201668	-1.162309
C	3.143474	1.660916	0.087176
C	4.335712	0.716700	0.175034
H	5.223604	1.319663	0.415985
H	4.200993	-0.031799	0.956185
H	4.504454	0.215282	-0.781862
O	2.628437	2.154801	1.123072
N	-0.669260	-0.738873	-3.298940
H	-0.669103	-0.510768	-4.289367
H	-0.705563	-1.747151	-3.140312
N	1.998923	0.007879	-3.285605
H	2.598651	-0.784464	-3.081313
H	1.873714	0.105389	-4.289198
N	-0.705223	-3.211313	-1.561159
H	0.216266	-3.638675	-1.530011
H	-1.413193	-3.942627	-1.579147
N	-1.295202	-2.926033	1.143308
H	-1.948722	-3.696745	1.037249
H	-0.462700	-3.200139	1.667942
N	1.413037	-2.612882	2.473058
H	2.155072	-3.064671	1.943877
H	1.617189	-2.716365	3.465127
N	2.525832	-0.156405	2.737986
H	2.412705	-0.043909	3.742505

H	2.685566	0.760625	2.297195

$R^1=R^2=R^3=H$

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.725991	0.007762	0.190879
N	-0.361261	0.141910	1.205110
C	0.252408	2.930094	1.076782
H	0.476637	2.944224	2.151315
H	0.013701	3.953932	0.772052
C	-0.081731	-2.803699	1.052806
C	3.430861	-0.083894	-0.214484
O	4.576326	-0.149873	-0.432816
P	1.595419	-2.192738	0.515483
P	1.726717	2.238082	0.199224
Si	-1.298791	-1.365692	1.234081
Si	-1.131060	1.686297	0.785343
C	-2.166380	-1.543340	2.894027
H	-2.898827	-0.745635	3.064309
H	-2.695917	-2.501936	2.963638
H	-1.440343	-1.510296	3.716464
C	-2.607562	2.054999	1.892098
H	-2.998537	3.061568	1.696701
H	-3.429572	1.348840	1.720634
H	-2.339521	2.005649	2.954269
H	-0.452354	-3.548316	0.339502
H	0.014681	-3.320001	2.014839
P	1.083523	-0.165944	-1.940800
C	-0.533700	-0.898178	-2.474076
H	-0.643323	-0.821396	-3.562655
H	-0.497549	-1.970860	-2.239800
Si	-2.058491	-0.157252	-1.623254
C	-3.463452	-0.110383	-2.876293
H	-3.227897	0.566617	-3.707012
H	-3.653628	-1.103625	-3.301485
H	-4.396635	0.239860	-2.418229
C	-2.546017	-1.258083	-0.168586
H	-2.768469	-2.266598	-0.543598
H	-3.491150	-0.877430	0.247130
C	-1.707603	1.596344	-1.000095

H	-0.974758	2.072089	-1.666627
H	-2.628825	2.188655	-1.090631
H	2.212042	0.145686	1.738233
H	0.174975	0.239817	2.069555
H	1.859886	-3.094716	-0.547769
H	2.429468	-2.842959	1.451835
H	1.942711	-0.893368	-2.802107
H	1.048438	1.007861	-2.744069
H	1.636236	2.963849	-1.019669
H	2.787940	2.988941	0.749901

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-1.631209	-0.012452	-0.131219
N	0.154935	-0.004599	-1.076304
C	-0.290870	2.850132	-1.323315
H	-0.613734	2.785292	-2.369455
H	0.027650	3.875804	-1.115294
C	0.135624	-2.893843	-0.496006
C	-3.381462	-0.048632	0.147174
O	-4.536995	-0.077942	0.305967
P	-1.582459	-2.266748	-0.400741
P	-1.665919	2.276779	-0.259742
Si	1.172380	-1.407010	-1.096304
Si	1.007169	1.501561	-1.019146
C	1.846550	-1.852826	-2.800940
H	2.503203	-1.073618	-3.204418
H	2.422870	-2.786561	-2.766789
H	1.025460	-1.993793	-3.515413
C	2.383207	1.706349	-2.297013
H	2.769278	2.733914	-2.276270
H	3.234029	1.039110	-2.112958
H	2.015830	1.510854	-3.311540
H	0.448659	-3.176521	0.515766
H	0.230775	-3.781413	-1.129543
P	-1.077424	-0.033706	2.029699
C	0.615117	-0.628479	2.471447
H	0.776510	-0.450412	3.541921
H	0.610901	-1.718739	2.342144
Si	2.119298	0.052082	1.499119

C	3.515382	0.197795	2.761515
H	3.274665	0.931424	3.541233
H	3.711904	-0.761829	3.256209
H	4.447934	0.519232	2.281346
C	2.595083	-1.168570	0.141035
H	2.899847	-2.131194	0.574556
H	3.483002	-0.770846	-0.372659
C	1.773944	1.729187	0.704986
H	1.115367	2.324148	1.354276
H	2.716662	2.289686	0.630114
H	-2.802218	2.995946	-0.692928
H	-1.439359	3.010935	0.927513
H	-2.126292	-2.706283	-1.628433
H	-2.261788	-3.189382	0.426598
H	-1.844790	-0.752312	2.977951
H	-1.087000	1.199190	2.730055

A3

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.791560	-1.330464	-0.020094
N	0.030769	0.841519	0.130352
C	0.770592	0.781948	-2.636357
H	1.680097	1.339033	-2.379302
H	0.553844	0.942237	-3.697065
C	-0.515929	-0.111969	2.882322
C	1.653544	-2.851940	-0.066952
O	2.271854	-3.845118	-0.086111
P	0.802190	-1.229078	2.208915
P	1.044887	-0.990304	-2.202101
Si	-0.866673	1.248516	1.610652
Si	-0.575055	1.365510	-1.456793
C	-0.244567	2.894824	2.267700
H	-0.407147	3.699540	1.540944
H	-0.751841	3.174037	3.199499
H	0.832837	2.854379	2.469445
C	-0.756091	3.235052	-1.538776
H	-0.985669	3.562615	-2.560681
H	-1.561392	3.601715	-0.890339
H	0.175214	3.725061	-1.232553
H	-1.417915	-0.721695	3.013498

H	-0.256499	0.295390	3.865782
P	-1.194370	-2.345406	-0.191916
C	-2.838066	-1.662231	0.344094
H	-3.638921	-2.327878	-0.000142
H	-2.865228	-1.691390	1.441178
Si	-3.202944	0.117210	-0.204796
C	-5.055468	0.270038	-0.511025
H	-5.378220	-0.369714	-1.341724
H	-5.629621	-0.022320	0.377157
H	-5.332445	1.302188	-0.759137
C	-2.692869	1.303584	1.172936
H	-3.289007	1.095838	2.072589
H	-2.954993	2.326333	0.864320
C	-2.242137	0.553024	-1.773880
H	-2.119896	-0.353247	-2.383059
H	-2.845564	1.245490	-2.377656
H	2.236667	-0.628714	0.016344
H	0.979705	1.219031	0.219290
C	4.416947	1.247672	-1.121006
H	5.487845	1.333715	-0.906993
H	4.206264	0.190105	-1.323954
H	4.162208	1.843977	-2.000018
C	3.585311	1.662942	0.065193
C	4.041333	1.169632	1.413730
H	4.972102	1.682008	1.690081
H	3.281778	1.374667	2.171121
H	4.247807	0.095598	1.374480
O	2.599901	2.373702	-0.060721
H	0.201429	-1.607747	-3.167763
H	2.263735	-1.289310	-2.851599
H	-1.585028	-2.754651	-1.497498
H	-1.313489	-3.633619	0.389293
H	1.930969	-0.715678	2.891860
H	0.641149	-2.365625	3.038928

A4

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.935032	-1.025954	-0.009256
N	-0.072316	0.804072	0.008675
C	0.450464	0.794676	-2.828617

H	1.256264	1.531630	-2.723590
H	0.092887	0.801220	-3.862358
C	-0.354810	0.256658	2.901752
C	2.104257	-2.352494	0.015802
O	2.869377	-3.232262	0.040607
P	0.834486	-0.992394	2.257325
P	1.108504	-0.823842	-2.288265
Si	-0.922913	1.325508	1.425648
Si	-0.835489	1.202678	-1.498505
C	-0.575360	3.121675	1.884110
H	-0.890899	3.815831	1.096824
H	-1.101806	3.404781	2.805103
H	0.497406	3.282813	2.048263
C	-1.293396	3.024874	-1.688037
H	-1.605421	3.231858	-2.720045
H	-2.121277	3.325063	-1.033917
H	-0.436382	3.671859	-1.465830
H	-1.207746	-0.257296	3.358377
H	0.106388	0.862308	3.689130
P	-0.795120	-2.439741	-0.114962
C	-2.424769	-1.932507	0.580809
H	-3.146319	-2.741995	0.416408
H	-2.298881	-1.847074	1.668412
Si	-3.162051	-0.287949	-0.061722
C	-5.021553	-0.564337	-0.216447
H	-5.249983	-1.333382	-0.965147
H	-5.463176	-0.884514	0.735504
H	-5.531860	0.356841	-0.523938
C	-2.791285	1.077031	1.183027
H	-3.289152	0.872080	2.140908
H	-3.234520	2.011148	0.806224
C	-2.417999	0.180857	-1.731893
H	-2.225616	-0.728479	-2.319622
H	-3.151222	0.764217	-2.306451
H	2.679917	0.179270	0.066140
H	1.408459	1.838509	-0.128422
C	4.340202	1.063491	-0.922932
H	4.898925	2.005942	-0.960602
H	5.032567	0.258420	-0.653027
H	3.945691	0.863561	-1.924988
C	3.201387	1.168368	0.080937
C	3.695811	1.395009	1.506662
H	4.261748	2.332274	1.562220
H	2.848024	1.475190	2.196645

H	4.341463	0.575571	1.844533
O	2.319694	2.183651	-0.314102
H	0.370784	-1.732504	-3.079954
H	2.341676	-0.963617	-2.963869
H	-1.207162	-2.911418	-1.386064
H	-0.645647	-3.713607	0.483854
H	2.021006	-0.694318	2.963227
H	0.512296	-2.166401	2.976293

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.035447	-1.007813	-0.029064
N	-0.127980	0.933537	0.084749
C	0.540157	0.994978	-2.690711
H	1.314767	1.725611	-2.424071
H	0.292622	1.107410	-3.750395
C	-0.439256	0.009345	2.898214
C	2.258145	-2.263757	-0.071406
O	3.128929	-3.042381	-0.097447
P	0.920890	-1.045323	2.204167
P	1.177932	-0.670634	-2.244015
Si	-1.061536	1.213555	1.571242
Si	-0.873301	1.300443	-1.487082
C	-0.777659	2.976315	2.152472
H	-1.171786	3.704739	1.434164
H	-1.260339	3.163504	3.119708
H	0.294812	3.176775	2.264874
C	-1.429802	3.093004	-1.593156
H	-1.745411	3.339560	-2.614945
H	-2.277024	3.306837	-0.930110
H	-0.611185	3.771280	-1.325866
H	-1.258376	-0.649293	3.209711
H	-0.105422	0.539522	3.796847
P	-0.680601	-2.431226	-0.207387
C	-2.383681	-2.078669	0.431361
H	-3.053144	-2.907192	0.170302
H	-2.324212	-2.062822	1.527878
Si	-3.148212	-0.435875	-0.145022
C	-4.993444	-0.713816	-0.399109
H	-5.181339	-1.453646	-1.187149

H	-5.471933	-1.076888	0.518941
H	-5.498235	0.215596	-0.690290
C	-2.871506	0.876015	1.182723
H	-3.397798	0.588662	2.103449
H	-3.342893	1.809400	0.841443
C	-2.350300	0.164142	-1.750405
H	-2.074215	-0.698071	-2.373182
H	-3.103130	0.722261	-2.324789
H	2.295079	0.043457	0.063622
H	0.724749	1.525479	0.132159
C	4.064654	1.124169	-1.026406
H	4.885830	1.854684	-1.028260
H	4.486619	0.124251	-0.893971
H	3.563413	1.186317	-1.995203
C	3.108361	1.498102	0.096542
C	3.666032	1.290230	1.496793
H	4.446104	2.046186	1.665534
H	2.883102	1.445477	2.243693
H	4.107732	0.298262	1.625207
O	2.257011	2.396510	-0.091869
H	0.442902	-1.484720	-3.144092
H	2.411284	-0.746850	-2.928579
H	-1.040247	-2.891153	-1.502734
H	-0.498240	-3.719775	0.353462
H	2.018455	-0.623614	2.988246
H	0.708796	-2.260025	2.901404

Mn(CO)-LYG19_A1

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.099308	-0.389999	0.989946
N	-1.037402	1.375726	-0.258341
C	1.100594	0.470249	-2.047355
H	1.817855	1.049331	-2.640222
H	1.018348	-0.504063	-2.539478
C	-2.583804	1.493606	2.174007
C	0.787996	-1.375645	2.118406
O	1.387888	-1.976755	2.929678
P	-1.772136	-0.138466	2.467497
P	1.673433	0.098597	-0.327358
Si	-2.664221	1.788092	0.320893
Si	-0.616975	1.264010	-1.976295
C	-3.033958	3.604540	-0.012348
H	-3.168389	3.805677	-1.081901
H	-3.954930	3.915513	0.497388
H	-2.223451	4.250056	0.348097
C	-0.549196	2.981785	-2.748729
H	-0.087387	2.948761	-3.743806
H	-1.550636	3.412378	-2.868005
H	0.033853	3.676581	-2.132111
H	-3.555287	1.581719	2.676493
H	-1.920612	2.261329	2.594451
C	-1.256493	-0.032654	4.230781
H	-2.080257	0.294483	4.875642
H	-0.908143	-1.012812	4.574056
H	-0.422430	0.669024	4.315089
C	-3.268188	-1.212726	2.689522
H	-2.966489	-2.241974	2.910823
H	-3.897723	-0.857041	3.514039
H	-3.875353	-1.226985	1.779910
P	-0.921641	-2.151632	-0.181313
C	-2.657751	-2.120488	-0.834929
H	-2.815870	-3.000564	-1.474765
H	-3.334516	-2.248403	0.019440
Si	-3.251115	-0.585162	-1.765875
C	-0.110257	-2.868305	-1.689557
H	-0.251747	-2.214585	-2.555076
H	0.964669	-2.991910	-1.528155
H	-0.540863	-3.846019	-1.937287

C	-0.981843	-3.706218	0.815594
H	-1.488501	-3.523145	1.767484
H	-1.498207	-4.516700	0.287376
H	0.039077	-4.030277	1.044373
C	-4.663718	-1.155637	-2.880229
H	-4.314470	-1.877222	-3.629450
H	-5.454698	-1.643799	-2.296699
H	-5.120244	-0.315091	-3.417544
C	-3.921667	0.715736	-0.574307
H	-4.590421	0.233245	0.150558
H	-4.561644	1.387511	-1.165422
C	-1.932554	0.234530	-2.844473
H	-1.460748	-0.513324	-3.495149
H	-2.476587	0.909111	-3.522848
H	0.360778	0.859921	1.901301
H	-0.367771	1.967919	0.238339
C	2.592679	1.628399	0.147497
C	3.211251	1.632763	1.405723
C	2.674294	2.778780	-0.638741
C	3.905571	2.748484	1.852891
H	3.132364	0.754895	2.041682
C	3.354185	3.910157	-0.181758
H	2.210753	2.814386	-1.619428
C	3.974324	3.896490	1.060920
H	4.385112	2.729542	2.827359
H	3.398641	4.798638	-0.805793
H	4.506934	4.773941	1.416463
C	3.096839	-1.032791	-0.643716
C	4.171560	-0.636958	-1.449637
C	3.106859	-2.316602	-0.095628
C	5.221883	-1.509517	-1.710844
H	4.192204	0.365422	-1.870212
C	4.160097	-3.193230	-0.353680
H	2.288807	-2.631502	0.542876
C	5.217449	-2.792399	-1.163286
H	6.048141	-1.188341	-2.338954
H	4.152829	-4.186647	0.085578
H	6.039012	-3.473797	-1.365419

Mn(CO)-LYG19_A2

Coordinates (Angstroms)		
X	Y	Z

Mn	-0.031454	0.161432	0.884856
N	-1.157008	0.779928	-0.723248
C	0.992521	-0.437021	-2.324523
H	1.533548	0.135519	-3.086634
H	1.118066	-1.499412	-2.562877
C	-3.077568	1.598034	1.373801
C	1.049360	0.070964	2.264654
O	1.733929	0.043903	3.218445
P	-1.455822	1.357350	2.173482
P	1.630933	-0.160447	-0.630802
Si	-2.767586	1.363603	-0.491922
Si	-0.863122	-0.014049	-2.227363
C	-3.106866	3.028670	-1.318300
H	-2.962823	2.990223	-2.404110
H	-4.134981	3.364988	-1.130687
H	-2.427287	3.796368	-0.925932
C	-1.288018	1.016564	-3.759609
H	-0.940461	0.509584	-4.669478
H	-2.368823	1.169104	-3.870014
H	-0.816932	2.006940	-3.729948
H	-3.753367	0.808468	1.725848
H	-3.535185	2.561450	1.630059
C	-0.746216	3.054762	2.222871
H	-1.433717	3.780990	2.672107
H	0.187279	3.041856	2.795860
H	-0.503863	3.372349	1.202982
C	-1.821636	1.050089	3.947456
H	-0.888119	0.889820	4.496802
H	-2.360879	1.891882	4.396310
H	-2.438353	0.151118	4.049462
P	-0.854503	-1.884874	1.190659
C	-2.620973	-2.111091	0.694997
H	-2.891658	-3.160950	0.879577
H	-3.219423	-1.520442	1.403373
Si	-3.233381	-1.653687	-1.060077
C	-0.031037	-3.294627	0.332207
H	0.133589	-3.060501	-0.722606
H	0.951272	-3.464450	0.784289
H	-0.613476	-4.220984	0.402872
C	-0.887691	-2.563955	2.903640
H	-1.448437	-1.891248	3.560106
H	-1.344929	-3.559431	2.945836
H	0.134242	-2.628212	3.292296

C	-4.524341	-2.968108	-1.480623
H	-4.073862	-3.967127	-1.543082
H	-5.315732	-3.007826	-0.721287
H	-5.003334	-2.762331	-2.445914
C	-4.016406	0.061944	-1.089763
H	-4.940066	0.102127	-0.496452
H	-4.310178	0.262894	-2.131523
C	-1.873496	-1.624039	-2.359592
H	-1.241716	-2.517786	-2.290066
H	-2.355058	-1.670765	-3.347595
C	2.381456	1.519056	-0.683286
C	3.392922	1.849561	0.226841
C	1.872313	2.520158	-1.516141
C	3.895238	3.145268	0.288460
H	3.791145	1.089806	0.894213
C	2.376694	3.816965	-1.455138
H	1.069628	2.298274	-2.212106
C	3.389416	4.133278	-0.554131
H	4.682678	3.383605	0.997750
H	1.973599	4.580774	-2.114168
H	3.782659	5.144690	-0.506074
C	3.099631	-1.248913	-0.481867
C	4.004113	-1.389657	-1.541610
C	3.333942	-1.948592	0.704050
C	5.113810	-2.218217	-1.418778
H	3.839560	-0.848125	-2.469723
C	4.447388	-2.777911	0.829434
H	2.644487	-1.842354	1.535437
C	5.337363	-2.914241	-0.231079
H	5.809033	-2.318540	-2.247380
H	4.617787	-3.313958	1.758655
H	6.204684	-3.561135	-0.135251

TSD4-5R

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.386251	0.079171	1.085521
N	1.079765	-1.190499	-0.714348
C	-1.166664	0.154567	-1.917174
H	-1.752247	-0.772037	-1.870534
H	-1.596481	0.755016	-2.725305

C	3.080139	-2.189375	1.213081
C	-0.241308	0.713371	2.588895
O	-0.622426	1.091310	3.631840
P	1.969080	-1.168153	2.296414
P	-1.281216	0.929556	-0.248066
Si	2.639064	-2.042273	-0.611110
Si	0.616402	-0.377182	-2.218079
C	2.495778	-3.767055	-1.339659
H	2.194269	-3.755275	-2.393560
H	3.458313	-4.291072	-1.275622
H	1.759741	-4.346365	-0.770863
C	0.691396	-1.514366	-3.716679
H	0.259970	-1.016573	-4.594957
H	1.726387	-1.776681	-3.969510
H	0.133859	-2.442264	-3.556865
H	4.124890	-1.903098	1.385664
H	2.988491	-3.239795	1.513167
C	1.357776	-2.413385	3.502019
H	2.196714	-2.881876	4.029814
H	0.705893	-1.927382	4.235653
H	0.800471	-3.171556	2.949093
C	3.230558	-0.404545	3.419309
H	2.734067	0.063538	4.275679
H	3.891866	-1.189855	3.802822
H	3.847009	0.347378	2.920268
P	1.869950	1.868338	0.904844
C	3.516931	1.458138	0.175042
H	4.171871	2.338162	0.237116
H	3.990949	0.676034	0.780405
Si	3.499763	0.818233	-1.620307
C	1.631957	3.500724	0.055128
H	1.461642	3.419537	-1.017373
H	0.782466	4.032139	0.487958
H	2.532603	4.106079	0.213162
C	2.278519	2.648172	2.534773
H	2.340840	1.924189	3.344092
H	3.215689	3.215071	2.486071
H	1.468048	3.342751	2.781903
C	4.824659	1.760388	-2.573575
H	4.588896	2.830608	-2.631126
H	5.805872	1.661827	-2.092773
H	4.920385	1.385063	-3.599946
C	3.899191	-1.020494	-1.569337
H	4.897287	-1.171640	-1.135190

H	3.953852	-1.402967	-2.599009
C	1.840737	1.017764	-2.511896
H	1.386798	1.983586	-2.274821
H	2.058235	1.046024	-3.589583
H	-0.740359	-1.288708	1.125491
H	0.387843	-1.894115	-0.442893
C	-1.135531	-2.836878	1.064707
O	-0.060811	-3.491155	0.997896
C	-3.050934	0.704636	0.223705
C	-4.063921	0.824911	-0.733214
C	-3.406680	0.474570	1.553105
C	-5.400515	0.693864	-0.373275
H	-3.810267	1.012206	-1.772988
C	-4.746556	0.349078	1.918957
H	-2.636892	0.375434	2.308538
C	-5.745633	0.450809	0.955869
H	-6.174546	0.779435	-1.130863
H	-5.003678	0.164475	2.958177
H	-6.789682	0.345812	1.237015
C	-1.403331	2.738832	-0.592947
C	-1.150784	3.329639	-1.831303
C	-1.760462	3.564458	0.482116
C	-1.240699	4.712590	-1.992444
H	-0.864756	2.722687	-2.684996
C	-1.860151	4.940877	0.322025
H	-1.957415	3.123913	1.456647
C	-1.594915	5.521352	-0.918513
H	-1.035747	5.155468	-2.963084
H	-2.141756	5.563056	1.166830
H	-1.670137	6.597253	-1.046067
C	-2.003219	-2.872848	-0.199362
C	-1.454554	-3.465273	-1.342710
C	-3.335884	-2.455084	-0.251228
C	-2.192978	-3.595683	-2.514005
H	-0.441130	-3.847805	-1.288516
C	-4.081347	-2.590247	-1.420758
H	-3.810317	-2.012221	0.616046
C	-3.512160	-3.150155	-2.560539
H	-1.743237	-4.060453	-3.387503
H	-5.113371	-2.252300	-1.435154
H	-4.094629	-3.254526	-3.471660
C	-1.923449	-2.802346	2.371782
H	-2.415167	-3.775928	2.503456
H	-1.252820	-2.632771	3.212555

H	-2.685515	-2.021536	2.381330

TSD4-5S

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.189369	-0.217001	0.700256
N	0.285127	-1.441324	-1.163950
C	0.873277	1.199811	-2.126520
H	-0.107147	1.148560	-2.610177
H	1.485829	1.895851	-2.708091
C	-0.164233	-3.573997	0.838933
C	-0.796810	0.587501	2.122370
O	-1.229728	1.065312	3.105180
P	-1.288611	-2.184679	1.287634
P	0.582311	1.694437	-0.376955
Si	0.449968	-3.201304	-0.914849
Si	1.488618	-0.575549	-2.135009
C	-0.594020	-4.096234	-2.193096
H	-0.179772	-3.945368	-3.197649
H	-0.620944	-5.176241	-2.002021
H	-1.624579	-3.725971	-2.207430
C	1.503843	-1.210566	-3.906018
H	2.122684	-0.573072	-4.550675
H	1.906411	-2.228858	-3.975737
H	0.489789	-1.221637	-4.322832
H	0.684141	-3.589875	1.530072
H	-0.661862	-4.549687	0.907254
C	-2.798576	-2.785182	0.422763
H	-2.881169	-3.872457	0.536176
H	-3.687417	-2.327008	0.860964
H	-2.767150	-2.525680	-0.637120
C	-1.863510	-2.512512	3.007124
H	-2.688343	-1.822796	3.218944
H	-2.236299	-3.538156	3.108044
H	-1.089199	-2.339152	3.755213
P	1.728331	-0.793698	1.915363
C	3.012970	-2.061825	1.427550
H	3.939630	-1.801942	1.957414
H	2.707685	-3.030232	1.845283
Si	3.425759	-2.358496	-0.393983
C	2.868244	0.576738	2.387712

H	3.407552	0.965061	1.520730
H	2.294677	1.397951	2.825246
H	3.600496	0.226467	3.124355
C	1.413467	-1.425407	3.625443
H	0.962530	-2.420098	3.584792
H	2.350806	-1.504307	4.187787
H	0.734730	-0.753503	4.159959
C	5.208301	-2.960842	-0.496352
H	5.911636	-2.200037	-0.135639
H	5.357157	-3.865067	0.106873
H	5.483163	-3.204243	-1.530209
C	2.260068	-3.672116	-1.070937
H	2.422642	-4.623855	-0.546025
H	2.501704	-3.855190	-2.127736
C	3.200237	-0.778469	-1.389129
H	3.445299	0.064224	-0.732321
H	3.932049	-0.757087	-2.208882
H	-1.561056	0.280436	-0.273055
H	-0.645261	-1.266307	-1.590263
C	-2.777088	1.491033	-2.102552
H	-3.626564	1.499024	-2.799723
H	-2.955150	2.256672	-1.347531
H	-1.882242	1.734131	-2.674224
C	-2.739678	0.083604	-1.526135
O	-2.303241	-0.853439	-2.237321
C	-0.555578	3.145465	-0.497610
C	-0.474519	4.030168	-1.577751
C	-1.493924	3.396271	0.504462
C	-1.337503	5.116983	-1.672333
H	0.261749	3.866994	-2.360029
C	-2.350422	4.492088	0.420235
H	-1.569980	2.726598	1.351746
C	-2.283280	5.347937	-0.674748
H	-1.272249	5.786200	-2.525635
H	-3.080437	4.664688	1.205916
H	-2.961348	6.193177	-0.750060
C	2.093150	2.691586	0.029269
C	3.267426	2.689420	-0.726987
C	2.049089	3.491663	1.179321
C	4.375713	3.439877	-0.331601
H	3.339634	2.103199	-1.637021
C	3.147579	4.245421	1.571895
H	1.143537	3.520226	1.781048
C	4.321786	4.216430	0.819909

H	5.280002	3.418125	-0.933584
H	3.089138	4.855092	2.469052
H	5.183569	4.802020	1.126721
C	-3.941378	-0.145572	-0.621478
C	-4.976121	-0.931404	-1.130269
C	-4.093041	0.453200	0.628453
C	-6.135264	-1.142516	-0.388903
H	-4.849855	-1.400150	-2.101991
C	-5.247564	0.238386	1.375274
H	-3.280820	1.051828	1.027587
C	-6.271390	-0.563501	0.870853
H	-6.928818	-1.766443	-0.791132
H	-5.346042	0.694338	2.356808
H	-7.171240	-0.733785	1.455437

D4R

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.740931	0.181547	1.200535
N	0.894312	-1.427348	-0.486182
C	-1.210203	0.191615	-1.520604
H	-1.901746	-0.597947	-1.206152
H	-1.712227	0.742768	-2.322481
C	3.037231	-2.308164	1.345135
C	0.488571	1.176622	2.607518
O	0.320654	1.814678	3.581140
P	1.766060	-1.446385	2.377349
P	-0.862456	1.193991	-0.007154
Si	2.322838	-2.485662	-0.400620
Si	0.387733	-0.669190	-2.006086
C	1.797930	-4.267027	-0.679360
H	1.301675	-4.384690	-1.650348
H	2.662283	-4.943069	-0.660441
H	1.092429	-4.598028	0.090797
C	0.065574	-1.957809	-3.342316
H	-0.456670	-1.515885	-4.200647
H	1.001833	-2.390359	-3.717107
H	-0.554089	-2.777620	-2.964649
H	3.933398	-1.675664	1.321047
H	3.331038	-3.277819	1.768465
C	0.705610	-2.869657	2.869219

H	1.289597	-3.682068	3.319677
H	-0.031090	-2.513052	3.596652
H	0.154057	-3.255546	2.006978
C	2.606377	-1.179622	3.996450
H	1.866195	-0.812518	4.716267
H	3.036888	-2.110972	4.382073
H	3.395748	-0.428270	3.926178
P	2.639642	1.377228	0.718226
C	3.981444	0.811698	-0.445003
H	4.624462	1.672121	-0.677180
H	4.619601	0.107260	0.105842
Si	3.479591	-0.050830	-2.049927
C	2.472487	3.120366	0.129540
H	1.987813	3.173816	-0.848605
H	1.852161	3.681018	0.834496
H	3.453159	3.606275	0.060586
C	3.719699	1.735028	2.179449
H	4.214542	0.817137	2.510304
H	4.497554	2.466743	1.931450
H	3.118809	2.120943	3.008829
C	4.734953	0.396874	-3.382262
H	4.715191	1.473499	-3.594270
H	5.756269	0.138347	-3.075875
H	4.528120	-0.129956	-4.322180
C	3.516146	-1.911390	-1.733436
H	4.538872	-2.207824	-1.461300
H	3.281636	-2.443887	-2.666681
C	1.752190	0.467742	-2.609486
H	1.577836	1.496845	-2.274612
H	1.721681	0.485888	-3.708167
H	-0.578807	-0.683846	1.524504
H	0.090883	-1.920668	-0.088827
C	-2.473216	-3.061693	0.599200
O	-1.440921	-3.654141	0.314929
C	-2.556876	1.364059	0.730475
C	-3.603878	1.891203	-0.035598
C	-2.822850	0.978449	2.045038
C	-4.884645	2.014561	0.492550
H	-3.416841	2.212820	-1.056960
C	-4.105289	1.103367	2.580177
H	-2.019350	0.571395	2.648153
C	-5.140839	1.615835	1.804191
H	-5.683790	2.425277	-0.118728
H	-4.289684	0.803142	3.608032

H	-6.139057	1.715845	2.221315
C	-0.737552	2.921242	-0.660471
C	-0.524916	3.251430	-2.000793
C	-0.791982	3.959894	0.279019
C	-0.349794	4.580465	-2.390261
H	-0.482861	2.476924	-2.760553
C	-0.627788	5.284253	-0.106547
H	-0.954804	3.726214	1.328807
C	-0.397910	5.599519	-1.445709
H	-0.179124	4.814404	-3.437640
H	-0.672380	6.072054	0.640195
H	-0.261540	6.633935	-1.748002
C	-3.357814	-2.552583	-0.492992
C	-3.145549	-3.029294	-1.791880
C	-4.333324	-1.577241	-0.268047
C	-3.888296	-2.532562	-2.853412
H	-2.387466	-3.789571	-1.948248
C	-5.076039	-1.078164	-1.334514
H	-4.491728	-1.172363	0.726952
C	-4.854385	-1.552072	-2.624504
H	-3.716814	-2.906855	-3.858271
H	-5.819572	-0.308621	-1.154677
H	-5.434159	-1.157712	-3.454142
C	-2.867170	-2.813917	2.030734
H	-3.933820	-2.993518	2.196299
H	-2.273758	-3.452472	2.686794
H	-2.652004	-1.766521	2.274952

D5Ra

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.527258	0.040041	1.067075
N	0.391839	-1.395647	-0.408960
C	-0.956177	0.643197	-1.931699
H	-1.930042	0.144928	-1.867857
H	-1.003429	1.322351	-2.788442
C	1.860640	-3.074851	1.515484
C	0.206032	1.035717	2.481570
O	0.008575	1.664946	3.451080
P	1.015114	-1.740884	2.428878
P	-0.669891	1.472552	-0.317949

Si	1.292055	-2.883321	-0.292832
Si	0.335571	-0.733290	-2.012051
C	0.297240	-4.420756	-0.741964
H	0.009977	-4.424860	-1.799451
H	0.882262	-5.330754	-0.554333
H	-0.627972	-4.476405	-0.157070
C	-0.229500	-1.967635	-3.327529
H	-0.537735	-1.449041	-4.244816
H	0.555271	-2.681653	-3.606059
H	-1.088046	-2.539550	-2.957216
H	2.942811	-2.910640	1.584902
H	1.650545	-4.065130	1.937971
C	-0.601882	-2.513829	2.839060
H	-0.467914	-3.457809	3.380281
H	-1.188992	-1.831858	3.463671
H	-1.161338	-2.713370	1.919600
C	1.808925	-1.709006	4.087545
H	1.382009	-0.904604	4.695610
H	1.660842	-2.663628	4.604888
H	2.885978	-1.539279	3.996762
P	2.633230	0.866510	0.906710
C	3.837050	-0.264049	0.081726
H	4.797471	0.264649	0.001626
H	4.015229	-1.104335	0.765903
Si	3.409610	-1.007656	-1.625818
C	3.075947	2.456913	0.085125
H	2.834149	2.446756	-0.979163
H	2.532153	3.285748	0.546235
H	4.151557	2.639954	0.193132
C	3.478318	1.194163	2.512215
H	3.417017	0.322761	3.167703
H	4.533565	1.451101	2.365288
H	2.979584	2.026694	3.019840
C	5.001421	-0.947889	-2.640230
H	5.315192	0.087122	-2.827333
H	5.826579	-1.458476	-2.127580
H	4.867331	-1.433916	-3.614747
C	2.843865	-2.788144	-1.383635
H	3.650141	-3.393382	-0.945872
H	2.633885	-3.226391	-2.370359
C	2.036448	-0.075328	-2.526679
H	2.119540	1.000380	-2.330114
H	2.171132	-0.204411	-3.610319
H	-3.211336	-0.662035	-0.200077

H	-1.483663	-1.995879	-0.289759
C	-3.459616	-1.726686	-0.095668
O	-2.312578	-2.516976	-0.365502
C	-2.380253	1.895329	0.228497
C	-3.211862	2.663562	-0.596755
C	-2.894435	1.397732	1.426211
C	-4.528023	2.920598	-0.233151
H	-2.824359	3.062933	-1.530891
C	-4.213918	1.657882	1.795578
H	-2.268097	0.788027	2.069447
C	-5.032486	2.416035	0.966090
H	-5.162498	3.516274	-0.883114
H	-4.599959	1.258389	2.728917
H	-6.062044	2.615499	1.249076
C	-0.040939	3.148264	-0.716094
C	0.504230	3.489835	-1.954836
C	-0.049514	4.106238	0.306162
C	1.039672	4.759660	-2.167447
H	0.534393	2.763380	-2.761069
C	0.477910	5.374366	0.092396
H	-0.468837	3.857169	1.277824
C	1.029979	5.702919	-1.145656
H	1.466645	5.007315	-3.135089
H	0.461437	6.107517	0.893630
H	1.448624	6.691354	-1.310774
C	-4.551482	-2.039520	-1.138048
C	-4.824132	-3.540891	-1.253556
C	-4.196565	-1.444033	-2.501316
H	-5.468135	-1.545217	-0.786470
H	-5.151551	-3.973731	-0.301715
H	-5.610769	-3.735923	-1.992006
H	-3.918811	-4.068424	-1.570503
H	-4.096411	-0.353087	-2.441000
H	-3.251573	-1.854731	-2.874233
H	-4.972910	-1.663902	-3.243833
C	-3.940590	-1.952766	1.336090
H	-4.883570	-1.425788	1.522701
H	-4.091547	-3.019947	1.532022
H	-3.202017	-1.582496	2.053782

D5Sa

Coordinates (Angstroms)

	X	Y	Z
Mn	0.721145	0.142894	1.021490
N	0.285113	-1.375013	-0.273068
C	-0.835671	0.720710	-1.979388
H	-1.913769	0.534333	-2.022702
H	-0.594060	1.327993	-2.856454
C	1.619812	-3.068990	1.737946
C	0.654702	1.305123	2.337412
O	0.620209	2.044021	3.248878
P	1.108870	-1.512533	2.541066
P	-0.449912	1.545577	-0.377103
Si	0.935144	-2.961443	-0.036095
Si	0.150504	-0.895812	-1.925475
C	-0.340815	-4.344369	-0.210926
H	-0.824929	-4.342802	-1.193580
H	0.122798	-5.330044	-0.071525
H	-1.126697	-4.238660	0.548678
C	-0.700689	-2.162733	-3.056455
H	-0.990329	-1.698310	-4.008530
H	-0.023452	-2.990153	-3.303003
H	-1.595062	-2.618410	-2.614411
H	2.716101	-3.095453	1.707801
H	1.282616	-3.957837	2.285583
C	-0.557254	-1.914729	3.209277
H	-0.557939	-2.849656	3.781920
H	-0.893363	-1.101496	3.862272
H	-1.266399	-2.003929	2.380693
C	2.095911	-1.417527	4.088944
H	1.889667	-0.477831	4.611713
H	1.858063	-2.254945	4.754776
H	3.165668	-1.456936	3.861448
P	2.855699	0.674716	0.566165
C	3.831986	-0.695132	-0.195680
H	4.838355	-0.314153	-0.421208
H	3.966965	-1.453739	0.588173
Si	3.168999	-1.603892	-1.742333
C	3.306558	2.096298	-0.517022
H	2.862606	1.999470	-1.509679
H	2.932127	3.024240	-0.073754
H	4.394708	2.171169	-0.627895
C	3.916101	1.112758	2.008554
H	3.889423	0.320104	2.760857
H	4.957927	1.280373	1.711832

H	3.531017	2.026199	2.474212
C	4.674194	-1.919352	-2.838802
H	5.111845	-0.978975	-3.197790
H	5.458807	-2.465589	-2.299597
H	4.404259	-2.515130	-3.719902
C	2.383237	-3.243596	-1.233759
H	3.129020	-3.919286	-0.792686
H	2.023555	-3.740693	-2.147146
C	1.868015	-0.617826	-2.687535
H	2.129889	0.447446	-2.700236
H	1.867019	-0.946661	-3.737012
H	-3.728552	-0.160750	-0.377068
H	-3.020543	-1.199961	-2.416530
C	-5.708461	-0.874200	-0.719318
H	-6.240220	-1.723399	-1.162227
H	-5.986534	-0.793186	0.335860
H	-6.042030	0.036549	-1.226254
C	-4.203465	-1.016652	-0.876738
O	-3.940642	-0.942987	-2.277885
C	-2.134515	1.921016	0.270191
C	-3.042921	2.657065	-0.500508
C	-2.553589	1.406362	1.498317
C	-4.343038	2.863697	-0.055975
H	-2.731615	3.063324	-1.459730
C	-3.856889	1.616886	1.948964
H	-1.862681	0.826554	2.103552
C	-4.753633	2.341282	1.170928
H	-5.038725	3.431442	-0.666935
H	-4.170281	1.206000	2.904441
H	-5.771240	2.499867	1.515989
C	0.160154	3.233671	-0.765274
C	0.620803	3.625476	-2.023280
C	0.253155	4.142573	0.297332
C	1.167243	4.892953	-2.217701
H	0.581498	2.941444	-2.865101
C	0.793624	5.408599	0.103333
H	-0.094256	3.855967	1.286280
C	1.256799	5.787113	-1.156379
H	1.525149	5.177693	-3.203090
H	0.854660	6.101434	0.937685
H	1.685040	6.773741	-1.307189
C	-3.855444	-2.365198	1.245683
C	-3.597716	-2.293146	-0.260074
H	-3.567337	-1.433359	1.746338

H	-4.914941	-2.549868	1.461056
H	-3.284854	-3.184980	1.697642
C	-4.058511	-3.572613	-0.959394
H	-2.508328	-2.202349	-0.395614
H	-3.922136	-3.507413	-2.043740
H	-3.491930	-4.437137	-0.595060
H	-5.120529	-3.771234	-0.770180

D4S

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.238182	-0.158837	1.004001
N	0.178515	-1.439991	-0.949846
C	0.388736	1.168446	-2.055263
H	-0.676140	1.066362	-2.292518
H	0.802111	1.904006	-2.753032
C	0.070426	-3.528684	1.136299
C	0.006885	0.736890	2.478456
O	-0.178782	1.312788	3.487297
P	-0.730303	-2.013308	1.830262
P	0.473143	1.664667	-0.276499
Si	0.369006	-3.190846	-0.703536
Si	1.082727	-0.571378	-2.202092
C	-0.919968	-4.110232	-1.716884
H	-0.852338	-3.846285	-2.778856
H	-0.785649	-5.195938	-1.630116
H	-1.936327	-3.872890	-1.382216
C	0.706655	-1.259974	-3.913718
H	1.142669	-0.630612	-4.700309
H	1.108435	-2.272267	-4.047831
H	-0.376528	-1.299555	-4.077770
H	1.028635	-3.667756	1.651140
H	-0.527227	-4.436087	1.295818
C	-2.469662	-2.279563	1.296300
H	-2.857196	-3.264885	1.584530
H	-3.099561	-1.499600	1.735311
H	-2.540547	-2.168473	0.211954
C	-0.927723	-2.374879	3.625877
H	-1.564962	-1.600971	4.067926
H	-1.398500	-3.350994	3.789137
H	0.031667	-2.350679	4.147622

P	2.371537	-0.657171	1.674090
C	3.452039	-1.991489	0.941128
H	4.490187	-1.798424	1.244554
H	3.177279	-2.939215	1.424334
Si	3.390285	-2.295417	-0.922154
C	3.608115	0.714058	1.739028
H	3.839006	1.094218	0.740457
H	3.189640	1.542648	2.317479
H	4.539345	0.385276	2.215474
C	2.517355	-1.183922	3.443654
H	2.060014	-2.169057	3.577346
H	3.566095	-1.252890	3.756544
H	1.998531	-0.471888	4.093087
C	5.085057	-2.899483	-1.485565
H	5.852068	-2.128113	-1.341447
H	5.398415	-3.789497	-0.925490
H	5.078175	-3.164345	-2.550385
C	2.107504	-3.641091	-1.249452
H	2.420451	-4.567484	-0.748091
H	2.090435	-3.865365	-2.326089
C	2.921750	-0.727262	-1.862114
H	3.282748	0.134111	-1.287712
H	3.454452	-0.708125	-2.823218
H	-1.267873	0.165543	0.524863
H	-0.811656	-1.221887	-1.092013
C	-3.321867	1.422350	-2.390478
H	-4.319838	1.830842	-2.577063
H	-2.845681	2.052338	-1.629797
H	-2.726133	1.465291	-3.304741
C	-3.393897	0.000702	-1.895513
O	-2.630766	-0.862206	-2.308336
C	-0.836640	2.977073	-0.195111
C	-0.825293	4.034548	-1.114220
C	-1.866765	2.923001	0.745694
C	-1.829434	4.996877	-1.110321
H	-0.023524	4.106524	-1.845066
C	-2.865500	3.897220	0.763826
H	-1.897238	2.103385	1.453711
C	-2.856040	4.929581	-0.169051
H	-1.810002	5.801260	-1.840369
H	-3.653019	3.842674	1.510913
H	-3.638474	5.683221	-0.160534
C	1.930151	2.805137	-0.229992
C	2.923887	2.865263	-1.209834

C	2.073495	3.606800	0.910642
C	4.039246	3.688777	-1.048139
H	2.846536	2.264325	-2.110986
C	3.178615	4.432706	1.071644
H	1.311993	3.576301	1.686680
C	4.171781	4.471908	0.093141
H	4.802952	3.716422	-1.820624
H	3.269186	5.043363	1.965644
H	5.039802	5.112491	0.220009
C	-4.444934	-0.337891	-0.890660
C	-4.958665	-1.637120	-0.857904
C	-4.891621	0.606697	0.037158
C	-5.910776	-1.989144	0.090343
H	-4.602017	-2.364074	-1.581031
C	-5.825749	0.245662	1.003099
H	-4.484335	1.613415	0.027262
C	-6.339397	-1.049332	1.027098
H	-6.315717	-2.996615	0.105687
H	-6.153604	0.975730	1.736925
H	-7.075049	-1.327213	1.776238

D5R

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.861948	0.151157	1.047928
N	0.613985	-1.435358	-0.285133
C	-1.141395	0.387191	-1.684935
H	-2.046254	-0.179407	-1.431051
H	-1.384085	0.983089	-2.570065
C	2.481977	-2.847958	1.498530
C	0.695176	1.224141	2.430800
O	0.622896	1.911744	3.377907
P	1.769574	-1.445718	2.434198
P	-0.676150	1.372489	-0.209174
Si	1.675964	-2.815147	-0.226332
Si	0.251816	-0.877093	-1.888834
C	0.804803	-4.471913	-0.469855
H	0.285443	-4.525464	-1.433865
H	1.538514	-5.288632	-0.444001
H	0.060629	-4.656625	0.313092
C	-0.363137	-2.205860	-3.083762

H	-0.683556	-1.740004	-4.025262
H	0.412094	-2.940307	-3.334454
H	-1.225370	-2.745480	-2.677676
H	3.562870	-2.685006	1.405941
H	2.341450	-3.802950	2.019748
C	0.340926	-2.191908	3.316898
H	0.651186	-3.027355	3.955679
H	-0.133293	-1.426365	3.941529
H	-0.392324	-2.553793	2.587938
C	2.940281	-1.189751	3.831115
H	2.626499	-0.336081	4.440871
H	2.977509	-2.082307	4.466072
H	3.951104	-1.000626	3.457485
P	2.825451	1.154012	0.488655
C	3.985790	0.022607	-0.386476
H	4.906329	0.577069	-0.616243
H	4.272393	-0.760760	0.327327
Si	3.376744	-0.855773	-1.971532
C	3.006545	2.672681	-0.543255
H	2.556227	2.558902	-1.529754
H	2.522070	3.520827	-0.052188
H	4.070749	2.902089	-0.672551
C	3.851811	1.734793	1.906438
H	3.992265	0.939720	2.640920
H	4.835230	2.084810	1.572013
H	3.337289	2.561790	2.407495
C	4.780514	-0.714354	-3.226532
H	4.982637	0.334796	-3.478301
H	5.711000	-1.147830	-2.838359
H	4.536450	-1.237537	-4.159338
C	3.040048	-2.657027	-1.539617
H	3.959771	-3.149883	-1.194990
H	2.731770	-3.187446	-2.452525
C	1.794158	-0.114149	-2.688100
H	1.801496	0.975475	-2.569864
H	1.777014	-0.305416	-3.770784
H	-2.284749	-0.923670	1.086435
H	-0.913196	-2.365900	0.342847
C	-2.705013	-1.931715	0.964113
O	-1.650423	-2.849204	0.790856
C	-2.296864	1.787683	0.573298
C	-3.290287	2.432325	-0.174667
C	-2.565506	1.455024	1.902033
C	-4.521497	2.736049	0.394306

H	-3.097811	2.697102	-1.211158
C	-3.801550	1.754123	2.474742
H	-1.809657	0.949853	2.495132
C	-4.780276	2.396290	1.722739
H	-5.282075	3.236474	-0.198127
H	-3.993918	1.486905	3.509695
H	-5.742401	2.631505	2.168385
C	-0.227877	3.041929	-0.826927
C	0.053372	3.325155	-2.163975
C	-0.113584	4.068487	0.119909
C	0.450651	4.605871	-2.547954
H	-0.016822	2.548155	-2.919017
C	0.277289	5.345943	-0.263050
H	-0.328021	3.865557	1.166355
C	0.566864	5.616923	-1.600319
H	0.669123	4.808936	-3.592493
H	0.358751	6.130321	0.483926
H	0.875832	6.614068	-1.900277
C	-3.635755	-1.900361	-0.240010
C	-4.576215	-0.874893	-0.375581
C	-3.562144	-2.882406	-1.226514
C	-5.418501	-0.827067	-1.481928
H	-4.640781	-0.101734	0.385869
C	-4.405656	-2.837581	-2.335256
H	-2.829141	-3.675126	-1.117554
C	-5.333718	-1.808591	-2.468727
H	-6.138655	-0.018584	-1.575609
H	-4.333252	-3.607749	-3.098523
H	-5.988566	-1.771006	-3.334932
C	-3.459803	-2.285839	2.241718
H	-3.869466	-3.299378	2.170321
H	-2.784467	-2.242213	3.102948
H	-4.287233	-1.589169	2.411935

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.188730	-0.362920	0.935540
N	1.248736	-0.884687	-1.002193
C	-1.076359	0.538770	-2.044947
H	-1.579423	-0.388482	-2.329093

H	-1.473119	1.320642	-2.700882
C	3.292115	-1.628393	1.029227
C	-0.629876	-0.230302	2.474769
O	-1.131962	-0.168122	3.533633
P	1.675360	-1.965007	1.846865
P	-1.423965	0.815393	-0.254405
Si	2.955895	-1.374027	-0.819702
Si	0.779539	0.292373	-2.243518
C	3.206083	-2.982057	-1.751902
H	3.062046	-2.832349	-2.829021
H	4.212467	-3.391006	-1.600040
H	2.474248	-3.729651	-1.426507
C	1.170920	-0.339046	-3.974613
H	0.743575	0.325319	-4.736736
H	2.253054	-0.380292	-4.151978
H	0.768568	-1.343382	-4.148528
H	3.709843	-0.706863	1.447904
H	4.023596	-2.426654	1.209053
C	1.604092	-3.798405	1.613552
H	2.607288	-4.222124	1.740206
H	0.952255	-4.249324	2.368206
H	1.197263	-4.033558	0.627477
C	2.017331	-2.013892	3.660388
H	1.146963	-2.465031	4.150080
H	2.892391	-2.638045	3.874608
H	2.163400	-1.030424	4.103155
P	1.585528	1.424255	1.585079
C	3.166771	1.945497	0.736599
H	3.326548	3.005889	0.976642
H	4.000469	1.416087	1.216779
Si	3.369391	1.722962	-1.129990
C	0.777785	3.075727	1.711792
H	0.506348	3.467995	0.729824
H	-0.136118	2.988077	2.304249
H	1.449056	3.792010	2.198454
C	2.255827	1.387470	3.309780
H	3.035364	0.627320	3.406090
H	2.702581	2.355257	3.564141
H	1.456659	1.169580	4.025151
C	4.575284	3.034878	-1.740834
H	4.168364	4.044004	-1.598877
H	5.531475	2.982169	-1.205641
H	4.786381	2.909568	-2.810052
C	4.054306	0.002453	-1.471297

H	5.051399	-0.096619	-1.019397
H	4.192698	-0.118773	-2.555072
C	1.706719	1.906857	-1.988380
H	1.106207	2.609131	-1.397720
H	1.849672	2.373281	-2.973316
H	-0.898642	-1.588212	0.253912
H	0.717749	-1.770963	-1.114541
C	-1.179942	-3.034035	-0.336862
O	-0.085254	-3.438651	-0.824500
C	-3.178381	0.253594	-0.082453
C	-4.114574	0.569721	-1.074365
C	-3.596167	-0.492432	1.019739
C	-5.427966	0.122690	-0.980658
H	-3.814872	1.163660	-1.934051
C	-4.915245	-0.931188	1.122444
H	-2.884226	-0.754585	1.791716
C	-5.831256	-0.633943	0.118697
H	-6.138908	0.366588	-1.764929
H	-5.219535	-1.516574	1.985666
H	-6.856079	-0.986577	0.192031
C	-1.796528	2.627257	-0.159093
C	-1.434277	3.563709	-1.129662
C	-2.452690	3.083282	0.992311
C	-1.693522	4.922236	-0.943702
H	-0.935753	3.250866	-2.041357
C	-2.716114	4.434232	1.178139
H	-2.753794	2.371980	1.757925
C	-2.328854	5.362253	0.211872
H	-1.397469	5.634376	-1.708854
H	-3.222589	4.765195	2.080285
H	-2.529319	6.419606	0.358072
C	-2.327848	-2.795762	-1.365422
C	-3.453577	-3.831919	-1.212062
C	-1.794796	-2.858008	-2.798003
H	-2.780212	-1.820796	-1.182434
H	-3.982462	-3.737402	-0.259633
H	-4.193146	-3.691525	-2.009299
H	-3.068547	-4.856056	-1.294702
H	-0.880854	-2.276407	-2.929906
H	-1.544349	-3.888882	-3.070436
H	-2.548858	-2.491087	-3.505199
C	-1.656456	-3.561804	1.019789
H	-0.897431	-3.411647	1.782957
H	-2.567239	-3.052841	1.344279

H	-1.864879	-4.637031	0.935910

D5S

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.339928	-0.217965	0.911552
N	0.207365	-1.353820	-0.830507
C	0.501917	1.177133	-2.180022
H	-0.536287	1.163872	-2.530635
H	1.058151	1.842763	-2.846483
C	0.034453	-3.630070	1.041197
C	-0.028302	0.697158	2.365827
O	-0.268753	1.258547	3.367578
P	-0.478570	-2.113383	1.918509
P	0.468897	1.700843	-0.423458
Si	0.325483	-3.090488	-0.763700
Si	1.047630	-0.632158	-2.166898
C	-0.963832	-3.976417	-1.817015
H	-0.882274	-3.714137	-2.877965
H	-0.845351	-5.064830	-1.733444
H	-1.980948	-3.721323	-1.496682
C	0.582092	-1.350783	-3.851726
H	0.989966	-0.729527	-4.660263
H	0.966880	-2.366930	-4.002233
H	-0.507578	-1.378884	-3.969334
H	0.968921	-3.994080	1.484205
H	-0.708372	-4.432067	1.134139
C	-2.285115	-2.073931	1.598932
H	-2.784219	-2.981717	1.956764
H	-2.739829	-1.205004	2.085582
H	-2.455949	-1.985989	0.523580
C	-0.441103	-2.539642	3.706672
H	-0.678251	-1.656297	4.308682
H	-1.169934	-3.326632	3.930006
H	0.548711	-2.902493	3.999351
P	2.494369	-0.464519	1.594798
C	3.332323	-1.977481	0.953943
H	4.368601	-1.968799	1.320245
H	2.852315	-2.839092	1.435889
Si	3.345974	-2.323667	-0.924245
C	3.828182	0.781721	1.334120

H	4.002236	0.976663	0.274940
H	3.556953	1.728247	1.808790
H	4.763421	0.421642	1.778337
C	2.726230	-0.675684	3.411716
H	2.100669	-1.487208	3.789549
H	3.772003	-0.894323	3.656386
H	2.428482	0.243494	3.927221
C	5.084778	-2.933216	-1.335438
H	5.835428	-2.163014	-1.116222
H	5.347638	-3.826957	-0.755250
H	5.176305	-3.189695	-2.398071
C	2.061690	-3.653401	-1.286020
H	2.323712	-4.594384	-0.782683
H	2.071090	-3.868767	-2.364618
C	2.924132	-0.809915	-1.969390
H	3.367986	0.091269	-1.529470
H	3.385193	-0.927171	-2.960850
H	-2.359132	0.523629	-0.552558
H	-1.558700	-1.143719	-1.510846
C	-3.436665	1.166706	-2.298549
H	-4.132659	0.752184	-3.036489
H	-3.916269	2.021800	-1.810638
H	-2.550297	1.528742	-2.827725
C	-3.061132	0.089369	-1.281268
O	-2.434608	-0.989135	-1.939080
C	-0.932796	2.905578	-0.366158
C	-1.066293	3.871249	-1.372244
C	-1.867751	2.882972	0.669523
C	-2.113648	4.784607	-1.346062
H	-0.343277	3.909272	-2.183042
C	-2.912953	3.805845	0.704274
H	-1.789414	2.138689	1.453940
C	-3.040714	4.754483	-0.304519
H	-2.205235	5.524991	-2.135500
H	-3.629024	3.777140	1.520915
H	-3.856389	5.471255	-0.280755
C	1.859723	2.883718	-0.224225
C	2.907145	3.005796	-1.138444
C	1.883918	3.664657	0.938465
C	3.961874	3.884964	-0.894334
H	2.922302	2.406272	-2.043581
C	2.930901	4.546751	1.178217
H	1.079173	3.580271	1.664864
C	3.977354	4.656356	0.262659

H	4.770321	3.964947	-1.615502
H	2.932245	5.146858	2.083620
H	4.796892	5.343676	0.450893
C	-4.299090	-0.356186	-0.514367
C	-4.901324	-1.589131	-0.760045
C	-4.855352	0.485877	0.451908
C	-6.033018	-1.977410	-0.044845
H	-4.462482	-2.246364	-1.503947
C	-5.983612	0.100777	1.168687
H	-4.393040	1.450774	0.645370
C	-6.576641	-1.136613	0.922974
H	-6.490723	-2.943062	-0.242603
H	-6.398400	0.765661	1.921610
H	-7.456317	-1.441827	1.482662

G4Ra

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.699110	0.277425	1.394810
N	0.916427	-1.607890	0.027365
C	-1.090741	-0.186156	-1.387902
H	-1.786305	-0.912869	-0.953069
H	-1.557788	0.204279	-2.297465
C	2.943684	-2.197070	2.097602
C	0.405773	1.525804	2.577753
O	0.222733	2.342664	3.400883
P	1.714916	-1.048836	2.878600
P	-0.815236	1.075358	-0.072462
Si	2.293396	-2.673993	0.382912
Si	0.499293	-1.154240	-1.638583
C	1.741547	-4.469629	0.436228
H	1.206161	-4.758636	-0.475789
H	2.608885	-5.134264	0.539162
H	1.082890	-4.660266	1.292147
C	0.158089	-2.688125	-2.672399
H	-0.208324	-2.428067	-3.673557
H	1.060027	-3.298559	-2.806689
H	-0.607047	-3.306059	-2.185602
H	3.883911	-1.642607	1.994946
H	3.152426	-3.075161	2.719396
P	2.652355	1.331341	0.812299

C	4.026648	0.533349	-0.158172
H	4.703366	1.325791	-0.506854
H	4.619846	-0.064748	0.547099
Si	3.605615	-0.607425	-1.607012
C	2.580559	2.961873	-0.047179
H	2.152849	2.864771	-1.048741
H	1.936296	3.636358	0.523737
H	3.577349	3.410976	-0.130625
C	3.644369	1.861739	2.281459
H	3.953888	0.987500	2.864966
H	4.544039	2.414167	1.986029
H	3.034954	2.497904	2.931365
C	4.968193	-0.435994	-2.897977
H	4.971457	0.568619	-3.338830
H	5.957374	-0.606769	-2.454753
H	4.841228	-1.157230	-3.714760
C	3.568057	-2.381688	-0.961549
H	4.563672	-2.653821	-0.584374
H	3.362227	-3.061511	-1.800987
C	1.930646	-0.185724	-2.369981
H	1.766343	0.892384	-2.253843
H	1.967315	-0.381757	-3.450739
H	-0.651553	-0.512955	1.828749
H	0.071450	-1.958088	0.480588
C	-3.576373	-2.444148	-0.016635
C	-2.544247	1.403386	0.504303
C	-3.550941	1.667423	-0.433609
C	-2.875229	1.409561	1.859553
C	-4.858988	1.911293	-0.028372
H	-3.310984	1.691450	-1.493946
C	-4.181177	1.676086	2.270764
H	-2.112646	1.186223	2.596192
C	-5.176573	1.919318	1.329824
H	-5.628090	2.104167	-0.771137
H	-4.418366	1.681802	3.330956
H	-6.195825	2.117975	1.649374
C	-0.590122	2.644479	-1.023800
C	-0.296742	2.703405	-2.388176
C	-0.659257	3.845769	-0.305465
C	-0.057673	3.926746	-3.015611
H	-0.244128	1.794896	-2.980029
C	-0.429998	5.065852	-0.929013
H	-0.886773	3.823515	0.757979
C	-0.119917	5.110112	-2.288277

H	0.172388	3.950307	-4.077375
H	-0.488885	5.985628	-0.353889
H	0.063547	6.062742	-2.776786
C	-4.330235	-1.995284	-1.257396
C	-5.817140	-2.367602	-1.134931
C	-3.743221	-2.535867	-2.557068
H	-4.267800	-0.896695	-1.268975
H	-6.276779	-1.948622	-0.233804
H	-6.374900	-1.987746	-1.997877
H	-5.942389	-3.456851	-1.106120
H	-2.705684	-2.219446	-2.693650
H	-3.755465	-3.630642	-2.569378
H	-4.325931	-2.174051	-3.412358
C	-4.023677	-1.844269	1.294784
H	-3.160324	-1.509334	1.879936
H	-4.680470	-0.984676	1.142338
H	-4.563911	-2.586890	1.896913
H	2.454450	-0.566796	3.986378
H	0.950463	-1.983306	3.616277
N	-2.624009	-3.286909	-0.132978
C	-1.944956	-3.728479	1.073621
H	-1.194306	-4.476153	0.804657
H	-1.443803	-2.898563	1.596326
H	-2.635796	-4.187381	1.795191

TSG4-5R

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.382239	-0.057432	1.153623
N	1.205526	-1.241420	-0.606675
C	-0.809364	0.348878	-1.976271
H	-1.461620	-0.528277	-2.064638
H	-1.083738	1.031749	-2.786484
C	2.977950	-2.437141	1.403143
C	-0.396563	0.499310	2.621193
O	-0.893135	0.813871	3.634042
P	1.770785	-1.409734	2.366020
P	-1.084647	1.016798	-0.288303
Si	2.732068	-2.157932	-0.452921
Si	0.953586	-0.299636	-2.085796
C	2.586005	-3.791969	-1.365229

H	2.698700	-3.654597	-2.447027
H	3.356365	-4.503140	-1.041745
H	1.601284	-4.232345	-1.174678
C	1.111314	-1.366111	-3.629581
H	0.764768	-0.821704	-4.517291
H	2.150613	-1.663294	-3.816208
H	0.511521	-2.280020	-3.545504
H	3.999953	-2.192763	1.712399
H	2.820936	-3.494121	1.638545
P	2.000081	1.618597	1.337247
C	3.679476	1.173873	0.719513
H	4.371085	1.999900	0.935335
H	4.040797	0.316291	1.302645
Si	3.821703	0.707832	-1.121811
C	1.921704	3.353585	0.704736
H	1.747457	3.408157	-0.369879
H	1.112437	3.895604	1.198371
H	2.866884	3.860575	0.930709
C	2.358032	2.082120	3.090482
H	2.591202	1.212989	3.709952
H	3.198657	2.783039	3.144275
H	1.473770	2.566868	3.517584
C	5.260315	1.687966	-1.841612
H	5.062647	2.766548	-1.793310
H	6.190864	1.497215	-1.292608
H	5.436815	1.431536	-2.893406
C	4.137116	-1.142295	-1.191633
H	5.076288	-1.386160	-0.676275
H	4.273734	-1.446519	-2.239186
C	2.263708	1.051506	-2.139620
H	1.831576	2.016334	-1.853943
H	2.580617	1.166993	-3.186773
H	-0.761081	-1.474693	1.060650
H	0.526809	-2.021544	-0.467196
C	-1.202291	-2.746481	0.931833
C	-2.912004	0.925349	-0.059960
C	-3.770744	1.124085	-1.145515
C	-3.461505	0.775615	1.214393
C	-5.147808	1.169752	-0.961074
H	-3.364090	1.245470	-2.145402
C	-4.840821	0.831435	1.402884
H	-2.814557	0.608306	2.067762
C	-5.687257	1.027196	0.315969
H	-5.801683	1.317812	-1.815775

H	-5.252559	0.713486	2.401274
H	-6.762910	1.069024	0.461842
C	-1.010141	2.849774	-0.492048
C	-0.590135	3.494851	-1.655907
C	-1.409914	3.632086	0.599345
C	-0.553350	4.887699	-1.724881
H	-0.273212	2.922556	-2.522023
C	-1.385628	5.019590	0.528888
H	-1.740217	3.151282	1.516935
C	-0.948659	5.653449	-0.633931
H	-0.215802	5.370883	-2.637436
H	-1.702650	5.608061	1.385176
H	-0.923354	6.737851	-0.689382
C	-2.294034	-2.573411	-0.134071
C	-1.993549	-2.841694	-1.475414
C	-3.621435	-2.275620	0.182622
C	-2.966489	-2.766918	-2.466389
H	-0.983643	-3.151783	-1.721291
C	-4.607124	-2.227551	-0.801708
H	-3.910723	-2.083156	1.208724
C	-4.284496	-2.458334	-2.133902
H	-2.698296	-2.972783	-3.499823
H	-5.630666	-1.998902	-0.519581
H	-5.051663	-2.415274	-2.902028
C	-1.767717	-2.915157	2.343988
H	-2.361240	-3.835500	2.411819
H	-0.961699	-2.975256	3.078776
H	-2.396074	-2.068261	2.631281
H	1.199668	-2.356268	3.238011
H	2.633402	-0.845807	3.332117
N	-0.221070	-3.575863	0.484945
C	0.335398	-4.542569	1.396617
H	1.159259	-5.071134	0.897858
H	0.747764	-4.162542	2.350535
H	-0.392713	-5.322677	1.687292

TSD4-5Sa

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.119183	-0.494432	0.769744
N	1.384869	-0.556856	-1.121476

C	-0.957907	0.803625	-2.118896
H	-1.285513	-0.151957	-2.538097
H	-1.411778	1.593028	-2.726260
C	3.336145	-1.485440	0.901721
C	-0.816302	-0.749923	2.223492
O	-1.397256	-0.968817	3.220204
P	1.696411	-2.133379	1.433906
P	-1.474808	0.808102	-0.352017
Si	3.116610	-0.928149	-0.896878
Si	0.918418	0.781393	-2.183442
C	3.598567	-2.300511	-2.084065
H	3.592463	-1.932507	-3.117458
H	4.604232	-2.683764	-1.872099
H	2.892418	-3.136124	-2.033484
C	1.469726	0.452124	-3.952263
H	1.050514	1.191172	-4.647133
H	2.561042	0.488824	-4.059097
H	1.135971	-0.540018	-4.279958
H	3.605961	-0.625425	1.521309
H	4.134098	-2.230460	1.011023
C	1.860264	-3.829778	0.703050
H	2.908585	-4.146509	0.745878
H	1.273021	-4.554592	1.274027
H	1.504148	-3.831754	-0.329926
C	1.881489	-2.629348	3.200098
H	1.004984	-3.228352	3.472685
H	2.777884	-3.242809	3.345328
H	1.915398	-1.777604	3.879913
P	1.312641	1.220119	1.845668
C	2.901588	2.009622	1.252473
H	2.956850	3.006604	1.711077
H	3.742377	1.453191	1.686833
Si	3.263656	2.185233	-0.596046
C	0.382609	2.765505	2.227213
H	0.162194	3.334117	1.320979
H	-0.564857	2.516494	2.711337
H	0.966020	3.402163	2.902155
C	1.851110	0.857759	3.578274
H	2.657573	0.120115	3.585268
H	2.222313	1.765574	4.067212
H	1.009834	0.463212	4.156926
C	4.386145	3.682044	-0.818145
H	3.892572	4.602777	-0.482969
H	5.314512	3.573557	-0.243700

H	4.662573	3.819360	-1.870789
C	4.125742	0.625273	-1.200036
H	5.100319	0.514757	-0.704597
H	4.332476	0.728380	-2.274878
C	1.672436	2.392424	-1.575983
H	0.960161	2.939837	-0.947887
H	1.862679	3.026992	-2.453077
H	-0.846087	-1.649840	-0.121165
H	0.924225	-1.427534	-1.457209
C	-2.206654	-2.581180	-1.972982
H	-2.602861	-3.510323	-2.406898
H	-3.003782	-2.114619	-1.396952
H	-1.918825	-1.940562	-2.808627
C	-0.982785	-2.963585	-1.150009
O	0.116554	-3.026377	-1.763083
C	-3.225401	0.218798	-0.413666
C	-4.014373	0.439597	-1.547964
C	-3.805460	-0.403771	0.692744
C	-5.339238	0.018841	-1.586732
H	-3.592812	0.934203	-2.417848
C	-5.136084	-0.817954	0.660318
H	-3.217195	-0.580399	1.585937
C	-5.903983	-0.615536	-0.481872
H	-5.931251	0.187586	-2.481888
H	-5.565873	-1.308447	1.528994
H	-6.937898	-0.947386	-0.512309
C	-1.917594	2.587622	-0.052521
C	-1.560994	3.644318	-0.893292
C	-2.653918	2.884474	1.102526
C	-1.899077	4.960469	-0.574871
H	-1.012930	3.461642	-1.811463
C	-2.998481	4.191896	1.419504
H	-2.955958	2.081508	1.770615
C	-2.613248	5.239993	0.584206
H	-1.604893	5.764850	-1.243398
H	-3.565296	4.394684	2.323771
H	-2.876243	6.264207	0.832052
C	-2.644434	-3.782460	0.650631
C	-1.285212	-3.971883	-0.014880
H	-2.750243	-2.760196	1.021460
H	-3.477621	-3.990990	-0.030660
H	-2.740530	-4.463255	1.505247
C	-1.121807	-5.393934	-0.563912
H	-0.535321	-3.811066	0.755230

H	-0.134150	-5.529151	-1.014883
H	-1.239981	-6.131396	0.239349
H	-1.876000	-5.617244	-1.329313

TSG4-5Ra

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.109619	-0.114100	0.985447
N	1.373876	-0.884057	-0.726703
C	-0.764569	0.523004	-2.243962
H	-1.277674	-0.307248	-2.737488
H	-0.940787	1.398518	-2.876156
C	3.199129	-1.773387	1.418275
C	-0.926174	0.106155	2.382249
O	-1.590041	0.199665	3.342376
P	1.700093	-1.132144	2.290977
P	-1.435240	0.693337	-0.532727
Si	3.051857	-1.446795	-0.437254
Si	1.079236	0.117953	-2.163236
C	3.361933	-3.008863	-1.426212
H	3.524270	-2.795376	-2.489110
H	4.244859	-3.546254	-1.058234
H	2.484206	-3.658402	-1.329875
C	1.535988	-0.802143	-3.739090
H	1.200648	-0.249364	-4.626112
H	2.618773	-0.946774	-3.835268
H	1.063792	-1.791599	-3.764274
H	4.101144	-1.311912	1.834430
H	3.280674	-2.849283	1.597790
P	1.203459	1.903261	1.400022
C	3.010571	1.913237	1.023508
H	3.438640	2.863809	1.370470
H	3.490941	1.130351	1.625119
Si	3.526785	1.637007	-0.789869
C	0.776234	3.590242	0.773919
H	0.730524	3.640416	-0.314020
H	-0.196178	3.901127	1.162873
H	1.531210	4.305001	1.121807
C	1.182115	2.353416	3.191106
H	1.508255	1.524260	3.823774
H	1.821540	3.220832	3.390069

H	0.154619	2.603589	3.476168
C	4.789971	2.968304	-1.213387
H	4.340207	3.968269	-1.166156
H	5.631954	2.952328	-0.510176
H	5.197531	2.833570	-2.222686
C	4.255511	-0.086530	-0.941626
H	5.171934	-0.178423	-0.342867
H	4.554325	-0.246473	-1.987681
C	2.104177	1.691767	-2.030061
H	1.451807	2.554036	-1.855364
H	2.560280	1.860176	-3.017401
H	-0.611513	-1.808698	0.715604
H	0.889299	-1.804966	-0.719899
C	-0.671869	-3.105896	0.628088
C	-3.116651	-0.061615	-0.629014
C	-3.830951	-0.125494	-1.828313
C	-3.718002	-0.542445	0.538076
C	-5.105445	-0.684632	-1.866434
H	-3.397077	0.262868	-2.745547
C	-4.998614	-1.086765	0.504800
H	-3.175391	-0.519867	1.476747
C	-5.691169	-1.169416	-0.699914
H	-5.640753	-0.739870	-2.810019
H	-5.444989	-1.465940	1.419434
H	-6.683000	-1.610877	-0.730620
C	-1.983300	2.449381	-0.369869
C	-1.820260	3.435716	-1.342504
C	-2.601103	2.799099	0.838739
C	-2.250244	4.742182	-1.111463
H	-1.339484	3.212361	-2.289458
C	-3.040168	4.097568	1.067150
H	-2.733793	2.051289	1.615504
C	-2.860030	5.077981	0.091951
H	-2.106958	5.497474	-1.879080
H	-3.519210	4.344781	2.010087
H	-3.195566	6.095384	0.270080
C	-1.792464	-3.280372	-0.438919
C	-2.371021	-4.699814	-0.373093
C	-1.289386	-3.018862	-1.851919
H	-2.596041	-2.574679	-0.214959
H	-2.917824	-4.885989	0.557202
H	-3.072623	-4.863983	-1.200310
H	-1.568640	-5.442878	-0.457068
H	-0.797689	-2.048256	-1.915627

H	-0.554568	-3.775610	-2.141765
H	-2.116890	-3.022347	-2.572213
C	-1.219928	-3.429911	2.025337
H	-0.561766	-3.070672	2.819465
H	-2.198649	-2.957924	2.169490
H	-1.336208	-4.511218	2.158968
H	1.334652	-2.229479	3.092054
H	2.302229	-0.396793	3.336717
N	0.525349	-3.628740	0.213692
C	1.237467	-4.493559	1.117422
H	2.226896	-4.723423	0.695397
H	1.423260	-4.116222	2.144193
H	0.744626	-5.476097	1.263758

TSG4-5Sa

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.083804	0.227460	0.959037
N	-1.402969	0.750267	-0.813296
C	0.763659	-0.507246	-2.237887
H	1.088470	0.460438	-2.636767
H	1.133356	-1.269039	-2.930948
C	-3.082750	2.004425	1.210277
C	1.016404	0.155178	2.315424
O	1.733559	0.134217	3.243667
P	-1.688601	1.285442	2.190192
P	1.451150	-0.622004	-0.535622
Si	-3.081015	1.272793	-0.531975
Si	-1.113067	-0.398334	-2.123574
C	-3.572069	2.640976	-1.719057
H	-3.597941	2.305904	-2.762005
H	-4.568388	3.029217	-1.470113
H	-2.846940	3.458537	-1.635562
C	-1.768913	0.203001	-3.783582
H	-1.424949	-0.456901	-4.590826
H	-2.865558	0.203765	-3.812514
H	-1.425022	1.217380	-4.014388
H	-4.037458	1.894878	1.735240
H	-2.903745	3.079349	1.092259
P	-1.051820	-1.777675	1.657919
C	-2.856674	-1.975349	1.323393

H	-3.197157	-2.925306	1.757421
H	-3.394819	-1.185106	1.863921
Si	-3.402536	-1.878423	-0.493989
C	-0.515333	-3.508261	1.286604
H	-0.558414	-3.746902	0.223804
H	0.511409	-3.668013	1.622927
H	-1.168361	-4.206350	1.823291
C	-0.994685	-1.968477	3.497588
H	-1.335113	-1.069647	4.017191
H	-1.609930	-2.814992	3.823277
H	0.040660	-2.155129	3.801054
C	-4.627839	-3.277333	-0.799507
H	-4.148235	-4.257138	-0.679257
H	-5.468021	-3.231229	-0.095534
H	-5.041485	-3.232476	-1.814471
C	-4.229468	-0.206879	-0.740536
H	-5.083657	-0.113057	-0.055711
H	-4.648976	-0.163383	-1.756483
C	-1.971763	-2.022181	-1.724024
H	-1.245948	-2.764252	-1.375220
H	-2.381467	-2.420469	-2.663609
H	0.555392	1.845648	0.494592
H	-0.929552	1.685822	-0.991715
C	2.086649	3.334565	-0.395628
H	2.309882	4.358911	-0.723174
H	2.693437	3.115459	0.483802
H	2.402259	2.657480	-1.191009
C	0.597813	3.219407	-0.101361
C	3.136186	0.116158	-0.697190
C	3.819728	0.106186	-1.917736
C	3.777744	0.643961	0.425985
C	5.105174	0.630624	-2.017145
H	3.350463	-0.312617	-2.803328
C	5.069555	1.154995	0.331742
H	3.261171	0.681399	1.378376
C	5.733639	1.157469	-0.891223
H	5.617164	0.624139	-2.975281
H	5.549118	1.566995	1.215062
H	6.736673	1.567261	-0.967939
C	1.995858	-2.378174	-0.377212
C	1.667978	-3.389091	-1.281534
C	2.769984	-2.708356	0.743123
C	2.094848	-4.700072	-1.069732
H	1.060270	-3.175265	-2.155215

C	3.205364	-4.011623	0.950696
H	3.029143	-1.939905	1.466849
C	2.863256	-5.015660	0.045128
H	1.823226	-5.474430	-1.781699
H	3.807044	-4.245534	1.824256
H	3.197352	-6.036098	0.208261
C	0.999930	3.778613	2.398396
C	0.156550	4.012571	1.147797
H	1.167145	2.713297	2.578946
H	1.978963	4.266268	2.316794
H	0.504145	4.200720	3.281139
C	0.106650	5.508256	0.808890
H	-0.874569	3.708349	1.345934
H	-0.519775	5.674750	-0.072370
H	-0.307009	6.079582	1.649105
H	1.106897	5.909065	0.602811
H	-1.358491	2.339541	3.070828
H	-2.434781	0.554094	3.145598
N	-0.292911	3.290908	-1.103406
C	0.198458	3.265275	-2.461426
H	0.804347	2.382055	-2.735101
H	-0.659628	3.284325	-3.145876
H	0.821294	4.141477	-2.710375

D4Ra

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.472237	-0.045548	1.156717
N	0.827560	-1.410117	-0.706080
C	-1.000417	0.437961	-1.828548
H	-1.730748	-0.375966	-1.772456
H	-1.340656	1.133315	-2.601808
C	2.649891	-2.638717	1.275108
C	0.032504	0.781771	2.623304
O	-0.270928	1.313817	3.627964
P	1.261573	-1.865514	2.219133
P	-0.919555	1.162689	-0.132967
Si	2.184313	-2.547940	-0.557626
Si	0.616557	-0.439111	-2.175344
C	1.628712	-4.245568	-1.145406
H	1.258305	-4.203209	-2.176835

H	2.449061	-4.973378	-1.112383
H	0.815315	-4.634721	-0.520511
C	0.412846	-1.538242	-3.691290
H	0.139131	-0.945395	-4.573827
H	1.332721	-2.082649	-3.938802
H	-0.384226	-2.272842	-3.526013
H	3.552885	-2.043890	1.459712
H	2.859967	-3.666666	1.598790
C	0.091191	-3.290232	2.299695
H	0.580981	-4.213785	2.632183
H	-0.714454	-3.042655	2.998166
H	-0.366357	-3.453089	1.319142
C	1.845676	-1.895237	3.966922
H	1.027771	-1.570513	4.619680
H	2.157278	-2.902013	4.268654
H	2.681145	-1.207436	4.117671
P	2.446392	1.110406	1.115801
C	3.941545	0.643152	0.101739
H	4.629972	1.499826	0.082355
H	4.473471	-0.147491	0.649277
Si	3.689157	0.005785	-1.659085
C	2.401010	2.923461	0.760105
H	2.080738	3.125214	-0.265300
H	1.677418	3.398369	1.429414
H	3.383694	3.384326	0.917404
C	3.296977	1.219515	2.757853
H	3.716696	0.245372	3.026152
H	4.116601	1.947608	2.737832
H	2.582401	1.512129	3.533346
C	5.174101	0.524917	-2.698237
H	5.236787	1.616832	-2.785490
H	6.113800	0.172093	-2.255279
H	5.111322	0.113951	-3.713594
C	3.592174	-1.879420	-1.604788
H	4.543544	-2.282167	-1.229813
H	3.483642	-2.258736	-2.631628
C	2.100490	0.681918	-2.418940
H	1.906253	1.673455	-1.993258
H	2.249404	0.828619	-3.497759
H	-0.882714	-0.884838	1.207537
H	-0.064880	-1.884748	-0.528686
C	-3.170983	-2.437813	-0.384053
O	-2.109428	-2.554567	-0.976744
C	-2.724117	1.208009	0.300850

C	-3.649479	1.730438	-0.612722
C	-3.195801	0.713914	1.517331
C	-5.010631	1.734680	-0.328762
H	-3.302205	2.143549	-1.556550
C	-4.559290	0.729208	1.812569
H	-2.489014	0.304441	2.229939
C	-5.470591	1.231335	0.888591
H	-5.713597	2.134500	-1.054335
H	-4.906512	0.342162	2.766816
H	-6.533389	1.237674	1.114573
C	-0.702916	2.969530	-0.459356
C	-0.246991	3.499363	-1.668872
C	-0.930076	3.848273	0.608261
C	-0.011898	4.867786	-1.806282
H	-0.056939	2.849784	-2.518146
C	-0.704761	5.212676	0.471855
H	-1.280319	3.456198	1.560430
C	-0.237173	5.727816	-0.737007
H	0.348566	5.259002	-2.753878
H	-0.889522	5.876287	1.311965
H	-0.055185	6.793242	-0.844266
C	-4.458175	-2.049863	-1.094548
C	-5.413260	-3.257688	-1.067960
C	-4.233346	-1.553589	-2.517569
H	-4.909304	-1.247566	-0.493873
H	-5.592491	-3.624215	-0.051839
H	-6.380873	-2.978743	-1.497364
H	-5.006744	-4.085199	-1.661363
H	-3.670962	-0.615911	-2.530994
H	-3.680869	-2.289917	-3.110375
H	-5.195603	-1.369371	-3.007932
C	-3.256116	-2.712616	1.097513
H	-2.483616	-2.111208	1.587792
H	-4.234573	-2.471686	1.519758
H	-3.032201	-3.768872	1.285805

G4Sa

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.273516	-0.043434	1.116091
N	0.014042	-1.492452	-0.686696

C	-0.049453	0.954590	-2.128837
H	-1.095921	0.824084	-2.423443
H	0.379674	1.654486	-2.851851
C	-0.078906	-3.457106	1.493476
C	0.003048	1.017413	2.470574
O	-0.269913	1.698217	3.388025
P	0.111552	-1.842991	2.400391
P	-0.076582	1.588445	-0.385159
Si	0.283623	-3.205934	-0.343812
Si	0.707086	-0.765617	-2.139028
C	-0.937545	-4.247640	-1.327960
H	-0.686022	-4.278031	-2.394364
H	-0.972994	-5.281931	-0.963075
H	-1.944987	-3.820888	-1.241093
C	0.136761	-1.675209	-3.689804
H	0.351914	-1.092260	-4.594806
H	0.640822	-2.643623	-3.800796
H	-0.943069	-1.865078	-3.661289
H	0.561619	-4.227370	1.937476
H	-1.110084	-3.812576	1.604249
P	2.538501	0.018760	1.363192
C	3.497059	-1.496577	0.897230
H	4.567135	-1.332189	1.086664
H	3.184512	-2.295873	1.585030
Si	3.256617	-2.152677	-0.863499
C	3.682443	1.323340	0.717915
H	3.673483	1.382951	-0.371740
H	3.370826	2.299875	1.101274
H	4.710776	1.129450	1.046406
C	3.038470	0.183316	3.136744
H	2.550048	-0.575914	3.754319
H	4.123993	0.093001	3.261972
H	2.723695	1.165352	3.505490
C	4.932504	-2.751938	-1.488149
H	5.649596	-1.923606	-1.551017
H	5.359445	-3.507614	-0.816784
H	4.854374	-3.200344	-2.486303
C	2.058974	-3.612408	-0.815639
H	2.460165	-4.381497	-0.140991
H	2.044095	-4.069220	-1.816580
C	2.580770	-0.851273	-2.060863
H	3.003477	0.129843	-1.818649
H	2.945881	-1.099119	-3.067812
H	-1.304367	-0.209802	1.077164

H	-1.003588	-1.320992	-0.706904
C	-5.358038	-0.608187	-0.290036
H	-5.937995	-0.841273	0.605172
H	-5.291411	0.482571	-0.382927
H	-5.920620	-0.973393	-1.157902
C	-3.974670	-1.213406	-0.251843
C	-1.685978	2.505301	-0.390923
C	-1.948635	3.471265	-1.371334
C	-2.674469	2.216826	0.549307
C	-3.177616	4.120043	-1.419618
H	-1.183565	3.718919	-2.103576
C	-3.904232	2.874784	0.511119
H	-2.473284	1.463204	1.302346
C	-4.161079	3.821301	-0.476164
H	-3.367470	4.863228	-2.189113
H	-4.660594	2.643918	1.256541
H	-5.120087	4.330902	-0.509582
C	1.071755	3.033035	-0.415905
C	2.002728	3.278605	-1.426607
C	1.062847	3.879209	0.701754
C	2.904772	4.337553	-1.326657
H	2.057502	2.630787	-2.296262
C	1.956175	4.939502	0.801041
H	0.355056	3.700539	1.507066
C	2.885374	5.170455	-0.213631
H	3.626339	4.505781	-2.121436
H	1.930909	5.584369	1.674871
H	3.588311	5.994734	-0.134403
C	-3.811785	-1.383510	2.282602
C	-3.602915	-2.079649	0.934595
H	-3.237751	-0.453917	2.335761
H	-4.867567	-1.159725	2.475928
H	-3.466221	-2.035933	3.093022
C	-4.366798	-3.409299	0.872085
H	-2.534226	-2.280486	0.825059
H	-4.181157	-3.933942	-0.071872
H	-4.057105	-4.066409	1.693207
H	-5.449199	-3.255532	0.965901
H	-0.954142	-1.922204	3.327830
H	1.111764	-2.238131	3.334415
N	-3.112506	-1.068916	-1.184558
C	-3.482214	-0.276559	-2.345412
H	-3.498825	0.794522	-2.099448
H	-2.745454	-0.431157	-3.139096

H	-4.467791	-0.539479	-2.753725

G5Sa

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.619372	0.048549	1.248662
N	0.528148	-1.458224	-0.127599
C	-0.835866	0.467045	-1.795364
H	-1.818683	-0.005565	-1.684691
H	-0.877295	1.084624	-2.698094
C	1.924282	-3.041874	1.919818
C	0.302731	1.183187	2.561836
O	0.117942	1.926890	3.447564
P	1.125304	-1.605967	2.729773
P	-0.534391	1.407287	-0.246983
Si	1.353533	-2.959614	0.099068
Si	0.441615	-0.926528	-1.767765
C	0.300853	-4.496930	-0.206805
H	-0.139269	-4.508671	-1.210181
H	0.900787	-5.410132	-0.098250
H	-0.520962	-4.554082	0.517094
C	-0.128179	-2.236919	-3.012181
H	-0.357125	-1.769272	-3.979133
H	0.639035	-2.998478	-3.200195
H	-1.030600	-2.762047	-2.676444
H	3.009496	-2.900784	1.977161
H	1.690263	-3.991728	2.411389
P	2.761539	0.775901	1.074716
C	3.940088	-0.399489	0.270478
H	4.896974	0.126346	0.143338
H	4.139292	-1.200064	0.995804
Si	3.493379	-1.251951	-1.379679
C	3.235426	2.348531	0.243078
H	2.997168	2.324588	-0.822499
H	2.693675	3.186245	0.690585
H	4.311744	2.523670	0.355494
C	3.611917	1.064133	2.686130
H	3.545395	0.173971	3.319626
H	4.669944	1.311400	2.543174
H	3.123971	1.889053	3.215896
C	5.091048	-1.303857	-2.386043

H	5.441472	-0.292505	-2.629195
H	5.895799	-1.811977	-1.839495
H	4.946670	-1.838746	-3.333019
C	2.898720	-3.004442	-1.006321
H	3.701208	-3.588547	-0.534256
H	2.670907	-3.510057	-1.956167
C	2.149890	-0.334437	-2.339392
H	2.266497	0.744580	-2.175373
H	2.282163	-0.506296	-3.417000
H	-3.345699	-0.631639	-0.117954
C	-5.249798	-1.520367	0.233255
H	-5.865478	-2.357113	-0.114932
H	-5.193674	-1.558997	1.325931
H	-5.762335	-0.588446	-0.026094
C	-3.855428	-1.572812	-0.389895
C	-2.233673	1.901144	0.265923
C	-3.024713	2.695192	-0.573909
C	-2.789802	1.405357	1.445927
C	-4.344844	2.978337	-0.242287
H	-2.604533	3.093998	-1.493996
C	-4.113445	1.688041	1.780582
H	-2.190886	0.783902	2.104089
C	-4.892832	2.471422	0.936583
H	-4.948789	3.594138	-0.902525
H	-4.533680	1.288123	2.698754
H	-5.925776	2.688486	1.193006
C	0.147145	3.028590	-0.762780
C	0.729126	3.254271	-2.011629
C	0.149305	4.063912	0.180889
C	1.313016	4.485489	-2.308017
H	0.748243	2.469187	-2.761474
C	0.724742	5.293546	-0.117322
H	-0.299145	3.905773	1.158410
C	1.315206	5.505725	-1.362826
H	1.768096	4.642835	-3.281748
H	0.716788	6.085382	0.626040
H	1.772034	6.463573	-1.593808
C	-2.543569	-2.475339	1.590018
C	-2.977912	-2.722443	0.146041
H	-2.001654	-1.526971	1.676204
H	-3.394909	-2.451335	2.281339
H	-1.870673	-3.271223	1.930823
C	-3.625917	-4.098094	-0.016640
H	-2.056418	-2.706719	-0.454202

H	-3.999184	-4.238228	-1.036125
H	-2.902377	-4.894174	0.195747
H	-4.468532	-4.226830	0.674198
H	-0.029695	-2.196744	3.289838
H	1.828873	-1.441225	3.945266
N	-3.958653	-1.690248	-1.848069
H	-3.020577	-1.815319	-2.219503
C	-4.558887	-0.534847	-2.497424
H	-4.382193	-0.597435	-3.576079
H	-5.643353	-0.528497	-2.343839
H	-4.165233	0.432980	-2.135959

D4Sa

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.197442	-0.146236	1.072569
N	0.603322	-1.414093	-0.847961
C	-0.617889	0.872108	-1.998878
H	-1.504142	0.235245	-2.101377
H	-0.699658	1.663711	-2.750300
C	1.740880	-3.154126	1.242045
C	-0.308438	0.600373	2.561643
O	-0.666926	1.059263	3.583842
P	0.360137	-2.188025	2.004098
P	-0.622426	1.473435	-0.251679
Si	1.660611	-2.825996	-0.622525
Si	0.836079	-0.298884	-2.203406
C	0.901178	-4.316075	-1.480898
H	0.748808	-4.123392	-2.549366
H	1.545558	-5.199111	-1.384853
H	-0.075457	-4.566844	-1.050842
C	0.700959	-1.186951	-3.858185
H	0.720462	-0.471843	-4.690732
H	1.525799	-1.893347	-4.015643
H	-0.239879	-1.746205	-3.918860
H	2.684192	-2.773717	1.652887
H	1.686288	-4.225821	1.474586
C	-1.054746	-3.315813	1.657709
H	-0.851230	-4.351082	1.958393
H	-1.936111	-2.949840	2.193540
H	-1.286236	-3.288233	0.589533

C	0.529826	-2.494621	3.812233
H	-0.339579	-2.065501	4.322460
H	0.575798	-3.566350	4.036740
H	1.421963	-2.009738	4.215306
P	2.348250	0.509889	1.499218
C	3.871038	-0.177710	0.670215
H	4.707895	0.505346	0.871248
H	4.128131	-1.115487	1.181516
Si	3.803857	-0.574111	-1.175809
C	2.753684	2.309071	1.397110
H	2.686174	2.682338	0.371705
H	2.034836	2.870405	2.000466
H	3.763068	2.506882	1.777400
C	2.895397	0.247918	3.248507
H	3.004994	-0.822582	3.446949
H	3.862044	0.728124	3.441912
H	2.153115	0.652669	3.943681
C	5.514018	-0.281625	-1.914312
H	5.788371	0.779728	-1.864352
H	6.285523	-0.849539	-1.379450
H	5.549560	-0.583669	-2.968386
C	3.335466	-2.394152	-1.354719
H	4.110642	-3.015315	-0.884748
H	3.332844	-2.660598	-2.421885
C	2.531578	0.493643	-2.072446
H	2.468270	1.458307	-1.555570
H	2.892421	0.705293	-3.088708
H	-1.312794	-0.622283	0.762847
H	-0.372996	-1.722102	-0.883903
C	-4.003602	-0.801695	-1.939869
H	-5.084527	-0.928697	-2.047962
H	-3.841077	0.045239	-1.261188
H	-3.560480	-0.563268	-2.909173
C	-3.336027	-2.018212	-1.347658
O	-2.215891	-2.355525	-1.699958
C	-2.393331	1.986782	-0.052860
C	-2.986957	2.823252	-1.007527
C	-3.171297	1.534475	1.013497
C	-4.328577	3.176012	-0.913030
H	-2.394054	3.205177	-1.834952
C	-4.513940	1.898709	1.119752
H	-2.727390	0.877083	1.751852
C	-5.098022	2.711773	0.153644
H	-4.773183	3.818074	-1.668409

H	-5.102465	1.537249	1.958583
H	-6.146075	2.987424	0.231864
C	0.088094	3.177321	-0.400801
C	0.820734	3.635604	-1.498357
C	-0.060878	4.031781	0.700177
C	1.407422	4.901860	-1.488863
H	0.953029	3.008883	-2.375001
C	0.513889	5.296612	0.709387
H	-0.626645	3.695927	1.566581
C	1.259630	5.734321	-0.385086
H	1.978257	5.235238	-2.351381
H	0.385612	5.940872	1.574704
H	1.717275	6.719315	-0.377117
C	-4.468927	-1.893664	0.891912
C	-4.093395	-2.800456	-0.285874
H	-3.585293	-1.384717	1.290436
H	-5.196958	-1.130882	0.593137
H	-4.918192	-2.491428	1.693019
C	-5.326737	-3.490596	-0.885903
H	-3.402713	-3.573402	0.063956
H	-5.063319	-4.107885	-1.752185
H	-5.784114	-4.144424	-0.135545
H	-6.086369	-2.765700	-1.198585

G5Ra

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.431562	-0.022135	1.196148
N	0.521766	-1.467499	-0.263749
C	-0.669242	0.514065	-1.956043
H	-1.610230	-0.054328	-1.924163
H	-0.695687	1.153196	-2.843907
C	1.649536	-3.161343	1.865294
C	-0.065746	1.014398	2.532875
O	-0.368675	1.677150	3.449928
P	0.813589	-1.728968	2.650075
P	-0.541849	1.414906	-0.370798
Si	1.348194	-2.964357	-0.010165
Si	0.667437	-0.818204	-1.863910
C	0.384833	-4.488769	-0.574689
H	0.148852	-4.449893	-1.644571

H	0.968036	-5.402821	-0.401671
H	-0.560728	-4.592259	-0.027843
C	0.325129	-2.031233	-3.276081
H	0.364911	-1.499844	-4.236283
H	1.058687	-2.844791	-3.329147
H	-0.674060	-2.473180	-3.191518
H	2.722267	-3.092688	2.078721
H	1.299182	-4.118767	2.264717
P	2.567648	0.743962	1.353547
C	3.848629	-0.403550	0.679490
H	4.820437	0.106336	0.738699
H	3.914854	-1.250391	1.375784
Si	3.645270	-1.145349	-1.068896
C	3.148251	2.349972	0.663753
H	2.983686	2.417066	-0.413178
H	2.602429	3.171789	1.134710
H	4.218155	2.479469	0.863560
C	3.189944	0.975365	3.076141
H	3.097392	0.049297	3.651594
H	4.242395	1.281372	3.080539
H	2.596509	1.744868	3.581141
C	5.361918	-1.132832	-1.856467
H	5.737072	-0.110544	-1.993006
H	6.089481	-1.674835	-1.239001
H	5.344509	-1.613670	-2.842389
C	3.033492	-2.921358	-0.886513
H	3.773456	-3.528583	-0.346592
H	2.944281	-3.367047	-1.888149
C	2.429779	-0.173081	-2.137598
H	2.512469	0.893387	-1.896138
H	2.712653	-0.274100	-3.194904
H	-2.497350	-0.980830	0.393545
C	-3.072644	-1.893293	0.183386
C	-2.261151	2.002518	-0.057215
C	-2.896343	2.823241	-0.998859
C	-2.968064	1.613569	1.081041
C	-4.208665	3.237076	-0.808220
H	-2.358374	3.142640	-1.887790
C	-4.283716	2.033576	1.277409
H	-2.496256	0.971747	1.817988
C	-4.906526	2.841993	0.333151
H	-4.688805	3.869780	-1.549121
H	-4.819249	1.722748	2.169792
H	-5.932584	3.165070	0.483410

C	0.250341	3.020506	-0.771949
C	0.933014	3.265587	-1.964841
C	0.196819	4.031404	0.196159
C	1.564105	4.490800	-2.180147
H	0.989247	2.500962	-2.733273
C	0.818320	5.255038	-0.021551
H	-0.331984	3.857670	1.130160
C	1.510346	5.485951	-1.210137
H	2.094243	4.664738	-3.112245
H	0.766408	6.028681	0.739055
H	2.000761	6.440237	-1.378821
C	-4.545892	-1.433377	0.068543
C	-5.598176	-2.542914	0.196037
C	-4.773004	-0.603224	-1.194455
H	-4.700876	-0.765395	0.927907
H	-5.521903	-3.071929	1.152012
H	-6.603531	-2.107621	0.145365
H	-5.526080	-3.286663	-0.604399
H	-4.031304	0.197113	-1.281083
H	-4.697016	-1.220939	-2.096098
H	-5.766652	-0.140024	-1.179652
C	-2.838753	-2.835546	1.371700
H	-3.198432	-2.385177	2.305518
H	-3.342135	-3.800824	1.253670
H	-1.766584	-3.030855	1.481874
H	-0.377551	-2.313432	3.135207
H	1.445151	-1.598376	3.908098
N	-2.494178	-2.372936	-1.073694
H	-1.487161	-2.398857	-0.925051
C	-2.957211	-3.646776	-1.595184
H	-3.941516	-3.536313	-2.063624
H	-2.266032	-3.977937	-2.377400
H	-3.027572	-4.460388	-0.854022

Mn(CO)-LYG20_A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.100607	-0.353008	1.205823
N	-1.188077	1.316715	-0.049648
C	0.823207	0.335040	-1.946558
H	1.473630	0.882179	-2.638441

H	0.723789	-0.674110	-2.359586
C	-2.592212	1.476319	2.482152
C	0.892431	-1.233060	2.338979
O	1.553620	-1.747123	3.159112
P	-1.729208	-0.139992	2.699299
P	1.548651	0.097287	-0.262669
Si	-2.777347	1.734330	0.627738
Si	-0.900931	1.098462	-1.786567
C	-3.189580	3.533404	0.265628
H	-3.380201	3.699952	-0.801472
H	-4.087200	3.848298	0.812726
H	-2.369209	4.197968	0.563558
C	-0.934933	2.763450	-2.667771
H	-0.548984	2.677757	-3.691635
H	-1.952460	3.167034	-2.734870
H	-0.323007	3.506177	-2.141493
H	-3.541334	1.539060	3.025448
H	-1.920302	2.249384	2.874183
P	-0.979775	-2.202561	0.227035
C	-2.778996	-2.205268	-0.215790
H	-3.028236	-3.156423	-0.707045
H	-3.340168	-2.198273	0.729601
Si	-3.468681	-0.776308	-1.247570
C	-0.318317	-3.028545	-1.295003
H	-0.523553	-2.429837	-2.187259
H	0.765353	-3.160539	-1.217372
H	-0.778922	-4.013120	-1.441152
C	-0.939228	-3.664602	1.353383
H	-1.401116	-3.405568	2.311666
H	-1.464234	-4.527537	0.926873
H	0.099846	-3.946782	1.552668
C	-4.935707	-1.457305	-2.218287
H	-4.617044	-2.225280	-2.934207
H	-5.677844	-1.913742	-1.551408
H	-5.442731	-0.666604	-2.785199
C	-4.079221	0.599157	-0.109255
H	-4.670978	0.150700	0.700753
H	-4.778950	1.221725	-0.685407
C	-2.249731	-0.018544	-2.475854
H	-1.806784	-0.803755	-3.101696
H	-2.861272	0.589339	-3.159858
H	0.367228	0.954316	2.038423
H	-0.496784	1.954449	0.352113
C	2.459407	1.675104	0.036144

C	3.133402	1.790774	1.259924
C	2.493507	2.755428	-0.847595
C	3.835228	2.945052	1.579844
H	3.089036	0.971468	1.972864
C	3.183885	3.924658	-0.519844
H	1.985632	2.704910	-1.805588
C	3.858484	4.020987	0.690772
H	4.354373	3.013245	2.531525
H	3.193250	4.755793	-1.219708
H	4.398412	4.928607	0.945167
C	2.965105	-1.025697	-0.626898
C	3.964099	-0.654150	-1.535049
C	3.039790	-2.281600	-0.022064
C	5.004690	-1.523645	-1.840336
H	3.933300	0.327526	-2.001307
C	4.083980	-3.155111	-0.324778
H	2.279266	-2.576663	0.693116
C	5.065667	-2.778978	-1.235410
H	5.771960	-1.221018	-2.547312
H	4.129619	-4.127368	0.157384
H	5.879602	-3.458332	-1.472238
H	-1.405724	-0.133842	4.073800
H	-2.871830	-0.984918	2.828073

Mn(CO)-LYG20_A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.069509	0.142705	1.107835
N	-1.260589	1.057832	-0.286701
C	0.850237	0.255817	-2.189624
H	1.362522	1.035610	-2.763185
H	0.961582	-0.688447	-2.734371
C	-3.158323	1.310778	1.973715
C	1.084771	-0.195633	2.391941
O	1.824659	-0.391610	3.279236
P	-1.500576	0.957519	2.662457
P	1.553881	0.073636	-0.501557
Si	-2.879815	1.534146	0.097772
Si	-1.001230	0.603499	-1.934995
C	-3.258364	3.341334	-0.297752
H	-3.085175	3.576694	-1.354022

H	-4.302164	3.590501	-0.066875
H	-2.617014	4.005489	0.296492
C	-1.518783	1.920870	-3.190956
H	-1.228343	1.621708	-4.206776
H	-2.603934	2.083182	-3.201122
H	-1.038755	2.884708	-2.980494
H	-3.792253	0.433335	2.143776
H	-3.644968	2.166749	2.452432
P	-0.898654	-1.936473	1.054754
C	-2.667037	-2.084114	0.531299
H	-2.913869	-3.155252	0.507539
H	-3.268743	-1.663241	1.349052
Si	-3.312358	-1.298311	-1.090886
C	-0.089184	-3.199900	-0.014577
H	0.019003	-2.828999	-1.037688
H	0.914775	-3.408534	0.367338
H	-0.658483	-4.136648	-0.037285
C	-0.938352	-2.861596	2.647479
H	-1.497942	-2.286965	3.393554
H	-1.401931	-3.849314	2.542444
H	0.082797	-2.985582	3.023685
C	-4.596950	-2.513075	-1.760033
H	-4.140831	-3.476824	-2.020155
H	-5.388160	-2.707603	-1.024456
H	-5.076971	-2.119655	-2.664722
C	-4.114337	0.377434	-0.761803
H	-5.035322	0.284371	-0.170557
H	-4.415099	0.788506	-1.737420
C	-1.964446	-0.982590	-2.364015
H	-1.299470	-1.850170	-2.455474
H	-2.444622	-0.861232	-3.346339
C	2.463184	1.656869	-0.253042
C	3.838164	1.718474	-0.012347
C	1.718191	2.844876	-0.246341
C	4.458826	2.944428	0.218838
H	4.433119	0.810162	-0.004651
C	2.342812	4.067814	-0.022885
H	0.642151	2.802628	-0.400872
C	3.715480	4.121197	0.210738
H	5.528830	2.977439	0.404089
H	1.754336	4.981214	-0.026246
H	4.202911	5.075451	0.388878
C	2.898273	-1.163159	-0.667335
C	3.590676	-1.325289	-1.873032

C	3.260188	-1.951722	0.429457
C	4.612045	-2.264003	-1.983805
H	3.334957	-0.710718	-2.731731
C	4.286149	-2.887670	0.320986
H	2.742274	-1.833679	1.375346
C	4.959979	-3.048903	-0.886441
H	5.136571	-2.381905	-2.927562
H	4.555343	-3.492913	1.181836
H	5.754723	-3.784285	-0.972362
H	-1.747343	0.371794	3.925840
H	-1.111245	2.228504	3.145142

TSE4-5S

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.294375	-0.146927	0.741715
N	0.002715	-1.495226	-1.066736
C	0.930888	0.969632	-2.166960
H	-0.034781	1.017312	-2.686334
H	1.643244	1.558134	-2.753899
C	-0.970978	-3.529697	0.841989
C	-0.813079	0.837186	2.087156
O	-1.190269	1.453577	3.012279
P	-1.546125	-1.889227	1.472552
P	0.642803	1.588345	-0.457706
Si	-0.151521	-3.255713	-0.844002
Si	1.324866	-0.866673	-2.058726
C	-1.245657	-3.954188	-2.196979
H	-0.779032	-3.846501	-3.183410
H	-1.454489	-5.019190	-2.037101
H	-2.196188	-3.409352	-2.222243
C	1.292619	-1.588808	-3.795945
H	2.019937	-1.084712	-4.445279
H	1.536765	-2.658110	-3.804284
H	0.301539	-1.467457	-4.249345
H	-0.237879	-3.930885	1.551035
H	-1.792890	-4.252149	0.788516
P	1.502597	-0.875221	1.996535
C	2.425183	-2.442237	1.615349
H	3.333381	-2.455854	2.233717
H	1.813178	-3.278688	1.977655

Si	2.890791	-2.841380	-0.177904
C	2.930990	0.239280	2.338987
H	3.495558	0.473344	1.433190
H	2.561742	1.180722	2.753869
H	3.610070	-0.222428	3.065204
C	1.064675	-1.232567	3.757674
H	0.328918	-2.040121	3.821598
H	1.949834	-1.530195	4.331621
H	0.627027	-0.342687	4.221115
C	4.571038	-3.693685	-0.168277
H	5.351569	-3.025231	0.216611
H	4.562207	-4.592050	0.461479
H	4.866843	-4.001547	-1.178835
C	1.575607	-3.997802	-0.874886
H	1.578113	-4.941311	-0.311520
H	1.837937	-4.258061	-1.910395
C	2.962260	-1.283208	-1.240702
H	3.307393	-0.454418	-0.612098
H	3.721033	-1.414587	-2.024808
H	-1.642267	0.357019	-0.198017
H	-0.891578	-1.198717	-1.507677
C	-2.914004	1.513260	-1.898635
H	-3.786456	1.554959	-2.565138
H	-3.023714	2.290879	-1.142846
H	-2.024116	1.713254	-2.496394
C	-2.877514	0.106025	-1.327366
O	-2.492122	-0.828157	-2.073973
C	-0.332334	3.136864	-0.713366
C	-0.181231	3.892165	-1.880698
C	-1.208036	3.597997	0.272171
C	-0.907213	5.063742	-2.070618
H	0.502608	3.562833	-2.657682
C	-1.924271	4.779654	0.091679
H	-1.346815	3.029924	1.184073
C	-1.783484	5.510607	-1.084057
H	-0.785935	5.629415	-2.990149
H	-2.602426	5.120197	0.869105
H	-2.350761	6.425125	-1.231656
C	2.239516	2.413654	-0.020917
C	3.434362	2.232545	-0.720935
C	2.248121	3.248134	1.104266
C	4.612054	2.847252	-0.294640
H	3.467013	1.603302	-1.604311
C	3.416976	3.869966	1.525179

H	1.329915	3.408467	1.664491
C	4.608154	3.664605	0.830125
H	5.531996	2.687785	-0.850267
H	3.399728	4.513149	2.400394
H	5.524237	4.145077	1.161081
C	-3.967347	-0.172999	-0.311950
C	-4.788383	-1.281480	-0.514146
C	-4.188461	0.646540	0.797405
C	-5.813988	-1.575596	0.383366
H	-4.605162	-1.913632	-1.377365
C	-5.202240	0.348908	1.699940
H	-3.529560	1.491216	0.976914
C	-6.019480	-0.764614	1.495171
H	-6.446977	-2.442836	0.215856
H	-5.352434	0.980880	2.570881
H	-6.811241	-0.996359	2.202161
H	-1.737159	-2.159380	2.848319
H	-2.905903	-1.942681	1.111877

E4R

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.363635	0.102693	1.276168
N	0.874386	-1.429772	-0.447193
C	-0.877587	0.314287	-1.828825
H	-1.625749	-0.483871	-1.734979
H	-1.174996	0.922867	-2.689024
C	2.425031	-2.612484	1.763895
C	-0.213294	1.026629	2.637002
O	-0.602193	1.617890	3.574595
P	1.128395	-1.554287	2.570211
P	-0.893912	1.219294	-0.219422
Si	2.181511	-2.585433	-0.114216
Si	0.783617	-0.551932	-1.981412
C	1.723498	-4.299868	-0.724551
H	1.529583	-4.301647	-1.804202
H	2.536105	-5.012029	-0.531698
H	0.827603	-4.658951	-0.206762
C	0.782037	-1.714251	-3.464464
H	0.587695	-1.161483	-4.392778
H	1.748971	-2.218397	-3.585460

H	0.008351	-2.484153	-3.372119
H	3.400577	-2.174465	2.006943
H	2.420110	-3.632410	2.163657
P	2.333054	1.263547	1.358780
C	3.898927	0.649694	0.571192
H	4.646019	1.455147	0.594775
H	4.296214	-0.145316	1.217273
Si	3.796959	-0.069954	-1.175961
C	2.402397	3.035942	0.845484
H	2.215729	3.162033	-0.224163
H	1.627117	3.589899	1.381996
H	3.378390	3.474526	1.084783
C	2.960841	1.499696	3.083765
H	3.135100	0.531819	3.564591
H	3.898399	2.067814	3.098289
H	2.213774	2.035718	3.678174
C	5.366358	0.406283	-2.105534
H	5.427012	1.491891	-2.253298
H	6.264631	0.094782	-1.557925
H	5.402794	-0.065447	-3.095219
C	3.703554	-1.946810	-1.015139
H	4.607360	-2.305432	-0.502737
H	3.727727	-2.394157	-2.019414
C	2.286807	0.562336	-2.122614
H	2.057461	1.575299	-1.773250
H	2.549023	0.654367	-3.185971
H	-0.993385	-0.755855	1.245224
H	-0.031493	-1.855844	-0.242948
C	-2.032470	-3.363769	1.167247
O	-1.026042	-4.055911	1.185164
C	-2.710435	1.403718	0.091546
C	-3.537463	1.944409	-0.900668
C	-3.286391	1.009878	1.299294
C	-4.907690	2.069118	-0.699186
H	-3.105325	2.280027	-1.840106
C	-4.658422	1.145273	1.510804
H	-2.657894	0.581755	2.071618
C	-5.473501	1.665826	0.510393
H	-5.534675	2.486247	-1.482470
H	-5.088800	0.838009	2.460124
H	-6.542641	1.768455	0.673731
C	-0.564491	2.970995	-0.711537
C	-0.028103	3.360876	-1.940857
C	-0.813018	3.960507	0.249313

C	0.268899	4.699831	-2.198595
H	0.173492	2.624681	-2.712940
C	-0.527094	5.295543	-0.007562
H	-1.229210	3.679348	1.214051
C	0.023713	5.669964	-1.233185
H	0.690981	4.980934	-3.159605
H	-0.728436	6.045854	0.751779
H	0.252754	6.712607	-1.433755
C	-2.629063	-2.931526	-0.137934
C	-2.106740	-3.457186	-1.325680
C	-3.691248	-2.025822	-0.201791
C	-2.644869	-3.088265	-2.553079
H	-1.286451	-4.165944	-1.271271
C	-4.219020	-1.643106	-1.430904
H	-4.101084	-1.594206	0.703635
C	-3.699896	-2.177248	-2.607616
H	-2.244179	-3.512134	-3.469233
H	-5.026974	-0.919256	-1.463754
H	-4.114853	-1.883418	-3.567378
C	-2.702410	-2.939571	2.449540
H	-3.776913	-3.150252	2.433639
H	-2.238527	-3.463923	3.286994
H	-2.562916	-1.860486	2.582907
H	0.233793	-2.552492	3.010901
H	1.726607	-1.328533	3.835656

E4S

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.015597	-0.145075	1.006522
N	0.096829	-1.523081	-0.868913
C	0.347373	1.033389	-2.094175
H	-0.698729	0.915112	-2.403060
H	0.809182	1.737112	-2.794267
C	-0.157922	-3.543044	1.256928
C	-0.327618	0.824117	2.414201
O	-0.587540	1.445516	3.377094
P	-0.906267	-1.972479	1.900862
P	0.307691	1.616625	-0.341453
Si	0.285276	-3.262352	-0.563723
Si	1.069230	-0.702674	-2.101844

C	-0.905698	-4.235426	-1.640915
H	-0.749026	-4.022402	-2.704503
H	-0.775752	-5.314437	-1.488857
H	-1.946072	-3.986137	-1.404803
C	0.817318	-1.478256	-3.798640
H	1.321210	-0.896589	-4.581366
H	1.211698	-2.500905	-3.848490
H	-0.250805	-1.514953	-4.042800
H	0.756223	-3.724251	1.834693
H	-0.811364	-4.411632	1.397694
P	2.088340	-0.581974	1.854906
C	3.204508	-1.956591	1.276823
H	4.213123	-1.774006	1.672435
H	2.861618	-2.880561	1.762471
Si	3.302325	-2.328819	-0.575677
C	3.322427	0.787539	1.949516
H	3.646148	1.104715	0.954069
H	2.859337	1.651152	2.435461
H	4.205151	0.487765	2.527294
C	2.054280	-1.008003	3.655966
H	1.479801	-1.926594	3.818964
H	3.063471	-1.156817	4.058192
H	1.564660	-0.203868	4.214893
C	5.050132	-2.911379	-0.973627
H	5.785634	-2.128992	-0.748006
H	5.321068	-3.799641	-0.389244
H	5.155242	-3.167367	-2.035158
C	2.068888	-3.709297	-0.946487
H	2.352743	-4.610131	-0.384629
H	2.141218	-3.977221	-2.010695
C	2.881354	-0.814629	-1.623517
H	3.192255	0.081275	-1.073083
H	3.480132	-0.837651	-2.544917
H	-1.457556	0.126737	0.423404
H	-0.887268	-1.341740	-1.086772
C	-3.544219	0.997699	-2.284623
H	-4.607570	1.236506	-2.392217
H	-3.107718	1.733956	-1.600348
H	-3.048285	1.076516	-3.253988
C	-3.353743	-0.390971	-1.732802
O	-2.587554	-1.182036	-2.267915
C	-1.014403	2.913494	-0.413362
C	-0.970693	3.893251	-1.412937
C	-2.076711	2.929937	0.492827

C	-1.974277	4.849677	-1.520996
H	-0.142521	3.911079	-2.117131
C	-3.075720	3.899640	0.397839
H	-2.133888	2.164734	1.258185
C	-3.032690	4.854455	-0.613570
H	-1.928367	5.595711	-2.309422
H	-3.889876	3.902919	1.117733
H	-3.814498	5.604767	-0.691786
C	1.749185	2.772927	-0.243978
C	2.809673	2.801944	-1.152604
C	1.801353	3.628775	0.864632
C	3.900531	3.649302	-0.951851
H	2.803593	2.160174	-2.028443
C	2.880817	4.480426	1.062243
H	0.988332	3.622813	1.587406
C	3.940910	4.488671	0.155976
H	4.715538	3.653744	-1.670605
H	2.897949	5.137164	1.927592
H	4.788027	5.150581	0.311345
C	-4.138703	-0.798154	-0.529125
C	-4.341422	-2.159739	-0.287367
C	-4.649400	0.143652	0.368438
C	-5.048918	-2.575767	0.834481
H	-3.950267	-2.882869	-0.995743
C	-5.333953	-0.273519	1.504390
H	-4.482680	1.202997	0.200668
C	-5.537765	-1.632496	1.736748
H	-5.213459	-3.634706	1.010496
H	-5.707078	0.461835	2.210806
H	-6.079233	-1.956035	2.621019
H	-2.273977	-2.241033	1.668105
H	-0.935773	-2.236722	3.293422

E5R

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.665720	0.118844	1.263762
N	0.666782	-1.480399	-0.069932
C	-0.940097	0.252429	-1.727737
H	-1.847730	-0.330901	-1.525402
H	-1.107491	0.794210	-2.663702

C	2.315148	-2.801426	1.972108
C	0.341570	1.275382	2.550725
O	0.174811	2.037992	3.424381
P	1.379664	-1.438457	2.769714
P	-0.654689	1.323019	-0.271084
Si	1.713674	-2.850762	0.160253
Si	0.492604	-0.979790	-1.721130
C	0.847359	-4.507278	-0.089964
H	0.429244	-4.599959	-1.099402
H	1.547216	-5.340738	0.055731
H	0.024159	-4.625939	0.624470
C	0.059474	-2.349793	-2.948078
H	-0.143057	-1.914135	-3.935552
H	0.867809	-3.079575	-3.077337
H	-0.842125	-2.888848	-2.636857
H	3.381809	-2.552971	2.011059
H	2.181920	-3.756571	2.490843
P	2.743709	1.020173	1.012717
C	4.011905	-0.035106	0.182563
H	4.908675	0.579902	0.024395
H	4.306059	-0.805343	0.907546
Si	3.589667	-0.944400	-1.439448
C	3.031709	2.636428	0.181210
H	2.680177	2.627130	-0.852652
H	2.487421	3.422320	0.711926
H	4.099992	2.881531	0.187566
C	3.611090	1.381727	2.601737
H	3.736906	0.465267	3.187378
H	4.601701	1.816320	2.425654
H	3.018737	2.082565	3.198665
C	5.126017	-0.833666	-2.530295
H	5.354940	0.208953	-2.786044
H	6.007093	-1.254275	-2.029437
H	4.986974	-1.381494	-3.470526
C	3.208531	-2.737503	-1.001542
H	4.086893	-3.217175	-0.547324
H	2.997106	-3.297088	-1.924529
C	2.106532	-0.187903	-2.325189
H	2.105372	0.894178	-2.143700
H	2.217975	-0.322408	-3.410406
H	-2.345081	-0.799578	1.394236
H	-0.801759	-2.267368	0.777607
C	-2.625533	-1.860277	1.301809
O	-1.471605	-2.660161	1.389348

C	-2.359704	1.818899	0.237342
C	-3.256296	2.291225	-0.729855
C	-2.793088	1.715208	1.559885
C	-4.555759	2.641043	-0.383294
H	-2.936133	2.382906	-1.764525
C	-4.097614	2.063867	1.910741
H	-2.116725	1.352575	2.325734
C	-4.981376	2.524183	0.940552
H	-5.240213	3.002398	-1.145411
H	-4.417873	1.970737	2.944410
H	-5.998563	2.792544	1.210981
C	-0.069729	2.931870	-0.934394
C	0.410570	3.103571	-2.234007
C	-0.061780	4.026989	-0.061310
C	0.908075	4.339334	-2.647276
H	0.415458	2.275060	-2.935350
C	0.426049	5.260345	-0.475687
H	-0.434019	3.910707	0.953688
C	0.921259	5.418246	-1.769658
H	1.285486	4.454587	-3.659358
H	0.425656	6.098241	0.215495
H	1.310015	6.379621	-2.092358
C	-3.342216	-2.027874	-0.031152
C	-4.299925	-1.095188	-0.440874
C	-3.046354	-3.102305	-0.869381
C	-4.940990	-1.230147	-1.668755
H	-4.534501	-0.247741	0.199127
C	-3.690327	-3.241726	-2.097647
H	-2.296649	-3.821080	-0.553992
C	-4.636140	-2.304466	-2.503583
H	-5.673609	-0.489424	-1.977425
H	-3.445233	-4.082387	-2.741410
H	-5.132042	-2.408689	-3.464542
C	-3.530077	-2.211314	2.476960
H	-3.816782	-3.267564	2.427902
H	-3.001713	-2.036947	3.420241
H	-4.441174	-1.603926	2.467556
H	0.306112	-2.126574	3.368804
H	2.102222	-1.154367	3.950487

E5S

Coordinates (Angstroms)

	X	Y	Z
Mn	-0.099082	-0.236099	0.848053
N	-0.015643	-1.400716	-0.884247
C	0.675739	1.070867	-2.179394
H	-0.330370	1.102316	-2.618206
H	1.332262	1.676881	-2.810974
C	-0.678797	-3.616314	0.942450
C	-0.577406	0.731309	2.236937
O	-0.889197	1.318525	3.202698
P	-1.176154	-2.043643	1.741522
P	0.508096	1.655337	-0.454088
Si	-0.082197	-3.134453	-0.803745
Si	1.083152	-0.771702	-2.067927
C	-1.295718	-3.894415	-2.030797
H	-1.051863	-3.633118	-3.067022
H	-1.293404	-4.989764	-1.954834
H	-2.317412	-3.546626	-1.836611
C	0.841246	-1.476402	-3.804726
H	1.455994	-0.926486	-4.529596
H	1.122504	-2.533736	-3.879503
H	-0.205088	-1.381792	-4.118789
H	0.146297	-4.052800	1.515784
H	-1.492178	-4.349314	0.929960
P	1.862779	-0.762280	1.897202
C	2.715391	-2.306833	1.348606
H	3.686741	-2.348793	1.860779
H	2.137967	-3.150417	1.748129
Si	2.982549	-2.660960	-0.506091
C	3.290607	0.396834	1.990413
H	3.665083	0.663396	0.999929
H	2.983161	1.318661	2.490844
H	4.107572	-0.058614	2.561850
C	1.695036	-1.103666	3.703715
H	0.976413	-1.909409	3.882991
H	2.655967	-1.393374	4.143728
H	1.327940	-0.208617	4.216143
C	4.693362	-3.444000	-0.656882
H	5.479627	-2.748709	-0.336285
H	4.776287	-4.349111	-0.041881
H	4.907851	-3.728846	-1.694397
C	1.647964	-3.866998	-1.069584
H	1.744442	-4.825701	-0.541066
H	1.799783	-4.086674	-2.136407

C	2.878700	-1.101810	-1.562928
H	3.301510	-0.258491	-1.003194
H	3.502374	-1.226563	-2.459365
H	-2.054382	0.749376	-0.654960
H	-1.610197	-1.005937	-1.751397
C	-3.592986	1.461325	-1.964701
H	-4.422736	1.066298	-2.561537
H	-3.989512	2.201875	-1.263366
H	-2.886836	1.961787	-2.634775
C	-2.897954	0.322256	-1.227614
O	-2.402598	-0.589364	-2.173275
C	-0.692469	3.056388	-0.587828
C	-0.682469	3.880679	-1.719451
C	-1.615716	3.323169	0.425542
C	-1.584680	4.932299	-1.841198
H	0.034042	3.699216	-2.515663
C	-2.518059	4.378895	0.307534
H	-1.640923	2.705721	1.315500
C	-2.509682	5.181140	-0.828870
H	-1.567539	5.556931	-2.729721
H	-3.233641	4.564863	1.103333
H	-3.220325	5.996604	-0.926661
C	2.031332	2.617136	-0.097464
C	3.176551	2.571920	-0.894611
C	2.044430	3.406365	1.059180
C	4.317525	3.289092	-0.535279
H	3.196547	1.971301	-1.798461
C	3.178273	4.127343	1.413137
H	1.161864	3.452305	1.692737
C	4.322560	4.065619	0.618601
H	5.202227	3.240349	-1.163735
H	3.170653	4.734997	2.313463
H	5.211154	4.624898	0.896393
C	-3.821922	-0.329736	-0.209432
C	-4.430697	-1.557133	-0.465670
C	-4.051631	0.296194	1.018456
C	-5.248657	-2.154055	0.493244
H	-4.244413	-2.043473	-1.418137
C	-4.864596	-0.296721	1.978780
H	-3.569319	1.248013	1.228827
C	-5.464887	-1.528912	1.719208
H	-5.714445	-3.113365	0.283979
H	-5.022479	0.197351	2.933543
H	-6.096130	-1.997638	2.468830

H	-2.568783	-2.045176	1.532581
H	-1.205583	-2.339008	3.123129

TSE4-5R

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.328899	0.034773	1.253034
N	1.129062	-1.345689	-0.409515
C	-0.916079	0.063557	-1.867106
H	-1.552506	-0.826582	-1.789372
H	-1.254751	0.617351	-2.748691
C	2.926336	-2.234367	1.761294
C	-0.390024	0.812909	2.643759
O	-0.840756	1.296416	3.611788
P	1.531823	-1.350549	2.601825
P	-1.103364	0.976576	-0.279745
Si	2.628840	-2.261385	-0.107818
Si	0.857872	-0.560797	-1.972966
C	2.439379	-4.032629	-0.695332
H	2.227538	-4.087373	-1.769923
H	3.357289	-4.605072	-0.510344
H	1.618385	-4.514162	-0.153398
C	1.005840	-1.760288	-3.415636
H	0.723645	-1.268056	-4.355331
H	2.028715	-2.136271	-3.539756
H	0.340252	-2.620333	-3.283492
H	3.857595	-1.702280	1.987313
H	3.034235	-3.249145	2.158187
P	2.042430	1.593091	1.290173
C	3.690065	1.180862	0.551930
H	4.323536	2.077189	0.604916
H	4.162993	0.442323	1.213214
Si	3.751253	0.465670	-1.205943
C	1.846671	3.316960	0.658914
H	1.632873	3.348857	-0.411351
H	1.015465	3.802509	1.176394
H	2.760571	3.891646	0.849140
C	2.587233	2.050904	2.997726
H	2.976264	1.180938	3.533848
H	3.372617	2.814661	2.966473
H	1.738138	2.443622	3.566036

C	5.201610	1.257725	-2.111645
H	5.043331	2.334785	-2.248634
H	6.140755	1.125932	-1.560263
H	5.337373	0.814573	-3.106165
C	4.012322	-1.391801	-1.041653
H	4.971498	-1.585174	-0.541375
H	4.097475	-1.836796	-2.043481
C	2.157414	0.781666	-2.171180
H	1.756066	1.755713	-1.870901
H	2.404138	0.866788	-3.239038
H	-0.903130	-1.205238	1.220815
H	0.390618	-2.023574	-0.192635
C	-1.261665	-2.756380	1.250524
O	-0.183445	-3.407449	1.215246
C	-2.918775	0.917599	0.046426
C	-3.830124	1.135510	-0.992894
C	-3.409503	0.694270	1.332699
C	-5.199435	1.106757	-0.754742
H	-3.468825	1.325581	-2.000204
C	-4.781858	0.679493	1.578235
H	-2.719552	0.509710	2.146203
C	-5.680071	0.875982	0.534262
H	-5.894664	1.267287	-1.573967
H	-5.145119	0.503557	2.586912
H	-6.749856	0.855997	0.722027
C	-1.025671	2.752167	-0.778538
C	-0.551950	3.203085	-2.012330
C	-1.439870	3.701342	0.164782
C	-0.468276	4.568259	-2.287875
H	-0.231108	2.497762	-2.772296
C	-1.366519	5.061034	-0.110708
H	-1.817783	3.371037	1.129669
C	-0.870611	5.500456	-1.337903
H	-0.089523	4.899481	-3.250912
H	-1.692985	5.780245	0.634907
H	-0.805317	6.563199	-1.552309
C	-2.113631	-2.814503	-0.018566
C	-1.566510	-3.458044	-1.134376
C	-3.419367	-2.326895	-0.110956
C	-2.280185	-3.567233	-2.323562
H	-0.574709	-3.889368	-1.045884
C	-4.139367	-2.438758	-1.298135
H	-3.886916	-1.842691	0.737685
C	-3.569697	-3.047406	-2.413363

H	-1.833439	-4.068602	-3.178144
H	-5.147818	-2.038927	-1.348063
H	-4.130718	-3.130654	-3.339964
C	-2.028417	-2.673366	2.565740
H	-2.529191	-3.635804	2.735865
H	-1.328281	-2.498290	3.385219
H	-2.778086	-1.879655	2.575233
H	0.872682	-2.411025	3.242761
H	2.187509	-0.845686	3.749178

E6Ra

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.078992	-0.162107	1.076595
N	1.285316	-0.984037	-0.595722
C	-0.728198	0.234286	-2.205422
H	-1.121121	-0.766704	-2.431403
H	-1.053099	0.894154	-3.015484
C	2.841732	-2.250496	1.531134
C	-0.980966	0.198669	2.426987
O	-1.661657	0.419390	3.356112
P	1.509025	-1.344986	2.438930
P	-1.380488	0.668569	-0.549251
Si	2.799711	-1.743298	-0.307257
Si	1.135467	-0.076081	-2.041273
C	3.066150	-3.346512	-1.277388
H	3.050912	-3.183288	-2.361424
H	4.035978	-3.797429	-1.027063
H	2.290231	-4.087105	-1.044924
C	1.633263	-0.983559	-3.627811
H	1.353544	-0.392962	-4.510990
H	2.715653	-1.153897	-3.687210
H	1.136878	-1.958113	-3.712730
H	3.815058	-2.077695	2.002682
H	2.648468	-3.326701	1.607108
P	1.314537	1.761906	1.493423
C	3.108147	1.608959	1.099559
H	3.617629	2.524084	1.432361
H	3.513024	0.795686	1.717875
Si	3.618944	1.237384	-0.702732
C	1.005472	3.477800	0.883683

H	0.982898	3.537380	-0.204578
H	0.043230	3.839236	1.255163
H	1.792967	4.145674	1.252220
C	1.368306	2.191227	3.290138
H	1.649417	1.327946	3.899025
H	2.080501	3.001650	3.483363
H	0.373446	2.515829	3.613166
C	5.028982	2.427944	-1.107511
H	4.683999	3.469952	-1.088459
H	5.849680	2.336307	-0.384794
H	5.442942	2.235570	-2.105082
C	4.216239	-0.550181	-0.743692
H	5.076041	-0.676042	-0.070927
H	4.580526	-0.789900	-1.753973
C	2.222726	1.474416	-1.960996
H	1.646186	2.373306	-1.714021
H	2.673516	1.662352	-2.946278
H	-2.382692	-2.323889	-0.227182
H	0.052120	-2.092531	-0.134650
C	-1.729905	-2.959657	0.384252
O	-0.524007	-2.259121	0.667064
C	-3.132633	0.075385	-0.593185
C	-3.805479	-0.138001	-1.801128
C	-3.817185	-0.161469	0.603421
C	-5.120938	-0.593967	-1.812347
H	-3.304135	0.049193	-2.745945
C	-5.134657	-0.611592	0.594176
H	-3.317097	-0.011591	1.553547
C	-5.788138	-0.836181	-0.614168
H	-5.625122	-0.758977	-2.760393
H	-5.645003	-0.796096	1.535167
H	-6.812764	-1.196745	-0.623058
C	-1.703698	2.479117	-0.611032
C	-1.283205	3.305140	-1.654585
C	-2.383100	3.055705	0.469754
C	-1.530259	4.677196	-1.617776
H	-0.741522	2.893658	-2.500273
C	-2.640450	4.421178	0.502088
H	-2.704144	2.434205	1.301664
C	-2.209059	5.238936	-0.542050
H	-1.188656	5.306198	-2.435036
H	-3.169721	4.849756	1.348257
H	-2.402416	6.307328	-0.514690
C	-1.437136	-4.233083	-0.430313

C	-0.451512	-5.172854	0.267093
C	-0.944825	-3.872673	-1.836872
H	-2.400052	-4.751959	-0.537771
H	-0.846075	-5.552736	1.215518
H	-0.228043	-6.038263	-0.367254
H	0.491699	-4.657256	0.478927
H	-1.658145	-3.214364	-2.348453
H	0.026451	-3.362932	-1.807869
H	-0.820612	-4.771920	-2.450488
C	-2.415770	-3.209954	1.715177
H	-2.588271	-2.259314	2.228081
H	-3.382308	-3.703812	1.567841
H	-1.795532	-3.833417	2.367915
H	0.908183	-2.360140	3.212400
H	2.241420	-0.753967	3.493911

TSE4-5Ra

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.098918	-0.268976	1.090842
N	1.247787	-1.184819	-0.665658
C	-0.815343	0.248134	-2.108451
H	-1.350399	-0.684165	-2.319891
H	-1.103747	0.957947	-2.890487
C	2.991534	-2.147324	1.515339
C	-0.857737	0.136136	2.497612
O	-1.466427	0.372976	3.471007
P	1.362772	-1.743208	2.292565
P	-1.302855	0.765624	-0.406607
Si	2.847411	-1.912660	-0.357472
Si	1.025187	-0.143820	-2.084383
C	2.929979	-3.564606	-1.237786
H	2.908163	-3.439307	-2.327125
H	3.842058	-4.118152	-0.982733
H	2.062056	-4.168270	-0.947824
C	1.508071	-1.004174	-3.689782
H	1.238273	-0.381957	-4.553263
H	2.588698	-1.184404	-3.747357
H	1.001304	-1.968747	-3.808717
H	3.744537	-1.460277	1.917802
H	3.310383	-3.162495	1.774365

P	1.561112	1.444825	1.629784
C	3.310129	1.468110	1.008466
H	3.746815	2.443536	1.263312
H	3.875862	0.731498	1.593767
Si	3.639818	1.098565	-0.822336
C	1.114681	3.213812	1.357525
H	1.008319	3.454774	0.297371
H	0.157861	3.422227	1.843083
H	1.879037	3.869643	1.790094
C	1.896173	1.572976	3.444020
H	2.384419	0.667293	3.815771
H	2.544786	2.427813	3.667107
H	0.953852	1.693295	3.987764
C	5.035474	2.222326	-1.404977
H	4.744812	3.279065	-1.353572
H	5.934853	2.093396	-0.790234
H	5.311718	2.004878	-2.444166
C	4.152747	-0.708594	-0.977202
H	5.092588	-0.875678	-0.433102
H	4.368993	-0.926550	-2.033219
C	2.100297	1.380783	-1.877794
H	1.522534	2.204260	-1.443143
H	2.410567	1.717117	-2.877356
H	-0.934969	-1.604197	0.669785
H	0.616083	-1.999154	-0.656033
C	-1.178111	-3.103289	0.460629
O	-0.054557	-3.658886	0.289307
C	-3.102862	0.349704	-0.365543
C	-3.906462	0.603773	-1.483338
C	-3.688657	-0.215714	0.767594
C	-5.258621	0.279803	-1.475005
H	-3.473273	1.057559	-2.370918
C	-5.045977	-0.533419	0.781862
H	-3.080631	-0.426637	1.638686
C	-5.831841	-0.292511	-0.340544
H	-5.866051	0.476989	-2.353828
H	-5.483940	-0.977100	1.671458
H	-6.888068	-0.546130	-0.332887
C	-1.489707	2.597582	-0.527935
C	-0.978682	3.378031	-1.566888
C	-2.155410	3.239206	0.524805
C	-1.112308	4.766749	-1.546480
H	-0.460225	2.918010	-2.402454
C	-2.295392	4.621280	0.543810

H	-2.563047	2.651021	1.343818
C	-1.766667	5.392169	-0.491044
H	-0.703976	5.357074	-2.362073
H	-2.813474	5.098792	1.370524
H	-1.871740	6.473070	-0.475618
C	-2.133858	-3.059142	-0.773761
C	-3.276402	-4.077158	-0.628326
C	-1.372031	-3.353370	-2.066084
H	-2.594093	-2.070090	-0.836565
H	-3.956284	-3.823896	0.190567
H	-3.870691	-4.103409	-1.549521
H	-2.888404	-5.088471	-0.454554
H	-0.484499	-2.728763	-2.184921
H	-1.024024	-4.391049	-2.082215
H	-2.018614	-3.191458	-2.937168
C	-1.894991	-3.303491	1.800106
H	-1.236902	-3.059182	2.634969
H	-2.796267	-2.688896	1.877871
H	-2.182101	-4.358418	1.893861
H	0.855135	-3.033935	2.504526
H	1.744729	-1.477559	3.628055

TSE4-5Sa

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.012597	-0.456247	0.906605
N	1.246694	-1.100877	-0.903876
C	-0.588151	0.706026	-2.208032
H	-1.131683	-0.152193	-2.617184
H	-0.775510	1.546053	-2.884451
C	2.771490	-2.480482	1.219577
C	-1.048570	-0.246168	2.296289
O	-1.721462	-0.157550	3.253533
P	1.060797	-2.215988	1.860129
P	-1.207183	0.957134	-0.491797
Si	2.790026	-1.946564	-0.597304
Si	1.216019	0.191060	-2.113438
C	2.919104	-3.449565	-1.709206
H	2.874904	-3.165690	-2.767680
H	3.863250	-3.984150	-1.545773
H	2.087876	-4.134444	-1.511603

C	1.753019	-0.436923	-3.805596
H	1.568427	0.318294	-4.580466
H	2.822683	-0.678395	-3.837866
H	1.197511	-1.340485	-4.085370
H	3.457440	-1.855582	1.801699
H	3.092459	-3.519678	1.347803
P	1.507923	1.012199	1.855207
C	3.299537	1.100444	1.364359
H	3.721749	2.010883	1.811265
H	3.819533	0.268517	1.857286
Si	3.773979	1.037384	-0.468892
C	1.144320	2.818072	1.950939
H	1.123191	3.283508	0.962542
H	0.164254	2.967072	2.411103
H	1.898591	3.326822	2.562402
C	1.736982	0.724246	3.668420
H	2.147135	-0.272860	3.856054
H	2.422536	1.462005	4.101150
H	0.772655	0.793822	4.181707
C	5.264418	2.162213	-0.717373
H	5.011376	3.208732	-0.505609
H	6.091627	1.880868	-0.053678
H	5.635812	2.112435	-1.748379
C	4.201700	-0.742770	-0.906233
H	5.081325	-1.069756	-0.334334
H	4.490151	-0.789534	-1.966135
C	2.350966	1.587879	-1.576386
H	1.784447	2.367749	-1.053711
H	2.762173	2.058043	-2.481077
H	-1.108460	-1.621567	0.267718
H	0.587138	-1.868187	-1.141675
C	-2.326906	-2.513542	-1.565529
H	-2.833081	-3.373959	-2.024527
H	-3.085091	-1.827339	-1.189175
H	-1.744160	-2.029656	-2.352224
C	-1.384022	-3.044708	-0.491874
O	-0.261092	-3.469346	-0.872649
C	-3.031209	0.722639	-0.669656
C	-3.676525	0.934149	-1.892808
C	-3.799941	0.354744	0.436417
C	-5.050875	0.753514	-2.012750
H	-3.107206	1.235718	-2.766941
C	-5.177564	0.182831	0.321579
H	-3.323268	0.189260	1.395076

C	-5.805676	0.372611	-0.905289
H	-5.533177	0.910368	-2.973441
H	-5.754884	-0.112872	1.192915
H	-6.877742	0.226061	-1.000183
C	-1.233246	2.796833	-0.300212
C	-0.583854	3.685781	-1.159707
C	-1.924577	3.321642	0.799210
C	-0.605028	5.059262	-0.916269
H	-0.044512	3.322463	-2.028194
C	-1.955468	4.689765	1.038976
H	-2.438549	2.651619	1.483983
C	-1.287341	5.565451	0.184161
H	-0.087481	5.731705	-1.594689
H	-2.497000	5.073697	1.898738
H	-1.305542	6.634838	0.372950
C	-3.329469	-3.091213	1.214423
C	-2.075664	-3.773640	0.679149
H	-3.110709	-2.061923	1.508477
H	-4.136379	-3.073250	0.472495
H	-3.703280	-3.624321	2.096751
C	-2.369871	-5.215132	0.238366
H	-1.347575	-3.827387	1.492158
H	-1.461246	-5.698276	-0.132900
H	-2.756208	-5.800558	1.081016
H	-3.125295	-5.246097	-0.556661
H	0.540453	-3.503846	1.648201
H	1.248965	-2.331300	3.257504

TSE5-6Ra

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.089258	-0.150650	1.096214
N	1.373186	-0.913817	-0.633008
C	-0.788442	0.089902	-2.181299
H	-1.073685	-0.954263	-2.370455
H	-1.198728	0.685523	-3.002397
C	3.001553	-2.034674	1.508690
C	-0.999602	0.075761	2.450340
O	-1.694723	0.214138	3.383478
P	1.639602	-1.196507	2.439295
P	-1.464594	0.500783	-0.525269

Si	2.979096	-1.492083	-0.312583
Si	1.097640	0.006417	-2.071216
C	3.438469	-3.020648	-1.321068
H	3.461161	-2.816096	-2.397737
H	4.432849	-3.389647	-1.035906
H	2.724399	-3.836516	-1.155632
C	1.693109	-0.822179	-3.662011
H	1.354815	-0.257797	-4.541296
H	2.787849	-0.874298	-3.716298
H	1.303773	-1.843390	-3.755358
H	3.967648	-1.864976	1.995883
H	2.821382	-3.115200	1.539146
P	1.098737	1.892359	1.524769
C	2.895927	1.937241	1.117654
H	3.306604	2.907371	1.430583
H	3.392883	1.182318	1.742760
Si	3.423834	1.594680	-0.682304
C	0.603954	3.571535	0.935525
H	0.596556	3.646826	-0.152496
H	-0.401106	3.811529	1.291428
H	1.302095	4.319365	1.329890
C	1.118993	2.301246	3.326560
H	1.481744	1.458505	3.920724
H	1.751004	3.173079	3.530241
H	0.098508	2.524595	3.655034
C	4.695140	2.916370	-1.129236
H	4.242246	3.916090	-1.133354
H	5.523510	2.930808	-0.409841
H	5.123790	2.743915	-2.124281
C	4.219108	-0.115017	-0.702592
H	5.063443	-0.133171	0.000535
H	4.648492	-0.304178	-1.697591
C	2.000064	1.661262	-1.931276
H	1.311402	2.468210	-1.656318
H	2.415252	1.938711	-2.910640
H	-2.021930	-2.492903	-0.248155
H	0.526634	-1.794089	-0.241397
C	-1.290749	-3.039880	0.367168
O	-0.172944	-2.232587	0.626500
C	-3.155923	-0.247213	-0.552254
C	-3.821727	-0.509270	-1.754533
C	-3.804049	-0.545993	0.649987
C	-5.094555	-1.072508	-1.754324
H	-3.346669	-0.279499	-2.703523

C	-5.080068	-1.102979	0.652068
H	-3.307222	-0.359958	1.595142
C	-5.726875	-1.372774	-0.550304
H	-5.593848	-1.274565	-2.697764
H	-5.563198	-1.333740	1.597149
H	-6.718006	-1.817040	-0.550274
C	-1.949339	2.272406	-0.638594
C	-1.574646	3.112275	-1.688749
C	-2.707547	2.807124	0.410675
C	-1.940550	4.458075	-1.687424
H	-0.978414	2.733732	-2.512930
C	-3.083510	4.145222	0.407345
H	-3.001373	2.173557	1.243638
C	-2.694469	4.978194	-0.641317
H	-1.633127	5.098767	-2.509165
H	-3.674955	4.540487	1.228197
H	-2.980370	6.025987	-0.641785
C	-0.885070	-4.290912	-0.443339
C	0.219462	-5.096742	0.242890
C	-0.470751	-3.900702	-1.865397
H	-1.782360	-4.922225	-0.517885
H	-0.111362	-5.511309	1.201381
H	0.542147	-5.935875	-0.384922
H	1.089326	-4.460468	0.437042
H	-1.277999	-3.359684	-2.375954
H	0.416453	-3.256919	-1.856267
H	-0.231664	-4.785672	-2.467363
C	-1.968883	-3.378632	1.689390
H	-2.228331	-2.456591	2.218046
H	-2.888232	-3.954897	1.530120
H	-1.300274	-3.955054	2.339062
H	1.136711	-2.229489	3.255013
H	2.379440	-0.533962	3.447914

E4Ra

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.463116	0.089768	1.296041
N	0.821549	-1.596344	-0.259420
C	-0.844172	0.088412	-1.820864
H	-1.623282	-0.675034	-1.716088

H	-1.082543	0.673449	-2.714313
C	2.453205	-2.608974	2.000416
C	-0.043681	1.182883	2.554951
O	-0.405550	1.882656	3.426480
P	1.257101	-1.399297	2.743057
P	-0.859187	1.048014	-0.243945
Si	2.069454	-2.787261	0.153602
Si	0.737434	-0.917627	-1.896630
C	1.405945	-4.513685	-0.179857
H	1.177488	-4.653442	-1.243086
H	2.127232	-5.286063	0.114098
H	0.479593	-4.689713	0.380962
C	0.530565	-2.275009	-3.186622
H	0.351049	-1.846099	-4.181069
H	1.419414	-2.913766	-3.264592
H	-0.326656	-2.911387	-2.937639
H	3.457830	-2.186408	2.121638
H	2.445770	-3.572038	2.523219
P	2.445882	1.192537	1.099209
C	3.960736	0.383377	0.385835
H	4.751821	1.141125	0.297008
H	4.324483	-0.338336	1.129891
Si	3.798000	-0.548082	-1.255039
C	2.578300	2.841478	0.273286
H	2.375247	2.770992	-0.797797
H	1.839892	3.526196	0.700862
H	3.578279	3.270375	0.411013
C	3.143113	1.699844	2.736517
H	3.304813	0.824596	3.374476
H	4.097183	2.228490	2.624402
H	2.433020	2.357939	3.247840
C	5.383277	-0.286074	-2.241193
H	5.529054	0.774110	-2.483430
H	6.263546	-0.620315	-1.677915
H	5.363702	-0.843287	-3.186097
C	3.583583	-2.389399	-0.885832
H	4.483997	-2.767694	-0.382219
H	3.517545	-2.929303	-1.841631
C	2.312253	0.034790	-2.266270
H	2.164819	1.110151	-2.114937
H	2.541543	-0.100669	-3.332750
H	-0.878686	-0.743852	1.493373
H	-0.104282	-1.989423	-0.053703
C	-3.071164	-2.539597	0.046449

O	-2.036060	-2.682156	-0.585734
C	-2.680412	1.163404	0.087986
C	-3.554087	1.579662	-0.925215
C	-3.211768	0.843192	1.338190
C	-4.923841	1.660174	-0.699112
H	-3.159206	1.850502	-1.901488
C	-4.583399	0.940711	1.574355
H	-2.544180	0.505485	2.122864
C	-5.442801	1.344069	0.556731
H	-5.586892	1.978533	-1.498684
H	-4.977912	0.697345	2.557202
H	-6.511382	1.416652	0.738904
C	-0.583305	2.790233	-0.785661
C	-0.050782	3.151622	-2.024793
C	-0.839454	3.800165	0.151532
C	0.227082	4.486574	-2.319675
H	0.170455	2.394464	-2.771318
C	-0.569577	5.131454	-0.142150
H	-1.246220	3.539194	1.125642
C	-0.028492	5.479109	-1.379878
H	0.646912	4.746986	-3.287507
H	-0.776012	5.899042	0.598338
H	0.187812	6.518680	-1.608670
C	-4.388177	-2.208145	-0.635748
C	-5.416784	-3.316076	-0.350496
C	-4.230322	-1.967399	-2.132144
H	-4.746622	-1.285928	-0.156965
H	-5.583972	-3.463475	0.721223
H	-6.378555	-3.055196	-0.803820
H	-5.091573	-4.271099	-0.780308
H	-3.571334	-1.119118	-2.334997
H	-3.812532	-2.847529	-2.632398
H	-5.204621	-1.746709	-2.581438
C	-3.085219	-2.728367	1.543956
H	-2.160772	-2.314565	1.957324
H	-3.947737	-2.252348	2.017861
H	-3.118954	-3.803100	1.764292
H	1.940586	-1.061445	3.940479
H	0.355858	-2.298530	3.360837

E4Sa

Coordinates (Angstroms)

	X	Y	Z
Mn	0.082432	-0.091014	1.137032
N	0.945458	-1.307009	-0.626382
C	-0.726032	0.462016	-2.079410
H	-1.396636	-0.392861	-2.235606
H	-0.926025	1.181992	-2.878972
C	2.320723	-2.627850	1.629683
C	-0.723918	0.635873	2.499747
O	-1.261127	1.100384	3.436433
P	0.810737	-1.815882	2.341385
P	-1.073182	1.099185	-0.382031
Si	2.282209	-2.411225	-0.252910
Si	0.999460	-0.282415	-2.073220
C	1.951144	-4.073849	-1.063242
H	1.852718	-3.970011	-2.149974
H	2.761624	-4.785613	-0.861953
H	1.017905	-4.515370	-0.692569
C	1.237681	-1.310023	-3.632903
H	1.119979	-0.693149	-4.533107
H	2.233128	-1.768517	-3.682354
H	0.489815	-2.109652	-3.676578
H	3.190826	-2.100272	2.038106
H	2.413482	-3.678457	1.927294
P	1.921597	1.187608	1.599492
C	3.630020	0.799935	0.971630
H	4.278665	1.663412	1.174656
H	4.026227	-0.017456	1.589679
Si	3.835303	0.274638	-0.833965
C	1.892098	3.009781	1.295223
H	1.823357	3.240524	0.229024
H	1.012280	3.440307	1.781853
H	2.789966	3.490688	1.701618
C	2.310963	1.258524	3.407315
H	2.518297	0.255923	3.796764
H	3.180891	1.894868	3.608068
H	1.449883	1.656209	3.953754
C	5.484818	0.940346	-1.457037
H	5.494736	2.037642	-1.455389
H	6.315217	0.600335	-0.825650
H	5.689937	0.608100	-2.482213
C	3.856561	-1.614440	-0.896300
H	4.720299	-1.983112	-0.325772
H	4.016119	-1.936051	-1.935824

C	2.429023	0.924581	-1.916525
H	2.092850	1.887062	-1.513281
H	2.819923	1.127483	-2.923333
H	-1.182783	-1.033231	0.835540
H	0.090253	-1.865692	-0.715937
C	-3.736857	-2.515719	-1.180809
H	-4.468126	-3.323606	-1.061661
H	-3.991953	-1.737070	-0.452984
H	-3.803683	-2.097864	-2.187054
C	-2.339384	-3.003314	-0.911718
O	-1.430491	-2.780790	-1.698380
C	-2.924077	1.040637	-0.321762
C	-3.678462	1.482296	-1.415353
C	-3.597399	0.556953	0.801488
C	-5.067914	1.417458	-1.397110
H	-3.177380	1.882937	-2.292848
C	-4.990907	0.510076	0.831660
H	-3.027662	0.194690	1.648752
C	-5.729092	0.929445	-0.270979
H	-5.635819	1.752534	-2.260656
H	-5.495268	0.131086	1.716221
H	-6.814353	0.880637	-0.253607
C	-0.888983	2.928768	-0.567290
C	-0.215934	3.547392	-1.623296
C	-1.385629	3.732830	0.467355
C	-0.029815	4.930041	-1.639748
H	0.182088	2.958265	-2.443896
C	-1.208068	5.110931	0.450149
H	-1.907562	3.271816	1.302657
C	-0.521585	5.715278	-0.602857
H	0.499163	5.391133	-2.469445
H	-1.601006	5.715267	1.263000
H	-0.376330	6.791698	-0.615185
C	-2.913066	-3.439408	1.546674
C	-2.080129	-3.843142	0.330600
H	-2.743020	-2.389066	1.803181
H	-3.984663	-3.592799	1.373420
H	-2.629632	-4.052115	2.410085
C	-2.299265	-5.319592	-0.040799
H	-1.018528	-3.700006	0.560726
H	-1.682852	-5.612680	-0.897221
H	-2.034705	-5.961647	0.806422
H	-3.348997	-5.515599	-0.290900
H	-0.019859	-2.949960	2.512225

H	1.177161	-1.717671	3.707684

E5Ra

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.095151	-0.232879	1.048716
N	1.348809	-0.984600	-0.825317
C	-0.731976	0.317788	-2.226608
H	-1.097761	-0.679115	-2.509246
H	-1.103939	1.013208	-2.985260
C	2.698925	-2.515378	1.225715
C	-0.969077	0.032213	2.411332
O	-1.668159	0.193620	3.338314
P	1.596909	-1.469772	2.274107
P	-1.388293	0.625564	-0.532525
Si	2.887962	-1.767180	-0.498575
Si	1.140504	0.104615	-2.181145
C	3.233074	-3.193382	-1.678896
H	3.388188	-2.852207	-2.708837
H	4.136185	-3.737636	-1.372853
H	2.403814	-3.911471	-1.687268
C	1.672762	-0.650555	-3.823631
H	1.373594	-0.011052	-4.664468
H	2.761329	-0.773538	-3.884150
H	1.215760	-1.636076	-3.975556
H	3.649987	-2.730920	1.723667
H	2.182653	-3.471412	1.081476
P	1.275083	1.694398	1.591445
C	3.079747	1.660338	1.194924
H	3.534734	2.602362	1.531247
H	3.537653	0.870272	1.806333
Si	3.595589	1.330737	-0.602769
C	0.895391	3.443969	1.133893
H	0.903176	3.605052	0.054940
H	-0.098008	3.714994	1.500650
H	1.631170	4.116100	1.591015
C	1.334730	1.967197	3.418770
H	1.649265	1.060274	3.942713
H	2.025901	2.777904	3.676022
H	0.335173	2.231302	3.779087
C	5.012305	2.510070	-0.999703

H	4.677440	3.554720	-0.967132
H	5.832121	2.401979	-0.278524
H	5.423684	2.325443	-1.999725
C	4.219508	-0.449350	-0.695858
H	5.011718	-0.580323	0.054500
H	4.704376	-0.603077	-1.671175
C	2.199087	1.622974	-1.855321
H	1.584869	2.461022	-1.506762
H	2.653685	1.954176	-2.799444
H	-2.464400	-2.379306	0.730768
H	0.580634	-1.683752	-0.704032
C	-1.525814	-2.954784	0.815976
O	-0.426023	-2.167156	0.536333
C	-3.127310	0.013267	-0.642448
C	-3.802127	-0.068202	-1.865093
C	-3.818078	-0.323251	0.525457
C	-5.127260	-0.490731	-1.920820
H	-3.295994	0.196794	-2.788424
C	-5.147835	-0.734541	0.473149
H	-3.315150	-0.278188	1.485374
C	-5.804192	-0.824979	-0.750331
H	-5.631507	-0.556181	-2.880782
H	-5.665016	-0.994363	1.392267
H	-6.838399	-1.154435	-0.793397
C	-1.749567	2.433071	-0.514397
C	-1.293186	3.327640	-1.484038
C	-2.491292	2.935485	0.562650
C	-1.562523	4.692106	-1.378308
H	-0.705898	2.975729	-2.326396
C	-2.770820	4.293084	0.663991
H	-2.848813	2.259611	1.335085
C	-2.301355	5.178674	-0.305714
H	-1.192685	5.373672	-2.139231
H	-3.350764	4.661997	1.505082
H	-2.512733	6.240776	-0.223387
C	-1.644932	-4.089547	-0.233285
C	-0.428939	-5.016796	-0.230699
C	-1.853991	-3.499394	-1.629048
H	-2.537630	-4.679714	0.024017
H	-0.316544	-5.549240	0.720557
H	-0.499942	-5.771153	-1.024307
H	0.481980	-4.431024	-0.398995
H	-2.696419	-2.797469	-1.641807
H	-0.956144	-2.955966	-1.948194

H	-2.053260	-4.282561	-2.371279
C	-1.490404	-3.500158	2.249136
H	-1.513844	-2.669339	2.962976
H	-2.350634	-4.150857	2.457228
H	-0.573314	-4.072901	2.433830
H	1.086140	-2.405123	3.195174
H	2.565221	-0.904748	3.143422

E5Sa

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.377413	0.145017	1.198591
N	0.743904	-1.346841	-0.156257
C	-0.880855	0.262258	-1.975922
H	-1.774989	-0.366067	-2.059676
H	-0.874482	0.909462	-2.858407
C	2.363395	-2.525393	2.004570
C	-0.282610	1.165765	2.476154
O	-0.685379	1.837799	3.346863
P	1.197505	-1.318812	2.739445
P	-0.974254	1.178379	-0.383917
Si	1.919856	-2.580535	0.147281
Si	0.657863	-0.826218	-1.801272
C	1.372190	-4.353671	-0.212299
H	1.021489	-4.488806	-1.241694
H	2.215358	-5.041022	-0.060705
H	0.566420	-4.672181	0.460058
C	0.535564	-2.235863	-3.068347
H	0.201247	-1.853183	-4.041615
H	1.507730	-2.717738	-3.231478
H	-0.156093	-3.033670	-2.768665
H	3.379952	-2.136987	2.133417
H	2.320672	-3.503812	2.493761
P	2.267969	1.398577	1.147859
C	3.760499	0.545620	0.473712
H	4.572478	1.284519	0.425029
H	4.075035	-0.191203	1.224623
Si	3.669743	-0.376937	-1.196533
C	2.395977	3.020410	0.284155
H	2.230295	2.909599	-0.789328
H	1.644273	3.715416	0.668887

H	3.390749	3.454213	0.439072
C	2.886886	1.929216	2.802839
H	3.013648	1.065339	3.462969
H	3.847453	2.450732	2.722756
H	2.157692	2.601389	3.267061
C	5.301139	-0.019083	-2.078162
H	5.411378	1.050639	-2.297676
H	6.160674	-0.321600	-1.466150
H	5.367217	-0.560662	-3.029956
C	3.502344	-2.221685	-0.842749
H	4.386220	-2.592739	-0.305139
H	3.478875	-2.763104	-1.799803
C	2.210140	0.162499	-2.265632
H	2.038948	1.240325	-2.146236
H	2.455873	0.003088	-3.325372
H	-2.627009	-1.478324	-0.338073
H	-2.049995	-2.527078	-2.364038
C	-4.511397	-2.481568	-0.322649
H	-4.978907	-3.399380	-0.695210
H	-4.653741	-2.426944	0.760798
H	-5.026091	-1.626938	-0.772154
C	-3.037671	-2.436309	-0.686736
O	-2.981082	-2.478989	-2.111767
C	-2.778847	1.194197	-0.004215
C	-3.685821	1.716774	-0.934208
C	-3.268364	0.659463	1.188775
C	-5.050714	1.709564	-0.672551
H	-3.319796	2.135917	-1.868217
C	-4.636689	0.655919	1.455336
H	-2.579033	0.236488	1.912972
C	-5.528993	1.181260	0.526686
H	-5.743736	2.116377	-1.403290
H	-5.002927	0.236269	2.387809
H	-6.595631	1.176948	0.731955
C	-0.725598	2.951430	-0.787317
C	-0.157709	3.402396	-1.979718
C	-1.065452	3.890549	0.195489
C	0.070998	4.762244	-2.186434
H	0.129750	2.699232	-2.755238
C	-0.842071	5.246461	-0.012131
H	-1.505711	3.557790	1.131841
C	-0.268974	5.686884	-1.204950
H	0.516744	5.096255	-3.119021
H	-1.115448	5.960906	0.758840

H	-0.091532	6.745949	-1.367227
C	-2.024510	-3.327142	1.449187
C	-2.163409	-3.532612	-0.058571
H	-1.690925	-2.306591	1.672021
H	-2.973300	-3.498385	1.972449
H	-1.287708	-4.020890	1.871761
C	-2.620265	-4.947649	-0.407010
H	-1.162747	-3.377630	-0.485360
H	-2.782783	-5.052147	-1.485083
H	-1.867268	-5.684587	-0.103735
H	-3.557154	-5.204589	0.102347
H	0.192756	-2.167761	3.256778
H	1.775253	-0.972924	3.982331

F5R

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.299488	0.224917	0.980271
N	0.784333	-1.395177	-0.155974
C	-1.160605	0.402738	-1.393879
H	-2.131498	0.001788	-1.091012
H	-1.339327	0.997218	-2.293206
C	2.992411	-2.701913	1.303108
C	1.346509	1.367714	2.311634
O	1.378003	2.087818	3.238465
P	2.391165	-1.285164	2.281064
P	-0.459650	1.359707	0.011597
Si	1.794633	-2.803147	-0.179489
Si	0.084058	-0.994070	-1.688615
C	0.872861	-4.444686	-0.006464
H	-0.018670	-4.494029	-0.641914
H	1.524852	-5.287009	-0.274212
H	0.550812	-4.603668	1.030681
C	-0.814218	-2.427927	-2.531027
H	-1.351913	-2.071257	-3.419176
H	-0.120342	-3.209947	-2.864891
H	-1.543075	-2.884329	-1.851209
H	4.002401	-2.465713	0.947117
H	3.055101	-3.629624	1.885511
C	1.102038	-2.046109	3.356129
H	1.495502	-2.897826	3.923240

H	0.720556	-1.297055	4.058907
H	0.267442	-2.389375	2.736295
C	3.706423	-0.937450	3.517391
H	3.431945	-0.065649	4.120816
H	3.859543	-1.796188	4.180799
H	4.654945	-0.723715	3.015111
P	3.073104	1.142903	-0.043584
C	4.024885	-0.021016	-1.115868
H	4.820903	0.548271	-1.616822
H	4.539040	-0.722207	-0.444123
Si	3.112349	-1.075410	-2.424595
C	2.901013	2.595823	-1.165717
H	2.153658	2.414428	-1.941418
H	2.574396	3.467841	-0.591482
H	3.857257	2.830953	-1.647556
C	4.408029	1.805354	1.040922
H	4.737458	1.038095	1.746535
H	5.274110	2.150204	0.464007
H	4.013293	2.644962	1.623187
C	4.251493	-1.123978	-3.932186
H	4.371616	-0.128858	-4.379485
H	5.251054	-1.492695	-3.668476
H	3.849847	-1.788851	-4.707182
C	2.846845	-2.821023	-1.761136
H	3.805669	-3.326319	-1.579140
H	2.338804	-3.402097	-2.545450
C	1.420842	-0.396596	-2.903082
H	1.444818	0.698568	-2.964892
H	1.177512	-0.754237	-3.914302
H	-4.456556	-1.686477	1.353563
C	-4.257094	-2.192732	0.391096
C	-1.832725	1.371407	1.240905
C	-2.742626	2.418467	1.401412
C	-1.952362	0.241743	2.060048
C	-3.745681	2.340539	2.366294
H	-2.670517	3.303518	0.776243
C	-2.957589	0.159306	3.018271
H	-1.244013	-0.578021	1.951610
C	-3.856247	1.212947	3.176382
H	-4.444531	3.164080	2.483485
H	-3.030732	-0.722093	3.649098
H	-4.635229	1.157201	3.931189
C	-0.342324	3.120412	-0.487215
C	-0.562795	3.576331	-1.787774

C	0.074748	4.040999	0.485102
C	-0.360812	4.916492	-2.115289
H	-0.885218	2.892570	-2.565842
C	0.262448	5.379987	0.162386
H	0.258068	3.707832	1.502584
C	0.052270	5.821259	-1.143649
H	-0.529841	5.249795	-3.135345
H	0.582364	6.078584	0.930049
H	0.209142	6.865206	-1.398979
C	-4.433203	-1.163571	-0.708921
C	-4.741539	0.159636	-0.394669
C	-4.231181	-1.506487	-2.050177
C	-4.839653	1.127393	-1.392841
H	-4.880467	0.441007	0.645560
C	-4.329077	-0.543985	-3.049712
H	-3.972499	-2.529285	-2.307544
C	-4.631242	0.778230	-2.723579
H	-5.064868	2.155950	-1.125257
H	-4.161209	-0.823386	-4.086261
H	-4.699247	1.531405	-3.503595
C	-5.255197	-3.345023	0.257186
H	-5.070881	-3.910418	-0.662533
H	-5.182273	-4.038799	1.101596
H	-6.279386	-2.958709	0.230421
N	-2.879724	-2.692145	0.349171
H	-2.250518	-1.900956	0.244220
C	-2.478568	-3.430887	1.533507
H	-2.940276	-4.423888	1.548295
H	-1.395175	-3.572019	1.503070
H	-2.739637	-2.924252	2.481320

F4S

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.389745	-0.073344	0.935489
N	0.022938	-1.286532	-1.031990
C	1.274893	1.034679	-2.123082
H	0.310529	1.383569	-2.511844
H	2.042240	1.515506	-2.738261
C	-1.039362	-3.156686	1.003835
C	0.396744	0.898123	2.381724

O	0.375174	1.538918	3.367064
P	-1.207945	-1.462751	1.729287
P	1.338658	1.521857	-0.334593
Si	-0.507460	-2.967664	-0.803553
Si	1.263906	-0.842560	-2.213796
C	-1.969292	-3.286986	-1.941356
H	-1.669742	-3.219285	-2.994694
H	-2.398376	-4.284405	-1.783306
H	-2.768997	-2.551986	-1.776746
C	0.814732	-1.401990	-3.957009
H	1.556454	-1.042435	-4.682052
H	0.787648	-2.495871	-4.038171
H	-0.162608	-1.019699	-4.272936
H	-0.257980	-3.686005	1.562473
H	-1.964576	-3.739908	1.100771
C	-2.927513	-1.055897	1.226742
H	-3.656616	-1.794315	1.581551
H	-3.187501	-0.073564	1.631529
H	-2.994202	-0.986691	0.137893
C	-1.519801	-1.774449	3.519021
H	-1.794490	-0.827171	3.996199
H	-2.341028	-2.486610	3.658711
H	-0.632418	-2.156089	4.027358
P	2.180565	-1.272406	1.734808
C	2.667836	-2.955746	1.098447
H	3.665253	-3.195076	1.492617
H	1.989331	-3.689087	1.554464
Si	2.640287	-3.271192	-0.765818
C	3.854363	-0.489702	1.798269
H	4.233200	-0.251974	0.801555
H	3.787562	0.449192	2.355225
H	4.574177	-1.146715	2.300641
C	2.078337	-1.709753	3.530998
H	1.323817	-2.486081	3.684553
H	3.035278	-2.093033	3.904701
H	1.794516	-0.831143	4.119225
C	4.024869	-4.479481	-1.185339
H	5.008430	-4.044661	-0.967463
H	3.935882	-5.408933	-0.609244
H	4.010373	-4.747241	-2.249295
C	0.974877	-4.046215	-1.215029
H	0.880115	-5.012917	-0.700964
H	0.967417	-4.271637	-2.291566
C	2.877126	-1.668661	-1.737893

H	3.500490	-0.991889	-1.142018
H	3.439511	-1.882156	-2.657507
H	-0.897510	0.725157	0.352612
H	-0.785897	-0.671222	-1.131977
C	-3.774199	2.449670	-1.247822
H	-4.570823	3.127750	-0.934201
H	-2.945824	2.532793	-0.531837
H	-3.399867	2.796379	-2.214782
C	-4.240009	1.016001	-1.318847
C	0.557793	3.202010	-0.398219
C	1.027459	4.151342	-1.315049
C	-0.498408	3.551940	0.444229
C	0.441929	5.409187	-1.403952
H	1.864744	3.906893	-1.964434
C	-1.079964	4.817795	0.365547
H	-0.875069	2.823045	1.153266
C	-0.617240	5.745745	-0.561760
H	0.814334	6.129704	-2.126957
H	-1.899584	5.074377	1.031316
H	-1.075849	6.728411	-0.628072
C	3.087162	2.085815	-0.118732
C	4.136180	1.768325	-0.984479
C	3.381485	2.812770	1.042851
C	5.446038	2.150420	-0.691896
H	3.951729	1.206672	-1.895490
C	4.683521	3.201824	1.332756
H	2.581989	3.068235	1.734572
C	5.724682	2.864250	0.468240
H	6.247444	1.886987	-1.376834
H	4.888282	3.762809	2.240357
H	6.744401	3.160298	0.696976
C	-5.365054	0.585706	-0.435662
C	-6.055602	-0.600387	-0.713439
C	-5.706544	1.308215	0.712249
C	-7.063760	-1.047942	0.130671
H	-5.782941	-1.164500	-1.599437
C	-6.709143	0.853499	1.565356
H	-5.172124	2.218561	0.966446
C	-7.392829	-0.323264	1.276089
H	-7.594180	-1.967017	-0.102338
H	-6.951353	1.419662	2.460204
H	-8.177359	-0.675695	1.939640
N	-3.696128	0.116464	-2.047131
C	-2.565884	0.478491	-2.878063

H	-1.793911	1.018224	-2.312897
H	-2.126165	-0.433892	-3.291459
H	-2.866779	1.114846	-3.722541

F5S

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.561835	-0.152143	0.967925
N	0.428463	-1.368712	-0.700880
C	0.492319	1.105924	-2.188610
H	-0.556677	1.050281	-2.499550
H	0.998170	1.772726	-2.893002
C	0.432067	-3.543880	1.284850
C	0.206813	0.826240	2.385173
O	-0.021685	1.434029	3.362539
P	-0.138948	-2.011796	2.094486
P	0.498021	1.687340	-0.447746
Si	0.631405	-3.085258	-0.553924
Si	1.129760	-0.672806	-2.116169
C	-0.637252	-4.114800	-1.499261
H	-0.615502	-3.911613	-2.576500
H	-0.437732	-5.185879	-1.362857
H	-1.650805	-3.909198	-1.134893
C	0.610528	-1.501756	-3.737790
H	0.952227	-0.909746	-4.597290
H	1.032776	-2.507645	-3.852721
H	-0.481102	-1.588974	-3.813181
H	1.402643	-3.817954	1.715432
H	-0.253670	-4.384970	1.446809
C	-1.955385	-2.054429	1.831272
H	-2.407366	-2.961720	2.249209
H	-2.420134	-1.181534	2.302063
H	-2.164588	-2.019660	0.757335
C	-0.026700	-2.334378	3.901356
H	-0.282742	-1.427068	4.458472
H	-0.711530	-3.137944	4.194473
H	0.987675	-2.635251	4.179238
P	2.750352	-0.247244	1.553947
C	3.678827	-1.711111	0.917261
H	4.733686	-1.586864	1.199988
H	3.322439	-2.589656	1.471761

Si	3.588482	-2.163579	-0.935094
C	3.966667	1.088842	1.186505
H	4.085089	1.241888	0.112377
H	3.629714	2.033018	1.622707
H	4.944720	0.833206	1.610342
C	3.085376	-0.387406	3.362612
H	2.565225	-1.250398	3.785040
H	4.157585	-0.495490	3.562393
H	2.717817	0.508383	3.873874
C	5.326194	-2.711343	-1.433474
H	6.042979	-1.881782	-1.381138
H	5.696868	-3.511996	-0.780812
H	5.338359	-3.093353	-2.462101
C	2.370164	-3.586106	-1.134079
H	2.717927	-4.475723	-0.590571
H	2.332468	-3.871128	-2.196144
C	3.022982	-0.732006	-2.029199
H	3.425227	0.211211	-1.637665
H	3.449183	-0.857680	-3.035005
H	-2.499726	0.164801	-0.385615
C	-3.439020	0.850417	-2.183230
H	-4.319322	0.644150	-2.802008
H	-3.548219	1.853161	-1.761144
H	-2.562493	0.866323	-2.839445
C	-3.263005	-0.210415	-1.082802
C	-1.003363	2.761253	-0.365157
C	-1.194620	3.757175	-1.332103
C	-1.960775	2.605845	0.637983
C	-2.314410	4.578467	-1.294933
H	-0.456015	3.892458	-2.118397
C	-3.081371	3.436133	0.683797
H	-1.840897	1.832476	1.389130
C	-3.261487	4.420724	-0.281975
H	-2.448356	5.345080	-2.052707
H	-3.815134	3.303228	1.473388
H	-4.134613	5.066102	-0.247949
C	1.788232	2.990774	-0.358115
C	2.795869	3.146599	-1.311292
C	1.783692	3.829996	0.763480
C	3.784056	4.116377	-1.145177
H	2.833205	2.503317	-2.185407
C	2.765327	4.800463	0.926511
H	1.007567	3.721014	1.517203
C	3.772516	4.944087	-0.027660

H	4.563163	4.222010	-1.894855
H	2.745292	5.445547	1.800218
H	4.541189	5.700771	0.099443
C	-4.549208	-0.399447	-0.273303
C	-4.955957	-1.667344	0.151001
C	-5.334114	0.699068	0.096839
C	-6.105836	-1.835214	0.918918
H	-4.353846	-2.525140	-0.129477
C	-6.480052	0.536246	0.870564
H	-5.048832	1.699131	-0.213891
C	-6.873532	-0.733623	1.285523
H	-6.400857	-2.833573	1.231408
H	-7.069035	1.406951	1.146906
H	-7.770704	-0.862782	1.884357
N	-2.736737	-1.486275	-1.554019
H	-1.719239	-1.447362	-1.576823
C	-3.299150	-2.001025	-2.787646
H	-3.130435	-1.367365	-3.674165
H	-2.870332	-2.986883	-2.992233
H	-4.382538	-2.128247	-2.674896

F4R

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.106425	0.324654	1.210805
N	0.984130	-1.466913	-0.315648
C	-1.315309	0.026914	-1.059078
H	-1.873720	-0.732746	-0.502716
H	-2.017508	0.455955	-1.781206
C	3.465613	-2.102221	1.160826
C	1.084225	1.466683	2.529068
O	1.075174	2.209861	3.438680
P	2.377940	-1.164792	2.326431
P	-0.709446	1.213573	0.215328
Si	2.433451	-2.493313	-0.380868
Si	0.156646	-0.891180	-1.778096
C	1.947441	-4.309742	-0.337372
H	1.217997	-4.543546	-1.121793
H	2.826861	-4.946505	-0.497648
H	1.510595	-4.592423	0.627608
C	-0.446070	-2.338177	-2.815667

H	-1.094229	-1.998354	-3.633401
H	0.383565	-2.898853	-3.265015
H	-1.030197	-3.024966	-2.189427
H	4.303950	-1.447599	0.892942
H	3.888160	-3.009808	1.612239
C	1.464279	-2.556104	3.121687
H	2.138762	-3.308453	3.548819
H	0.822815	-2.152345	3.911242
H	0.809333	-3.040990	2.391989
C	3.477358	-0.737519	3.742132
H	2.860958	-0.319537	4.545837
H	4.001519	-1.620369	4.125336
H	4.214111	0.018703	3.463859
P	2.854847	1.457253	0.243242
C	3.943660	0.770751	-1.106513
H	4.502558	1.605581	-1.551438
H	4.700225	0.134496	-0.627640
Si	3.173183	-0.268810	-2.485068
C	2.562278	3.137979	-0.463335
H	1.900516	3.099889	-1.332568
H	2.081587	3.765793	0.291896
H	3.507204	3.606613	-0.762451
C	4.202512	1.933300	1.420825
H	4.750497	1.040504	1.736503
H	4.917954	2.622482	0.956915
H	3.776974	2.409439	2.309888
C	4.153090	0.030167	-4.066944
H	4.043414	1.066263	-4.411114
H	5.223222	-0.158319	-3.914990
H	3.812346	-0.626607	-4.876983
C	3.324361	-2.080239	-1.978663
H	4.387406	-2.340877	-1.880584
H	2.923563	-2.716686	-2.780754
C	1.357602	0.158348	-2.768275
H	1.219894	1.222192	-2.540776
H	1.124540	0.033694	-3.835166
H	-0.106496	-0.527144	1.863704
H	0.285181	-1.866093	0.312925
C	-3.183328	-2.918789	0.399483
C	-2.246874	1.495276	1.219149
C	-3.350562	2.140588	0.645854
C	-2.350313	1.046375	2.537816
C	-4.524825	2.327898	1.366529
H	-3.293798	2.504518	-0.376168

C	-3.530253	1.225590	3.260701
H	-1.500568	0.548766	2.992761
C	-4.620723	1.864212	2.677928
H	-5.367617	2.833822	0.903193
H	-3.590873	0.869416	4.285519
H	-5.538152	2.008621	3.241812
C	-0.716679	2.833902	-0.674588
C	-0.792013	2.971427	-2.062375
C	-0.585293	3.993140	0.102139
C	-0.712603	4.229666	-2.661488
H	-0.909851	2.098257	-2.696436
C	-0.517193	5.247826	-0.489987
H	-0.526303	3.907631	1.184954
C	-0.572247	5.370130	-1.878524
H	-0.768512	4.314425	-3.743371
H	-0.414183	6.133131	0.131194
H	-0.511155	6.349340	-2.344528
C	-4.001386	-2.115867	-0.561014
C	-4.062727	-2.493503	-1.909099
C	-4.663156	-0.951717	-0.159662
C	-4.763824	-1.726461	-2.829463
H	-3.549101	-3.396245	-2.220418
C	-5.365470	-0.181806	-1.083832
H	-4.608076	-0.610315	0.869409
C	-5.419021	-0.564690	-2.419668
H	-4.802999	-2.035127	-3.870403
H	-5.859909	0.726191	-0.752617
H	-5.967957	0.036642	-3.138860
C	-3.347134	-2.632002	1.872448
H	-4.393372	-2.446130	2.129655
H	-2.983782	-3.454071	2.492100
H	-2.774571	-1.733632	2.139674
N	-2.363361	-3.764086	-0.098757
C	-1.538743	-4.574726	0.775273
H	-2.141947	-5.238741	1.410189
H	-0.885535	-5.202070	0.163629
H	-0.908779	-3.965987	1.437519

TSF4-5S

Coordinates (Angstroms)		
X	Y	Z

Mn	-0.138166	-0.197842	0.734569
N	0.311112	-1.444128	-1.105322
C	0.883164	1.205819	-2.131419
H	-0.089288	1.203126	-2.631340
H	1.530804	1.883075	-2.697492
C	-0.036281	-3.541744	0.962596
C	-0.691554	0.644120	2.159870
O	-1.057113	1.152930	3.154133
P	-1.197304	-2.182036	1.407971
P	0.576823	1.715469	-0.387162
Si	0.531262	-3.193852	-0.812770
Si	1.498298	-0.573564	-2.095278
C	-0.517403	-4.133828	-2.053149
H	-0.104956	-4.018413	-3.063435
H	-0.548165	-5.207057	-1.827947
H	-1.544970	-3.753562	-2.068361
C	1.621648	-1.271820	-3.841301
H	2.100882	-2.258980	-3.836838
H	0.644798	-1.377821	-4.323765
H	2.237209	-0.619959	-4.474969
H	0.828004	-3.516923	1.633042
H	-0.499841	-4.531442	1.063346
C	-2.710025	-2.863084	0.609759
H	-2.736886	-3.949559	0.756186
H	-3.601600	-2.433965	1.071313
H	-2.726897	-2.626614	-0.457910
C	-1.712635	-2.470451	3.153627
H	-2.572425	-1.820482	3.352077
H	-2.024778	-3.510385	3.302423
H	-0.937506	-2.221353	3.878219
P	1.813313	-0.714918	1.948375
C	3.114056	-1.970757	1.476067
H	4.041772	-1.680694	1.987705
H	2.831903	-2.935522	1.916829
Si	3.499589	-2.279355	-0.348493
C	2.927817	0.689657	2.378247
H	3.441732	1.081996	1.498066
H	2.342630	1.500856	2.818587
H	3.680842	0.364867	3.105381
C	1.529961	-1.308978	3.677139
H	1.109357	-2.317755	3.671059
H	2.475745	-1.343606	4.229661
H	0.839034	-0.641712	4.201247
C	5.293085	-2.838955	-0.490161

H	5.986168	-2.062121	-0.144209
H	5.478333	-3.740620	0.106708
H	5.549859	-3.073410	-1.530788
C	2.350190	-3.626082	-0.986030
H	2.539244	-4.562890	-0.443051
H	2.581575	-3.828510	-2.041249
C	3.210030	-0.702888	-1.331487
H	3.409400	0.142008	-0.662803
H	3.944326	-0.634976	-2.146265
H	-1.572644	0.230037	-0.339140
H	-0.655316	-1.337800	-1.496690
C	-2.886258	1.357674	-1.996843
H	-3.764160	1.314928	-2.656220
H	-3.067616	2.130069	-1.249311
H	-2.032213	1.658608	-2.605627
C	-2.726404	-0.020254	-1.357618
C	-0.606476	3.125667	-0.536731
C	-0.574912	3.968872	-1.651971
C	-1.526326	3.392104	0.478518
C	-1.468681	5.028541	-1.767161
H	0.146886	3.794506	-2.445091
C	-2.414136	4.460393	0.372509
H	-1.562571	2.758627	1.355940
C	-2.396562	5.273474	-0.756601
H	-1.441180	5.664377	-2.647648
H	-3.130338	4.644229	1.168127
H	-3.099815	6.096148	-0.848267
C	2.056784	2.755084	0.019201
C	3.240859	2.766608	-0.721460
C	1.981089	3.566169	1.159611
C	4.329490	3.541194	-0.318729
H	3.337480	2.169936	-1.622292
C	3.060037	4.344569	1.558684
H	1.067924	3.582312	1.749932
C	4.245149	4.328357	0.823826
H	5.242904	3.528844	-0.906964
H	2.978010	4.962278	2.448397
H	5.091902	4.932212	1.136895
C	-3.850910	-0.210079	-0.347784
C	-4.972932	-0.935162	-0.754765
C	-3.869526	0.395709	0.906994
C	-6.072550	-1.080450	0.087440
H	-4.954108	-1.413927	-1.729390
C	-4.964027	0.253956	1.754409

H	-2.998099	0.953291	1.227099
C	-6.070695	-0.491526	1.350009
H	-6.930479	-1.661498	-0.240810
H	-4.947956	0.721836	2.735289
H	-6.923898	-0.609625	2.012442
N	-2.426055	-1.083171	-2.110034
C	-2.057922	-0.861303	-3.490800
H	-1.229193	-0.152917	-3.661790
H	-1.749222	-1.818031	-3.930188
H	-2.900362	-0.488890	-4.099074

TSF4-5R

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.464527	-0.060831	1.011615
N	1.162755	-1.153472	-0.851244
C	-1.042277	0.418717	-1.974266
H	-1.701473	-0.449514	-2.074347
H	-1.376908	1.148434	-2.718385
C	3.281794	-2.164243	0.954840
C	-0.193515	0.384928	2.572103
O	-0.595064	0.614154	3.649450
P	2.111133	-1.318997	2.128543
P	-1.194845	0.975477	-0.230010
Si	2.773837	-1.927253	-0.856601
Si	0.714461	-0.191563	-2.273623
C	2.673167	-3.555297	-1.797332
H	3.375265	-4.301233	-1.405306
H	1.662943	-3.971908	-1.740302
H	2.911072	-3.403021	-2.856581
C	0.736385	-1.237299	-3.840775
H	0.270741	-0.698042	-4.675759
H	1.760356	-1.487299	-4.145708
H	0.191730	-2.178976	-3.707911
H	4.278548	-1.728453	1.098585
H	3.379322	-3.224436	1.214583
C	1.602594	-2.650303	3.301332
H	0.906799	-2.228179	4.034294
H	1.110578	-3.476106	2.794667
H	2.476665	-3.044700	3.831444
C	3.330635	-0.567727	3.309765

H	2.810849	-0.231247	4.212925
H	4.054183	-1.335318	3.606124
H	3.881613	0.275859	2.890511
P	1.918245	1.792913	1.006828
C	3.583240	1.455102	0.286686
H	4.235951	2.322572	0.453822
H	4.051342	0.611117	0.803997
Si	3.594449	1.019381	-1.571237
C	1.727338	3.481314	0.258383
H	1.584449	3.465972	-0.820846
H	0.884985	4.012622	0.701846
H	2.640503	4.049358	0.473405
C	2.239402	2.457808	2.706460
H	2.222953	1.687476	3.473950
H	3.189974	3.001404	2.758101
H	1.430629	3.160170	2.937739
C	4.897677	2.106829	-2.388961
H	4.630613	3.168524	-2.310993
H	5.878560	1.977092	-1.914898
H	5.010306	1.871217	-3.454236
C	4.023765	-0.802013	-1.709087
H	5.021900	-0.996284	-1.293217
H	4.073818	-1.070917	-2.773781
C	1.949714	1.217149	-2.482947
H	1.469578	2.174995	-2.261883
H	2.206362	1.258360	-3.552498
H	-0.740352	-1.521630	0.831941
H	0.516133	-1.978314	-0.745284
C	-1.275196	-2.805115	0.538535
C	-2.983602	0.788049	0.179418
C	-3.963901	1.064474	-0.777942
C	-3.377981	0.530081	1.493145
C	-5.309428	1.085486	-0.428729
H	-3.678447	1.270610	-1.805770
C	-4.725203	0.560856	1.847575
H	-2.633259	0.302073	2.246731
C	-5.693685	0.839404	0.888270
H	-6.059750	1.294609	-1.185879
H	-5.014150	0.361725	2.875889
H	-6.744710	0.863909	1.162545
C	-1.270781	2.820308	-0.333182
C	-1.042953	3.557855	-1.494633
C	-1.597257	3.510490	0.842574
C	-1.126185	4.950477	-1.483688

H	-0.781416	3.060126	-2.423108
C	-1.689461	4.896865	0.854771
H	-1.778792	2.958090	1.761227
C	-1.447628	5.624084	-0.311157
H	-0.938944	5.505489	-2.398760
H	-1.944990	5.411732	1.776530
H	-1.516657	6.708009	-0.303467
C	-2.495558	-2.527960	-0.351450
C	-2.368746	-2.642577	-1.741689
C	-3.781305	-2.337679	0.159784
C	-3.464740	-2.521125	-2.588048
H	-1.389422	-2.875776	-2.143296
C	-4.889393	-2.241953	-0.680656
H	-3.944587	-2.264670	1.227443
C	-4.738537	-2.319214	-2.059577
H	-3.325083	-2.609975	-3.662512
H	-5.873465	-2.096597	-0.244887
H	-5.601857	-2.239918	-2.714670
C	-1.679811	-3.137341	1.977305
H	-2.275130	-4.059659	2.007231
H	-0.810051	-3.266016	2.616786
H	-2.264979	-2.324182	2.412996
N	-0.390989	-3.559149	-0.149549
C	0.469968	-4.466971	0.553508
H	0.027709	-4.920249	1.456184
H	0.730384	-5.302690	-0.111446
H	1.434910	-4.029892	0.861835

F4Sa

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.209607	-0.117826	1.042077
N	0.439764	-1.467027	-0.876434
C	-0.169828	1.041996	-2.080509
H	-1.183376	0.668386	-2.273000
H	0.015882	1.832230	-2.815310
C	1.052117	-3.389572	1.282780
C	-0.199192	0.750630	2.495256
O	-0.482756	1.309690	3.490006
P	-0.108452	-2.141470	2.000107
P	-0.164885	1.630552	-0.323912

Si	1.135245	-3.077105	-0.581686
Si	0.990697	-0.431652	-2.203610
C	0.106291	-4.371322	-1.474403
H	0.116876	-4.208896	-2.559148
H	0.493512	-5.380965	-1.287766
H	-0.938638	-4.348973	-1.139652
C	0.802011	-1.264497	-3.884848
H	1.093028	-0.576140	-4.689004
H	1.441827	-2.151701	-3.971999
H	-0.230135	-1.576558	-4.077939
H	2.038751	-3.224860	1.732602
H	0.754132	-4.421056	1.512975
C	-1.724992	-2.958740	1.672115
H	-1.719709	-4.012043	1.979087
H	-2.498853	-2.431918	2.238571
H	-1.993894	-2.892420	0.613155
C	-0.023911	-2.448689	3.815369
H	-0.757517	-1.805417	4.313736
H	-0.253602	-3.493931	4.051949
H	0.959692	-2.204788	4.221850
P	2.434016	0.073094	1.587562
C	3.803113	-0.954033	0.845766
H	4.760163	-0.471239	1.087518
H	3.817623	-1.914742	1.378031
Si	3.752383	-1.355310	-0.999944
C	3.229377	1.737969	1.496233
H	3.292966	2.105003	0.468820
H	2.624136	2.450188	2.064500
H	4.238886	1.714487	1.923605
C	2.824035	-0.266870	3.364939
H	2.680053	-1.329717	3.578085
H	3.863992	-0.012442	3.601716
H	2.159662	0.308412	4.017154
C	5.523153	-1.457585	-1.637618
H	6.035211	-0.493213	-1.528812
H	6.106066	-2.207499	-1.088677
H	5.550359	-1.728569	-2.700357
C	2.900746	-3.026949	-1.219004
H	3.491222	-3.801886	-0.710362
H	2.903538	-3.290963	-2.286665
C	2.806877	-0.035198	-1.962893
H	2.935219	0.922249	-1.445090
H	3.265087	0.085030	-2.954470
H	-1.348025	-0.279064	0.646969

H	-0.581351	-1.509278	-0.873221
C	-4.316887	-0.096436	-1.591494
H	-5.169723	0.426524	-1.153168
H	-3.430830	0.525280	-1.408640
H	-4.470353	-0.156446	-2.674139
C	-4.111542	-1.463252	-0.980257
C	-1.797657	2.503643	-0.240213
C	-2.158533	3.403545	-1.251906
C	-2.694566	2.279610	0.804625
C	-3.392677	4.043142	-1.232137
H	-1.465393	3.612041	-2.063064
C	-3.925511	2.934565	0.837394
H	-2.435137	1.575079	1.585381
C	-4.282237	3.808590	-0.184076
H	-3.659122	4.730391	-2.030349
H	-4.609089	2.749780	1.661445
H	-5.245564	4.310450	-0.163530
C	0.899274	3.143829	-0.403217
C	1.804281	3.418475	-1.431222
C	0.844002	4.023861	0.686080
C	2.649507	4.526576	-1.364189
H	1.871539	2.765436	-2.295743
C	1.677842	5.133518	0.751623
H	0.144319	3.831197	1.496281
C	2.592844	5.383909	-0.270903
H	3.352012	4.716826	-2.171066
H	1.619046	5.803057	1.605134
H	3.251442	6.246001	-0.217157
C	-4.610885	-0.720178	1.385832
C	-4.848340	-1.782195	0.306284
H	-3.542326	-0.521034	1.516963
H	-5.101212	0.227234	1.134653
H	-5.022911	-1.059440	2.343741
C	-6.347102	-1.972004	0.034868
H	-4.442461	-2.738387	0.652940
H	-6.520242	-2.770523	-0.694990
H	-6.868724	-2.239970	0.960916
H	-6.808243	-1.053822	-0.349174
N	-3.363624	-2.373332	-1.475561
C	-2.690061	-2.111912	-2.734497
H	-1.921478	-2.873401	-2.895579
H	-3.394799	-2.170810	-3.576156
H	-2.210681	-1.124807	-2.779234

TSF4-5Sa

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.132964	-0.410800	0.837701
N	1.400491	-0.527595	-1.032590
C	-0.971848	0.724272	-2.107913
H	-1.271786	-0.263001	-2.470161
H	-1.442775	1.465897	-2.760861
C	3.382349	-1.299851	1.027078
C	-0.800465	-0.632139	2.299733
O	-1.369171	-0.809841	3.311430
P	1.768646	-1.993287	1.576537
P	-1.497688	0.815087	-0.345794
Si	3.144631	-0.822809	-0.791459
Si	0.907255	0.763490	-2.140998
C	3.675361	-2.214326	-1.933775
H	3.617304	-1.889929	-2.980260
H	4.709182	-2.524779	-1.738127
H	3.025673	-3.088824	-1.820492
C	1.540583	0.480680	-3.892788
H	1.091119	1.201930	-4.587848
H	2.628074	0.615547	-3.950044
H	1.309530	-0.523920	-4.262008
H	3.616360	-0.403514	1.608142
H	4.208817	-2.007667	1.166959
C	2.013908	-3.709222	0.910925
H	3.077745	-3.968324	0.961452
H	1.466756	-4.440982	1.512593
H	1.652591	-3.769545	-0.121013
C	1.954347	-2.405417	3.363338
H	1.111362	-3.044209	3.650362
H	2.883368	-2.957650	3.545084
H	1.929530	-1.525535	4.006424
P	1.269647	1.365134	1.869599
C	2.832095	2.193862	1.260134
H	2.833858	3.212886	1.671415
H	3.690559	1.697166	1.731043
Si	3.192204	2.303211	-0.593549
C	0.271692	2.880317	2.191676
H	0.041108	3.411525	1.265495
H	-0.671646	2.603182	2.668751

H	0.816618	3.560524	2.855909
C	1.811538	1.078978	3.615082
H	2.644947	0.372502	3.648632
H	2.147672	2.015651	4.074129
H	0.983852	0.673396	4.205385
C	4.258566	3.827974	-0.887450
H	3.725717	4.745732	-0.608760
H	5.185283	3.790062	-0.301159
H	4.539901	3.916384	-1.944094
C	4.105401	0.751509	-1.139358
H	5.075138	0.686188	-0.626587
H	4.325859	0.826315	-2.213491
C	1.585241	2.419350	-1.561734
H	0.856875	2.945071	-0.934366
H	1.738140	3.045886	-2.451727
H	-0.827781	-1.634852	-0.095138
H	0.978235	-1.453673	-1.299928
C	-2.304911	-2.707649	-1.638637
H	-2.599685	-3.663398	-2.093651
H	-3.101778	-2.393909	-0.967176
H	-2.244544	-1.978413	-2.448024
C	-0.978458	-2.913766	-0.914682
C	-3.230282	0.176911	-0.370586
C	-4.011925	0.259584	-1.527510
C	-3.805920	-0.346542	0.788709
C	-5.322665	-0.205834	-1.536236
H	-3.594784	0.678983	-2.438333
C	-5.121631	-0.804870	0.785798
H	-3.225109	-0.412854	1.701942
C	-5.880070	-0.746640	-0.379347
H	-5.908412	-0.147553	-2.449355
H	-5.546293	-1.221033	1.694815
H	-6.901317	-1.116678	-0.386272
C	-1.981987	2.598907	-0.146932
C	-1.644388	3.617076	-1.041686
C	-2.734438	2.940210	0.985371
C	-2.016830	4.939649	-0.796830
H	-1.083385	3.399067	-1.944201
C	-3.113445	4.253711	1.228939
H	-3.023481	2.168006	1.693794
C	-2.747012	5.263880	0.340377
H	-1.736366	5.713743	-1.505623
H	-3.692747	4.490683	2.116791
H	-3.036019	6.293292	0.530944

C	-2.411783	-3.604220	1.132909
C	-1.139612	-3.839086	0.322106
H	-2.540912	-2.542502	1.352401
H	-3.310234	-3.961859	0.615921
H	-2.349807	-4.138368	2.088729
C	-1.033483	-5.304530	-0.110748
H	-0.311695	-3.619726	0.987889
H	-0.088652	-5.486550	-0.630568
H	-1.091634	-5.970851	0.759265
H	-1.850288	-5.582300	-0.789532
N	0.144349	-3.083311	-1.629627
C	0.082338	-2.904730	-3.063054
H	-0.290680	-1.924220	-3.412512
H	1.093902	-3.014693	-3.475105
H	-0.547803	-3.660024	-3.564802

F5Sa

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.894001	0.106083	1.068328
N	0.446756	-1.379036	-0.260246
C	-1.016059	0.646950	-1.700494
H	-2.009119	0.249867	-1.469762
H	-1.122909	1.293179	-2.576727
C	2.032198	-3.061727	1.561387
C	0.847917	1.224087	2.424952
O	0.826421	1.946192	3.349477
P	1.433937	-1.600845	2.476912
P	-0.449904	1.504714	-0.176284
Si	1.205204	-2.928846	-0.151842
Si	0.145221	-0.835081	-1.870247
C	-0.008583	-4.369907	-0.290607
H	-0.529117	-4.379276	-1.254833
H	0.497592	-5.337584	-0.177354
H	-0.770146	-4.300161	0.497613
C	-0.686067	-2.100772	-3.012255
H	-1.037774	-1.611805	-3.930776
H	0.012498	-2.888253	-3.321532
H	-1.545060	-2.597455	-2.546292
H	3.120278	-2.975193	1.453024
H	1.824943	-4.005698	2.080740

C	-0.187991	-2.171594	3.135164
H	-0.107204	-3.139980	3.642938
H	-0.581089	-1.434495	3.844294
H	-0.895834	-2.260022	2.306178
C	2.432036	-1.531242	4.019523
H	2.161780	-0.642125	4.599162
H	2.261346	-2.422268	4.634099
H	3.499994	-1.476954	3.787361
P	2.977801	0.752903	0.518771
C	3.952094	-0.502322	-0.424908
H	4.908503	-0.042605	-0.712409
H	4.207465	-1.302318	0.283414
Si	3.196750	-1.348302	-1.963029
C	3.320842	2.273128	-0.465447
H	2.855244	2.221970	-1.451493
H	2.911674	3.147129	0.050079
H	4.400252	2.412288	-0.597922
C	4.120208	1.098000	1.923950
H	4.151522	0.246888	2.609192
H	5.138316	1.307114	1.575993
H	3.752492	1.964412	2.483908
C	4.605605	-1.520213	-3.210835
H	4.976085	-0.539683	-3.536547
H	5.454033	-2.071751	-2.786110
H	4.274871	-2.061748	-4.105970
C	2.560943	-3.060080	-1.477273
H	3.388091	-3.695289	-1.130483
H	2.159731	-3.546728	-2.378573
C	1.773652	-0.365605	-2.721612
H	1.973649	0.709476	-2.630623
H	1.716640	-0.579849	-3.798276
H	-3.855598	-0.240678	-0.116382
C	-5.778647	-1.154694	-0.206090
H	-6.298505	-1.999419	-0.671526
H	-5.885067	-1.226533	0.880900
H	-6.286839	-0.234862	-0.513888
C	-4.306053	-1.120367	-0.613532
C	-2.050192	1.879358	0.655355
C	-2.978258	2.759930	0.086443
C	-2.405337	1.177151	1.808564
C	-4.235775	2.927328	0.656659
H	-2.717011	3.313070	-0.812586
C	-3.665199	1.343922	2.382157
H	-1.695316	0.488266	2.258792

C	-4.582786	2.215515	1.805006
H	-4.947666	3.611978	0.204599
H	-3.927649	0.788667	3.278158
H	-5.565498	2.344309	2.249260
C	0.113122	3.170588	-0.688356
C	0.467571	3.486539	-2.001373
C	0.293239	4.135233	0.311643
C	0.995875	4.739013	-2.309958
H	0.356392	2.752631	-2.794032
C	0.812454	5.387249	0.002449
H	0.032480	3.901903	1.340799
C	1.169859	5.691217	-1.311024
H	1.270760	4.967264	-3.335843
H	0.941964	6.126000	0.788133
H	1.582108	6.666628	-1.552323
C	-3.561287	-2.542014	1.368604
C	-3.494752	-2.350678	-0.147271
H	-3.315278	-1.616282	1.901585
H	-4.557901	-2.864734	1.692863
H	-2.852904	-3.315559	1.687141
C	-3.887220	-3.643920	-0.866370
H	-2.442849	-2.133521	-0.390640
H	-3.849468	-3.531357	-1.953986
H	-3.212024	-4.459179	-0.580421
H	-4.906791	-3.951364	-0.602612
N	-4.194379	-0.998912	-2.070650
H	-3.234858	-1.196008	-2.339438
C	-4.565715	0.301125	-2.603634
H	-4.258393	0.358508	-3.653098
H	-5.652602	0.433576	-2.576047
H	-4.112415	1.152113	-2.063692

F4Ra

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.620771	0.017915	1.205168
N	0.959656	-1.421716	-0.629062
C	-1.057033	0.271662	-1.679509
H	-1.738800	-0.569370	-1.498137
H	-1.509104	0.882519	-2.467651
C	2.917725	-2.465464	1.328522

C	0.220332	0.892237	2.660337
O	-0.043162	1.462307	3.653253
P	1.554006	-1.704643	2.320252
P	-0.871910	1.138741	-0.062300
Si	2.368314	-2.494185	-0.484650
Si	0.581254	-0.531871	-2.117027
C	1.896980	-4.256861	-0.942544
H	1.499446	-4.317868	-1.962562
H	2.774013	-4.914887	-0.890596
H	1.141758	-4.668275	-0.261214
C	0.328294	-1.684185	-3.583561
H	0.079237	-1.109806	-4.485374
H	1.222457	-2.276899	-3.813591
H	-0.505861	-2.371949	-3.400537
H	3.799649	-1.822176	1.436183
H	3.194690	-3.464718	1.690202
C	0.473076	-3.175658	2.585764
H	1.017536	-4.015268	3.035220
H	-0.356327	-2.892347	3.241443
H	0.041612	-3.504784	1.635802
C	2.248050	-1.587761	4.023185
H	1.448099	-1.285264	4.708045
H	2.652534	-2.549607	4.358635
H	3.035921	-0.834530	4.082914
P	2.548091	1.253879	0.998724
C	3.991959	0.782914	-0.084003
H	4.647767	1.659654	-0.176815
H	4.581505	0.033384	0.461621
Si	3.662550	0.063906	-1.801360
C	2.426331	3.043535	0.556495
H	2.032653	3.188531	-0.452475
H	1.739514	3.534995	1.251436
H	3.405643	3.531597	0.625529
C	3.493988	1.482063	2.574418
H	3.968973	0.541281	2.867050
H	4.282836	2.235530	2.462264
H	2.820522	1.794853	3.378518
C	5.051577	0.608464	-2.953327
H	5.045066	1.696380	-3.095755
H	6.034490	0.330547	-2.553055
H	4.952471	0.144354	-3.942537
C	3.674431	-1.818730	-1.648894
H	4.668423	-2.146368	-1.313569
H	3.527390	-2.261948	-2.644747

C	1.999470	0.639348	-2.484626
H	1.793139	1.632272	-2.068384
H	2.077110	0.768038	-3.572922
H	-0.716889	-0.888632	1.322466
H	0.111126	-1.884128	-0.300698
C	-3.578411	-2.450751	-0.514361
C	-2.633154	1.251668	0.507026
C	-3.579250	1.920184	-0.281928
C	-3.049439	0.685466	1.712276
C	-4.905791	2.017983	0.122534
H	-3.274881	2.378825	-1.219209
C	-4.378081	0.790782	2.126039
H	-2.328138	0.147126	2.317251
C	-5.308948	1.455102	1.333615
H	-5.624805	2.536918	-0.505148
H	-4.682131	0.348442	3.070775
H	-6.343864	1.535528	1.654333
C	-0.680824	2.911803	-0.551395
C	-0.348836	3.346307	-1.836636
C	-0.820587	3.872513	0.459579
C	-0.142177	4.700618	-2.102606
H	-0.239699	2.633384	-2.647967
C	-0.624630	5.222243	0.196186
H	-1.076925	3.556324	1.468407
C	-0.276844	5.641634	-1.088100
H	0.119530	5.016037	-3.109046
H	-0.737353	5.950331	0.994608
H	-0.117132	6.696045	-1.294343
C	-4.722189	-1.553457	-0.947107
C	-6.064100	-2.263270	-0.701588
C	-4.621356	-1.085696	-2.394949
H	-4.690189	-0.674364	-0.291102
H	-6.186604	-2.575634	0.341149
H	-6.895544	-1.592416	-0.944781
H	-6.151561	-3.154612	-1.334800
H	-3.681888	-0.559006	-2.582037
H	-4.667930	-1.930696	-3.089862
H	-5.446464	-0.401441	-2.624696
C	-3.465791	-2.727068	0.968645
H	-2.512286	-2.333810	1.345839
H	-4.266285	-2.242045	1.531462
H	-3.492896	-3.803227	1.178585
N	-2.783098	-2.919260	-1.396880
C	-1.727380	-3.818532	-0.973238

H	-0.946023	-3.848372	-1.737518
H	-1.265589	-3.541795	-0.015310
H	-2.116636	-4.840295	-0.862059

TSF4-5Ra

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.184229	-0.181218	0.904771
N	1.167350	-0.871041	-1.007507
C	-0.911579	0.741794	-2.187480
H	-1.447566	-0.151678	-2.531705
H	-1.218533	1.556978	-2.850191
C	3.048063	-2.202022	0.875605
C	-0.706331	0.027503	2.403483
O	-1.268777	0.129736	3.424490
P	1.692674	-1.605086	1.985902
P	-1.364359	0.976572	-0.416902
Si	2.732351	-1.740428	-0.921887
Si	0.911629	0.291704	-2.331275
C	2.570080	-3.294786	-1.951046
H	1.709645	-3.869100	-1.577127
H	2.399519	-3.080364	-3.012436
H	3.461521	-3.929245	-1.873332
C	1.199030	-0.478117	-4.023562
H	0.937275	0.238688	-4.813026
H	2.250416	-0.752125	-4.173694
H	0.591479	-1.376264	-4.179031
H	4.000053	-1.769715	1.207141
H	3.143237	-3.289540	0.981124
C	0.896617	-3.165704	2.462433
H	1.614366	-3.876395	2.887958
H	0.102636	-2.974349	3.189833
H	0.461027	-3.585438	1.541326
C	2.642779	-1.244886	3.527852
H	1.954968	-1.031802	4.353149
H	3.230234	-2.130007	3.797292
H	3.327559	-0.399895	3.411085
P	1.570296	1.651032	1.373321
C	3.319121	1.401341	0.828630
H	3.930579	2.228893	1.214025
H	3.709050	0.491151	1.297579

Si	3.627636	1.259744	-1.050869
C	1.422112	3.440979	0.913764
H	1.354807	3.613923	-0.158971
H	0.537006	3.880742	1.377045
H	2.305374	3.969341	1.292140
C	1.700477	1.986211	3.185216
H	1.744013	1.074535	3.777585
H	2.570451	2.610799	3.418483
H	0.796145	2.527152	3.485987
C	5.057387	2.412470	-1.461788
H	4.795865	3.455854	-1.244050
H	5.949687	2.165741	-0.873054
H	5.331672	2.352746	-2.521962
C	4.052727	-0.526004	-1.487037
H	5.014228	-0.811195	-1.039220
H	4.189171	-0.589037	-2.576066
C	2.131059	1.700756	-2.120649
H	1.633704	2.609715	-1.771012
H	2.522274	1.939030	-3.120587
H	-0.812793	-1.975155	0.421879
H	0.449574	-1.598698	-1.056275
C	-1.504126	-3.017234	0.141368
C	-3.180336	0.631663	-0.373374
C	-3.975338	0.728393	-1.519830
C	-3.792594	0.322854	0.843767
C	-5.345961	0.498612	-1.454800
H	-3.527111	0.975960	-2.477454
C	-5.166608	0.104657	0.912466
H	-3.196977	0.235793	1.746271
C	-5.946132	0.185484	-0.237393
H	-5.946116	0.566366	-2.357682
H	-5.622726	-0.142863	1.866594
H	-7.015580	0.003220	-0.186752
C	-1.497323	2.802157	-0.192575
C	-1.177108	3.744195	-1.170231
C	-1.963591	3.255931	1.048600
C	-1.310964	5.108827	-0.914028
H	-0.804148	3.431983	-2.140351
C	-2.110294	4.614440	1.301221
H	-2.206024	2.541186	1.830727
C	-1.778564	5.547953	0.319383
H	-1.049369	5.827307	-1.685650
H	-2.477049	4.945698	2.268439
H	-1.886604	6.610368	0.516978

C	-2.214994	-2.584096	-1.182525
C	-3.584710	-3.260667	-1.328298
C	-1.399674	-2.903550	-2.436511
H	-2.395958	-1.508091	-1.131548
H	-4.296149	-2.926944	-0.566828
H	-4.022923	-3.027073	-2.306775
H	-3.484904	-4.351084	-1.257448
H	-0.379141	-2.513713	-2.410375
H	-1.301715	-3.985767	-2.551258
H	-1.891817	-2.492760	-3.328796
C	-2.481120	-2.981576	1.328177
H	-1.941363	-3.039424	2.276987
H	-3.060296	-2.054675	1.329229
H	-3.181988	-3.823193	1.293946
N	-0.712431	-4.132798	-0.030675
C	-0.950355	-5.273667	0.816634
H	-0.193544	-6.040215	0.594552
H	-0.896813	-5.111413	1.916321
H	-1.932566	-5.762009	0.647847

F5Ra

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.705035	-0.026142	1.080608
N	0.261443	-1.413777	-0.381495
C	-0.744472	0.831894	-1.854293
H	-1.772198	0.481280	-1.698967
H	-0.760300	1.506206	-2.716032
C	1.400709	-3.314972	1.555086
C	0.617988	1.049316	2.468662
O	0.576789	1.748964	3.409215
P	0.783332	-1.847374	2.444187
P	-0.208716	1.613171	-0.285567
Si	0.870700	-3.028742	-0.256228
Si	0.288419	-0.745845	-1.977470
C	-0.400645	-4.371223	-0.640724
H	-0.814258	-4.275622	-1.650778
H	0.049370	-5.369563	-0.559392
H	-1.235480	-4.329641	0.070877
C	-0.502458	-1.818014	-3.319800
H	-0.477426	-1.291931	-4.283405

H	0.005498	-2.779453	-3.464903
H	-1.554960	-2.012799	-3.081078
H	2.494688	-3.326292	1.632859
H	1.028066	-4.257869	1.974762
C	-0.991555	-2.248154	2.722333
H	-1.133367	-3.244071	3.158548
H	-1.438957	-1.503271	3.389837
H	-1.507982	-2.198764	1.759672
C	1.445294	-1.967683	4.154480
H	1.150564	-1.083374	4.729408
H	1.065600	-2.863699	4.658174
H	2.537932	-2.019450	4.144823
P	2.928664	0.327908	0.923082
C	3.886422	-0.966529	0.018005
H	4.918330	-0.605250	-0.094854
H	3.947735	-1.841234	0.679339
Si	3.262555	-1.602302	-1.669607
C	3.637457	1.858366	0.183223
H	3.358055	1.963850	-0.867159
H	3.258318	2.734125	0.717082
H	4.731356	1.846229	0.253035
C	3.847651	0.367368	2.522454
H	3.721016	-0.578582	3.055683
H	4.919121	0.534672	2.363149
H	3.454146	1.168094	3.157259
C	4.800918	-1.857735	-2.735890
H	5.317072	-0.906981	-2.921250
H	5.516231	-2.536617	-2.254469
H	4.541813	-2.289152	-3.710664
C	2.379939	-3.245725	-1.388748
H	3.074869	-3.991338	-0.977497
H	2.053565	-3.636509	-2.363982
C	2.076591	-0.401318	-2.513835
H	2.367716	0.626543	-2.263115
H	2.174176	-0.495103	-3.604616
H	-3.249726	-0.492993	0.357587
C	-3.973435	-1.220441	-0.030991
C	-1.764316	2.356927	0.364648
C	-2.362812	3.461438	-0.253532
C	-2.424705	1.742106	1.430827
C	-3.595232	3.934934	0.183853
H	-1.864243	3.951264	-1.085845
C	-3.663405	2.210140	1.865789
H	-1.969812	0.887075	1.924455

C	-4.250836	3.306347	1.242080
H	-4.048874	4.792489	-0.304670
H	-4.165337	1.717597	2.693790
H	-5.215000	3.674395	1.580974
C	0.726160	3.116085	-0.760520
C	1.289719	3.294409	-2.025703
C	0.947405	4.090566	0.221453
C	2.069121	4.417098	-2.302081
H	1.139672	2.552420	-2.804134
C	1.714993	5.215303	-0.057619
H	0.516639	3.966190	1.211836
C	2.284471	5.378397	-1.320026
H	2.506533	4.538055	-3.289003
H	1.872686	5.964402	0.713032
H	2.888201	6.254777	-1.537200
C	-5.111303	-0.364454	-0.643347
C	-6.230228	-1.159763	-1.325193
C	-4.557090	0.677906	-1.613276
H	-5.557242	0.174356	0.205672
H	-6.625332	-1.964498	-0.695125
H	-7.068117	-0.496008	-1.570493
H	-5.880048	-1.599163	-2.266154
H	-3.828996	1.329919	-1.121401
H	-4.063785	0.186691	-2.459710
H	-5.358495	1.315359	-2.006324
C	-4.466298	-2.041540	1.168535
H	-4.879227	-1.377048	1.936711
H	-5.248947	-2.756772	0.893686
H	-3.647506	-2.609443	1.624156
N	-3.221677	-1.984293	-1.034928
H	-2.242066	-2.013584	-0.758528
C	-3.679674	-3.331631	-1.333956
H	-3.065735	-3.742410	-2.142019
H	-3.631962	-4.038664	-0.488733
H	-4.713022	-3.316168	-1.689486

G4S

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.003153	-0.048313	-0.939130
N	0.255148	-1.424452	0.955291

C	-0.931550	0.874942	2.132689
H	0.066600	1.117791	2.521170
H	-1.652390	1.367726	2.793049
C	1.358538	-3.189884	-1.133595
C	0.128588	1.027856	-2.302380
O	0.253559	1.740135	-3.228370
P	1.523500	-1.457244	-1.779806
P	-0.961698	1.482393	0.386497
Si	0.708481	-3.114872	0.643179
Si	-1.040758	-1.002896	2.083527
C	2.057979	-3.645358	1.833549
H	1.696175	-3.643619	2.869188
H	2.412056	-4.659103	1.607692
H	2.911071	-2.958232	1.770483
C	-0.747913	-1.703240	3.808595
H	-1.504368	-1.331403	4.512043
H	-0.809890	-2.798706	3.818015
H	0.234370	-1.420982	4.203442
H	0.629552	-3.708745	-1.767782
H	2.302155	-3.742803	-1.204582
P	-1.738760	-1.119451	-1.953972
C	-2.324492	-2.818344	-1.468841
H	-3.295535	-3.000590	-1.949849
H	-1.631232	-3.542596	-1.917912
Si	-2.442336	-3.247143	0.369641
C	-3.372869	-0.277327	-2.131313
H	-3.853129	-0.117923	-1.161882
H	-3.222484	0.703074	-2.592486
H	-4.048468	-0.864700	-2.764683
C	-1.440670	-1.445293	-3.751360
H	-0.565062	-2.090092	-3.881290
H	-2.302184	-1.933594	-4.222112
H	-1.241368	-0.503058	-4.271892
C	-3.914010	-4.399796	0.613152
H	-4.857430	-3.896047	0.367841
H	-3.834507	-5.286735	-0.027762
H	-3.983771	-4.747372	1.651406
C	-0.852995	-4.136916	0.865201
H	-0.765974	-5.068015	0.287885
H	-0.928717	-4.439569	1.919823
C	-2.657159	-1.704330	1.440355
H	-3.206648	-0.955774	0.857717
H	-3.290515	-1.954774	2.303177
H	1.268383	0.654290	-0.241097

H	1.094545	-0.874433	1.153156
C	3.303776	1.937724	1.874005
H	3.863326	2.705947	1.336933
H	2.237387	2.110087	1.684349
H	3.482536	2.073438	2.945268
C	3.684668	0.545188	1.434200
C	-0.164373	3.145776	0.561505
C	-0.610068	4.035553	1.547003
C	0.890169	3.537374	-0.264886
C	-0.001684	5.274359	1.717425
H	-1.445369	3.759999	2.186428
C	1.493608	4.784389	-0.105538
H	1.249179	2.852751	-1.024083
C	1.055318	5.651841	0.889911
H	-0.355233	5.949167	2.492078
H	2.311613	5.073006	-0.760083
H	1.530813	6.619962	1.020089
C	-2.700243	2.076629	0.174640
C	-3.765231	1.730344	1.009366
C	-2.967068	2.874000	-0.946534
C	-5.064353	2.152397	0.723542
H	-3.599829	1.121720	1.893221
C	-4.257776	3.303810	-1.228437
H	-2.153571	3.153984	-1.612315
C	-5.315693	2.936499	-0.396815
H	-5.878539	1.867053	1.384210
H	-4.441381	3.920261	-2.103952
H	-6.326740	3.265254	-0.619224
C	4.345270	0.372899	0.108547
C	5.194369	-0.716753	-0.113147
C	4.092499	1.258407	-0.943307
C	5.780246	-0.914720	-1.358860
H	5.387330	-1.405200	0.703268
C	4.663870	1.050862	-2.194976
H	3.409067	2.088340	-0.799650
C	5.513052	-0.033138	-2.405317
H	6.445895	-1.759090	-1.514390
H	4.437297	1.734386	-3.007998
H	5.965630	-0.190122	-3.380278
H	2.892660	-1.236289	-1.531719
H	1.658661	-1.701652	-3.169151
N	3.470212	-0.512076	2.122554
C	2.851679	-0.390869	3.427872
H	2.617762	-1.391373	3.802699

H	3.529411	0.085175	4.150864
H	1.922112	0.195607	3.413793

G5S

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.156093	-0.194744	-0.827637
N	-0.437883	-1.331014	0.872704
C	-0.618668	1.174027	2.256672
H	0.338163	0.984494	2.756589
H	-1.162545	1.906373	2.860093
C	-0.207889	-3.638982	-0.951203
C	0.505548	0.687528	-2.197317
O	0.920521	1.231567	-3.150974
P	0.483686	-2.163433	-1.790877
P	-0.234049	1.706381	0.549567
Si	-0.682259	-3.044265	0.797765
Si	-1.382366	-0.544447	2.088167
C	0.382256	-3.995991	2.029889
H	0.130374	-3.745071	3.067176
H	0.259031	-5.080753	1.914177
H	1.443197	-3.756551	1.880658
C	-1.344414	-1.317898	3.817550
H	-1.867407	-0.657792	4.522887
H	-1.850506	-2.290013	3.857727
H	-0.326702	-1.457994	4.197690
H	-1.102373	-3.970510	-1.490026
H	0.503243	-4.471326	-0.947489
P	-2.197154	-0.225985	-1.829882
C	-3.292601	-1.629464	-1.337629
H	-4.261153	-1.490783	-1.838614
H	-2.859698	-2.538861	-1.775327
Si	-3.607991	-1.987246	0.510340
C	-3.392062	1.175038	-1.797992
H	-3.693761	1.428432	-0.780194
H	-2.931654	2.062694	-2.240299
H	-4.289438	0.919454	-2.373685
C	-2.142068	-0.468255	-3.658470
H	-1.563563	-1.361392	-3.913978
H	-3.148420	-0.574493	-4.079512
H	-1.653432	0.391018	-4.129284

C	-5.434857	-2.441539	0.663627
H	-6.082110	-1.599804	0.385311
H	-5.696472	-3.290509	0.019264
H	-5.683571	-2.720717	1.695288
C	-2.526299	-3.438637	1.048791
H	-2.804398	-4.349008	0.499256
H	-2.729869	-3.649891	2.108831
C	-3.212166	-0.499789	1.602263
H	-3.465467	0.428700	1.076246
H	-3.839962	-0.529743	2.504089
H	3.126808	0.658532	0.851893
C	4.943081	-0.052510	1.711053
H	5.448209	-0.992214	1.963819
H	5.591699	0.518995	1.039510
H	4.815618	0.534900	2.626126
C	3.599417	-0.322884	1.025581
C	1.330356	2.677284	0.731306
C	1.752214	3.158553	1.975857
C	2.140439	2.922633	-0.382765
C	2.962941	3.833376	2.107914
H	1.140188	3.004810	2.858867
C	3.345871	3.608217	-0.254972
H	1.845528	2.562043	-1.361293
C	3.767314	4.055751	0.993498
H	3.276242	4.187440	3.085939
H	3.960017	3.779354	-1.134397
H	4.715370	4.574889	1.098537
C	-1.429870	3.040968	0.146069
C	-2.581607	3.298265	0.892639
C	-1.205954	3.780434	-1.021738
C	-3.490982	4.271388	0.478620
H	-2.793741	2.732285	1.794453
C	-2.105746	4.758041	-1.428482
H	-0.327310	3.582434	-1.629347
C	-3.256504	5.003224	-0.680758
H	-4.386013	4.454608	1.066368
H	-1.912865	5.321659	-2.336785
H	-3.965473	5.760564	-1.001932
C	3.839334	-0.975646	-0.324193
C	4.193655	-2.326559	-0.403199
C	3.758595	-0.233867	-1.502707
C	4.466128	-2.917601	-1.633288
H	4.238285	-2.909309	0.511896
C	4.021011	-0.823836	-2.738412

H	3.478650	0.814189	-1.451691
C	4.379514	-2.167462	-2.806838
H	4.739378	-3.968406	-1.679545
H	3.938366	-0.233497	-3.646417
H	4.583031	-2.631258	-3.767942
H	1.864486	-2.388483	-1.654849
H	0.389700	-2.460698	-3.169539
N	2.742176	-1.187442	1.837911
H	1.820379	-1.236920	1.398213
C	2.563195	-0.750893	3.210109
H	1.741046	-1.322694	3.649123
H	3.458328	-0.958229	3.806827
H	2.334952	0.325829	3.320927

G4R

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.252676	-0.243839	1.228505
N	-0.815849	-1.248775	-0.623949
C	0.307326	1.031879	-1.872436
H	-0.713543	1.436011	-1.876530
H	0.850869	1.540741	-2.675135
C	-1.561718	-3.161117	1.482772
C	0.757331	0.627169	2.651426
O	1.060501	1.213241	3.623067
P	-1.108282	-1.592281	2.370103
P	0.972060	1.358749	-0.182915
Si	-1.437884	-2.895669	-0.390808
Si	0.114380	-0.825700	-2.070153
C	-3.118242	-3.104745	-1.196549
H	-3.054787	-2.950894	-2.280979
H	-3.510394	-4.116213	-1.027536
H	-3.837201	-2.382333	-0.791138
C	-0.844098	-1.202633	-3.646466
H	-0.328211	-0.801091	-4.528087
H	-0.969506	-2.280841	-3.805433
H	-1.840410	-0.747295	-3.609596
H	-0.828123	-3.919855	1.781812
H	-2.545189	-3.535842	1.787860
P	2.044205	-1.641799	1.455406
C	2.109067	-3.319072	0.662855

H	3.117884	-3.734857	0.793231
H	1.440931	-3.975219	1.237827
Si	1.588701	-3.464982	-1.151129
C	3.761998	-1.069264	1.089250
H	3.898050	-0.837697	0.029830
H	3.964160	-0.155384	1.654057
H	4.495351	-1.831389	1.378380
C	2.342854	-2.147198	3.210469
H	1.477684	-2.685181	3.611326
H	3.223811	-2.793843	3.298511
H	2.496687	-1.256065	3.827555
C	2.708704	-4.734303	-1.979316
H	3.754312	-4.400853	-1.972824
H	2.665866	-5.700177	-1.460798
H	2.422378	-4.905467	-3.024395
C	-0.197164	-4.065829	-1.184151
H	-0.259480	-5.046972	-0.692984
H	-0.497702	-4.230610	-2.229164
C	1.706315	-1.821590	-2.078839
H	2.532146	-1.237021	-1.657993
H	1.973790	-2.030908	-3.124384
H	-1.046154	0.696066	1.103715
H	-1.563574	-0.564180	-0.488433
C	-4.172273	0.441734	0.807770
C	0.456737	3.116066	0.090929
C	0.790348	4.095297	-0.853168
C	-0.273837	3.494771	1.216959
C	0.388327	5.415713	-0.684563
H	1.376641	3.825642	-1.728278
C	-0.671210	4.819923	1.394503
H	-0.548668	2.742944	1.947977
C	-0.347791	5.781735	0.442505
H	0.653591	6.161112	-1.429053
H	-1.236888	5.096564	2.280087
H	-0.658388	6.813797	0.579649
C	2.765958	1.688492	-0.480710
C	3.449296	1.361355	-1.653760
C	3.491693	2.251748	0.577638
C	4.824536	1.573770	-1.762235
H	2.920805	0.929045	-2.498029
C	4.858692	2.473767	0.469108
H	2.979138	2.510115	1.501492
C	5.533016	2.128006	-0.701847
H	5.338296	1.309028	-2.682371

H	5.400410	2.912888	1.302097
H	6.602743	2.295738	-0.787297
C	-3.755161	1.204900	-0.413894
C	-3.992078	0.677767	-1.691240
C	-3.131964	2.452425	-0.315521
C	-3.627555	1.385999	-2.830574
H	-4.480040	-0.286839	-1.777061
C	-2.765972	3.163976	-1.455160
H	-2.909791	2.881845	0.653455
C	-3.014728	2.634482	-2.717418
H	-3.828427	0.964943	-3.811868
H	-2.270416	4.124064	-1.345525
H	-2.730589	3.186506	-3.608796
C	-4.040323	1.148134	2.134565
H	-4.524837	2.129437	2.095095
H	-4.492527	0.586596	2.952842
H	-2.978264	1.304552	2.360604
H	-2.393514	-1.125443	2.723133
H	-0.801266	-2.107890	3.655240
N	-4.617355	-0.741789	0.626530
C	-5.091168	-1.564888	1.717566
H	-6.148693	-1.345797	1.916725
H	-5.030863	-2.615147	1.413071
H	-4.540583	-1.454287	2.660425

G5R

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.891037	0.048918	-1.247208
N	-0.585090	-1.472378	0.066599
C	0.852423	0.450928	1.644831
H	1.815765	-0.021926	1.421768
H	0.991298	1.054594	2.546208
C	-2.046145	-3.124028	-1.881061
C	-0.680622	1.190864	-2.574296
O	-0.559843	1.933244	-3.472086
P	-1.577044	-1.552647	-2.710086
P	0.378882	1.404281	0.153232
Si	-1.389400	-3.000912	-0.092151
Si	-0.414716	-0.948947	1.712715
C	-0.286958	-4.497946	0.241377

H	-0.145282	-4.658358	1.316465
H	-0.729273	-5.415748	-0.167818
H	0.709313	-4.366004	-0.198974
C	0.200347	-2.267539	2.922063
H	0.522063	-1.794274	3.859026
H	-0.583202	-2.991231	3.178575
H	1.052342	-2.822022	2.518398
H	-3.140056	-3.191942	-1.865553
H	-1.679468	-4.002230	-2.422111
P	-3.005751	0.781730	-0.889340
C	-4.088646	-0.477418	-0.087862
H	-5.070930	-0.018800	0.093150
H	-4.260436	-1.273783	-0.825880
Si	-3.492625	-1.325157	1.518667
C	-3.447742	2.282339	0.084134
H	-3.073109	2.228998	1.107556
H	-3.013329	3.169943	-0.383134
H	-4.537087	2.399674	0.117478
C	-3.975352	1.184403	-2.407206
H	-3.962558	0.352184	-3.117069
H	-5.018606	1.417701	-2.165052
H	-3.527522	2.052460	-2.902708
C	-5.000247	-1.419516	2.653328
H	-5.348846	-0.417807	2.936045
H	-5.837402	-1.938954	2.169694
H	-4.767260	-1.960166	3.579196
C	-2.889263	-3.057874	1.079334
H	-3.708261	-3.641391	0.635787
H	-2.613955	-3.578657	2.007845
C	-2.097838	-0.385479	2.381442
H	-2.239929	0.692907	2.243109
H	-2.156832	-0.569824	3.463770
H	3.703952	-1.007911	-1.564328
C	3.677759	-1.896486	-0.907480
C	1.985471	1.979692	-0.541918
C	2.770501	2.913638	0.145177
C	2.455934	1.462085	-1.749695
C	3.990504	3.331187	-0.373310
H	2.419415	3.324771	1.087877
C	3.679112	1.880715	-2.273561
H	1.861787	0.729709	-2.289531
C	4.445929	2.817960	-1.588495
H	4.586364	4.060634	0.167913
H	4.029487	1.472213	-3.217132

H	5.395357	3.150802	-1.998106
C	-0.299443	2.999398	0.750753
C	-0.711881	3.219360	2.065892
C	-0.462216	4.025651	-0.189456
C	-1.285953	4.436475	2.433378
H	-0.604254	2.440702	2.814804
C	-1.025321	5.241536	0.178699
H	-0.150225	3.869487	-1.218987
C	-1.445494	5.448173	1.492515
H	-1.605724	4.590721	3.459999
H	-1.141101	6.027108	-0.562496
H	-1.891533	6.395788	1.779897
C	3.904480	-1.415669	0.512561
C	4.465614	-0.159702	0.751342
C	3.569798	-2.220592	1.604445
C	4.671051	0.293582	2.051796
H	4.723823	0.479548	-0.088599
C	3.771414	-1.768964	2.906204
H	3.128596	-3.196188	1.423149
C	4.317971	-0.507863	3.134706
H	5.094823	1.280463	2.215169
H	3.490584	-2.401200	3.744016
H	4.467304	-0.152566	4.150484
C	4.820339	-2.821146	-1.344290
H	4.801697	-3.748140	-0.760291
H	4.748296	-3.078785	-2.406388
H	5.786252	-2.329549	-1.187757
H	-0.576845	-1.973182	-3.614119
H	-2.586124	-1.370994	-3.683944
N	2.389148	-2.580154	-0.999418
H	1.661785	-2.021875	-0.549019
C	1.964344	-2.862121	-2.357065
H	2.612688	-3.613708	-2.819743
H	0.955131	-3.284066	-2.329970
H	1.951150	-1.974386	-3.018046

TSG4-5S

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.215724	-0.180072	-0.769413
N	-0.233724	-1.523735	0.992513

C	-0.797933	1.053122	2.170868
H	0.167534	0.999839	2.686115
H	-1.443106	1.709709	2.763700
C	0.304038	-3.606098	-1.030481
C	0.824500	0.759905	-2.108771
O	1.232131	1.342025	-3.043072
P	1.198974	-2.078807	-1.552206
P	-0.444869	1.656738	0.468975
Si	-0.408216	-3.275492	0.694415
Si	-1.429028	-0.714522	2.018113
C	0.583604	-4.221307	1.972031
H	0.182761	-4.074753	2.982212
H	0.579298	-5.298624	1.764227
H	1.620298	-3.864161	1.960772
C	-1.555785	-1.494996	3.727402
H	-2.006729	-2.494092	3.682019
H	-0.575439	-1.591472	4.206706
H	-2.188444	-0.884467	4.384742
H	-0.507931	-3.789857	-1.742924
H	0.957583	-4.485051	-1.046699
P	-1.667310	-0.616766	-2.042609
C	-2.882112	-1.975619	-1.673762
H	-3.794407	-1.769032	-2.250291
H	-2.478630	-2.906269	-2.093944
Si	-3.353919	-2.339986	0.123183
C	-2.848818	0.748276	-2.412870
H	-3.384792	1.074416	-1.517881
H	-2.298344	1.606340	-2.807069
H	-3.581527	0.425465	-3.161468
C	-1.270137	-1.077048	-3.789521
H	-0.729269	-2.027961	-3.827845
H	-2.184749	-1.181576	-4.384215
H	-0.635500	-0.310972	-4.245907
C	-5.152857	-2.897716	0.150588
H	-5.825376	-2.088396	-0.160327
H	-5.316875	-3.744900	-0.527075
H	-5.457603	-3.214232	1.155802
C	-2.234015	-3.716778	0.752185
H	-2.401701	-4.629214	0.163006
H	-2.512600	-3.963430	1.786651
C	-3.118637	-0.814286	1.203318
H	-3.300192	0.070471	0.581990
H	-3.883862	-0.804360	1.992270
H	1.676236	0.085138	0.254624

H	0.742522	-1.442354	1.381225
C	3.152645	1.010268	1.793454
H	4.064154	0.880924	2.392158
H	3.339920	1.794403	1.059473
H	2.357906	1.352967	2.459292
C	2.826093	-0.327807	1.135500
C	0.765539	3.027140	0.735754
C	0.794194	3.734889	1.941459
C	1.651939	3.399670	-0.277910
C	1.705907	4.767267	2.140307
H	0.107534	3.476706	2.742292
C	2.555095	4.442957	-0.087211
H	1.653321	2.868737	-1.222241
C	2.592073	5.122987	1.126389
H	1.722552	5.295783	3.089253
H	3.238886	4.712772	-0.886937
H	3.305643	5.927038	1.281280
C	-1.900532	2.721715	0.062184
C	-3.101931	2.719907	0.774377
C	-1.791036	3.559795	-1.055018
C	-4.173765	3.515222	0.367556
H	-3.224480	2.094629	1.652653
C	-2.852966	4.360388	-1.456144
H	-0.866678	3.578344	-1.627176
C	-4.054352	4.335017	-0.749054
H	-5.101504	3.493784	0.932457
H	-2.745037	5.001718	-2.326124
H	-4.888094	4.955615	-1.064042
C	3.819131	-0.638842	0.026893
C	4.622133	-1.774841	0.126965
C	3.998266	0.213674	-1.065179
C	5.567731	-2.068007	-0.855590
H	4.474814	-2.430378	0.979232
C	4.938003	-0.074089	-2.047389
H	3.368306	1.093020	-1.158527
C	5.726544	-1.221670	-1.948329
H	6.178617	-2.962539	-0.765857
H	5.051600	0.594675	-2.896341
H	6.459191	-1.449120	-2.717863
H	1.423635	-2.308423	-2.929212
H	2.496866	-2.387948	-1.107996
N	2.464358	-1.376538	1.887258
C	2.193325	-1.149214	3.289736
H	1.409074	-0.403943	3.514519

H	1.863063	-2.094077	3.739283
H	3.086042	-0.824144	3.850728

R_1=R_2=R_3=NMeiPr

A5

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.144288	-0.565698	-0.581659
N	0.153367	-0.996004	1.576528
C	2.965281	-0.371061	1.354870
H	3.856600	-0.875886	1.743005
H	3.237250	0.677654	1.198098
C	-2.508145	-1.905786	1.068214
C	0.284432	-0.636254	-2.334235
O	0.440262	-0.820603	-3.480853
P	-2.365064	-0.911553	-0.447716
P	2.426151	-0.973759	-0.285369
Si	-1.310866	-1.279516	2.399305
Si	1.458930	-0.425281	2.513502
C	-1.313197	-2.694578	3.663942
H	-0.722047	-2.473022	4.559193
H	-2.339674	-2.900228	3.998175
H	-0.916111	-3.620253	3.228244
C	1.914309	-1.483997	4.023620
H	2.927074	-1.240649	4.372678
H	1.234682	-1.294029	4.863509
H	1.879742	-2.559494	3.812480
H	-3.528179	-2.090846	1.416103
H	-2.081030	-2.883510	0.809211
P	0.032816	1.915984	-0.302939
C	-1.144708	2.242519	1.052998
H	-1.432599	3.297621	1.095765
H	-2.046819	1.688473	0.766529
Si	-0.737405	1.737675	2.847797
C	-1.226362	3.246594	3.885736
H	-0.652763	4.139848	3.605392
H	-2.291014	3.485346	3.762622
H	-1.052690	3.067077	4.954321
C	-1.857590	0.292513	3.322216
H	-2.904828	0.569863	3.144657
H	-1.768932	0.116530	4.404959
C	1.069437	1.309341	3.169308
H	1.701434	2.033385	2.648432
H	1.284147	1.399265	4.243474

H	0.142008	-2.328228	-0.202494
H	-0.188110	-2.333117	-0.910153
N	2.795852	-2.660485	-0.230003
N	3.633022	-0.414517	-1.349935
N	-2.958447	-1.967447	-1.659144
N	-3.521092	0.347532	-0.178155
N	-0.777751	2.643158	-1.649408
N	1.349458	2.944176	0.159906
C	-2.694461	-1.666032	-3.054006
H	-3.582605	-1.285538	-3.578035
H	-1.922543	-0.905205	-3.125126
H	-2.330718	-2.548834	-3.596451
C	-3.781993	1.109766	-1.390390
H	-4.231702	2.078568	-1.153087
H	-2.832130	1.310518	-1.891043
H	-4.449271	0.588088	-2.095112
C	-1.638596	3.805646	-1.506604
H	-1.105594	4.738121	-1.268113
H	-2.184158	3.972859	-2.440695
H	-2.391863	3.639178	-0.733698
C	2.631404	2.719702	-0.483685
H	3.451790	3.046674	0.167445
H	2.771772	1.657974	-0.669203
H	2.745403	3.245407	-1.443851
C	3.345978	0.181120	-2.639237
H	3.350295	-0.543876	-3.465305
H	2.368439	0.659169	-2.618666
H	4.080890	0.962776	-2.868716
C	2.505435	-3.369248	-1.463873
H	1.495769	-3.807226	-1.500063
H	2.594004	-2.682789	-2.310661
H	3.228831	-4.176507	-1.627575
C	-3.909327	-3.061407	-1.423670
C	-3.228771	-4.424043	-1.598755
C	-5.166651	-2.961266	-2.294407
H	-4.231204	-2.992283	-0.382439
H	-2.373677	-4.518634	-0.920701
H	-3.929888	-5.239162	-1.383902
H	-2.863689	-4.560232	-2.623276
H	-5.605087	-1.958910	-2.244677
H	-4.954657	-3.189872	-3.344801
H	-5.918415	-3.678843	-1.947527
C	-4.626305	0.299899	0.790247
C	-5.885259	-0.412174	0.286195

C	-4.975922	1.703802	1.299860
H	-4.252079	-0.248492	1.655425
H	-5.685253	-1.461245	0.052139
H	-6.668910	-0.383565	1.052132
H	-6.285113	0.069704	-0.613493
H	-4.073988	2.259098	1.576326
H	-5.529812	2.292053	0.559659
H	-5.611357	1.623348	2.188683
C	-0.197622	2.458824	-2.990434
C	0.549100	3.682209	-3.533635
C	-1.240370	1.988568	-4.008924
H	0.536585	1.658865	-2.890934
H	1.393875	3.952897	-2.895898
H	0.945705	3.461970	-4.531161
H	-0.106791	4.556067	-3.627242
H	-1.732002	1.074129	-3.673222
H	-2.012186	2.747271	-4.187816
H	-0.760207	1.777307	-4.970300
C	1.155670	4.332774	0.633120
C	1.494840	5.405380	-0.410266
C	1.938750	4.623219	1.920127
H	0.097129	4.446981	0.872352
H	0.968436	5.242127	-1.352465
H	1.202638	6.390354	-0.029371
H	2.569758	5.443383	-0.620949
H	1.602459	4.000682	2.751066
H	3.014389	4.461380	1.786155
H	1.799644	5.671340	2.209491
C	5.041099	-0.719954	-1.067741
C	5.826956	0.544057	-0.705969
C	5.708431	-1.495707	-2.205979
H	5.043478	-1.381282	-0.196391
H	5.391950	1.028412	0.173946
H	6.871963	0.300728	-0.480335
H	5.827307	1.269646	-1.527977
H	5.135840	-2.397098	-2.448552
H	5.801345	-0.891236	-3.115769
H	6.717916	-1.803703	-1.911294
C	2.869378	-3.474011	0.986352
C	4.073086	-4.422166	0.938600
C	1.575457	-4.230880	1.305817
H	3.047043	-2.783125	1.811633
H	4.986164	-3.872821	0.684273
H	4.216511	-4.900044	1.914327

H	3.938751	-5.222290	0.201474
H	0.754175	-3.519183	1.432065
H	1.318729	-4.949381	0.518215
H	1.687284	-4.793672	2.240105

TSA5-1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.032436	-0.471502	-0.467507
N	0.095426	-0.969172	1.757561
C	2.943941	-0.544819	1.337088
H	3.786832	-1.147615	1.693281
H	3.331094	0.464522	1.168829
C	-2.606074	-1.669018	1.263338
C	0.035977	-0.823965	-2.184315
O	0.078869	-1.202601	-3.291915
P	-2.418706	-0.734849	-0.300432
P	2.264194	-1.090413	-0.276869
Si	-1.411839	-1.030818	2.584185
Si	1.506244	-0.419504	2.573417
C	-1.482527	-2.325247	3.962630
H	-0.858788	-2.053946	4.822257
H	-2.509672	-2.444771	4.333330
H	-1.140419	-3.304546	3.604331
C	1.942841	-1.429170	4.115258
H	2.976726	-1.233662	4.429477
H	1.295968	-1.168747	4.961957
H	1.840472	-2.507643	3.945025
H	-3.634452	-1.758074	1.623821
H	-2.238857	-2.688105	1.088568
P	0.160575	1.995576	-0.331955
C	-0.945238	2.471605	1.053758
H	-1.123444	3.550800	1.098841
H	-1.915895	2.011809	0.842328
Si	-0.535237	1.958545	2.845063
C	-0.858351	3.502219	3.892071
H	-0.210792	4.342351	3.611384
H	-1.898458	3.836520	3.783980
H	-0.688992	3.299693	4.957309
C	-1.806556	0.653486	3.342003
H	-2.795664	1.017526	3.034688

H	-1.832579	0.559247	4.437038
C	1.237286	1.372293	3.116278
H	1.897452	2.025673	2.536297
H	1.502316	1.502853	4.174947
H	-0.220779	-2.137304	-0.272805
H	-0.021300	-1.819701	0.613037
N	3.433160	-0.635123	-1.422802
N	2.500557	-2.799884	-0.214944
N	-3.074741	-1.797074	-1.483015
N	-3.636489	0.470509	-0.119421
N	-0.583471	2.771135	-1.685942
N	1.571649	2.910514	0.084516
C	-3.035911	-1.315698	-2.852217
H	-2.507356	-0.359683	-2.894979
H	-2.500037	-2.000223	-3.521413
H	-4.043522	-1.153007	-3.262469
C	-3.562509	1.624160	-1.002756
H	-3.990933	2.512671	-0.519247
H	-2.519867	1.834828	-1.239089
H	-4.093348	1.473450	-1.954259
C	-1.201173	4.084166	-1.633917
H	-0.521874	4.904475	-1.906205
H	-2.059567	4.123434	-2.315417
H	-1.591114	4.290684	-0.637065
C	2.857187	2.513283	-0.456884
H	3.661434	2.722095	0.261669
H	2.868609	1.446621	-0.657409
H	3.118190	3.027103	-1.393581
C	3.080404	-0.017704	-2.686307
H	2.993099	-0.739255	-3.510497
H	2.124508	0.495750	-2.584689
H	3.827404	0.734852	-2.967658
C	2.011343	-3.490845	-1.396708
H	2.209067	-2.886555	-2.286986
H	2.537103	-4.443401	-1.528590
H	0.929884	-3.690845	-1.370822
C	-3.442750	-3.199106	-1.289325
C	-2.272469	-4.146953	-1.581767
C	-4.684308	-3.573330	-2.104303
H	-3.717327	-3.318071	-0.238364
H	-1.426555	-3.919923	-0.924519
H	-2.562452	-5.193198	-1.425839
H	-1.926385	-4.042704	-2.616660
H	-5.508159	-2.880591	-1.898581

H	-4.487052	-3.564774	-3.182123
H	-5.013048	-4.584365	-1.839482
C	-5.014029	0.064212	0.230123
C	-6.019002	0.185079	-0.920574
C	-5.490225	0.834040	1.463034
H	-4.985348	-0.998100	0.483661
H	-5.645276	-0.303739	-1.825852
H	-6.956258	-0.305709	-0.635402
H	-6.255185	1.227910	-1.159959
H	-4.858968	0.606971	2.327914
H	-5.451117	1.916010	1.288977
H	-6.525395	0.573621	1.714639
C	-0.203146	2.322598	-3.032254
C	0.937550	3.127951	-3.663809
C	-1.397757	2.258841	-3.990474
H	0.150879	1.301811	-2.903611
H	1.838087	3.095376	-3.043793
H	1.192604	2.706995	-4.643516
H	0.661985	4.178157	-3.819129
H	-2.257139	1.770968	-3.522450
H	-1.711875	3.251513	-4.334466
H	-1.123267	1.679780	-4.878864
C	1.498636	4.347561	0.418525
C	2.016506	5.268465	-0.695965
C	2.229992	4.668937	1.726897
H	0.446229	4.592442	0.572090
H	1.616087	4.988268	-1.673750
H	1.718406	6.302197	-0.488726
H	3.110427	5.253341	-0.761337
H	1.802576	4.125921	2.572664
H	3.295093	4.417645	1.664776
H	2.159169	5.741738	1.941734
C	4.828914	-1.052093	-1.249207
C	5.746375	0.148679	-0.998847
C	5.324048	-1.917191	-2.409765
H	4.849877	-1.682491	-0.354834
H	5.424912	0.698706	-0.108106
H	6.779885	-0.181409	-0.841286
H	5.748356	0.844491	-1.846166
H	4.661752	-2.776296	-2.558618
H	5.374912	-1.352588	-3.348227
H	6.330380	-2.295085	-2.197262
C	2.575708	-3.602662	1.010148
C	3.777980	-4.552861	0.959411

C	1.286856	-4.363388	1.344221
H	2.756184	-2.910513	1.833232
H	4.697539	-3.997752	0.745491
H	3.900432	-5.068449	1.919121
H	3.659206	-5.321834	0.187035
H	0.445043	-3.672590	1.440708
H	1.045641	-5.112482	0.581430
H	1.401786	-4.890037	2.298746

A6

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.142779	-0.144196	-0.625003
N	-0.250995	-1.146011	1.406414
C	2.263271	-2.226360	0.618105
H	1.607740	-3.034437	0.258967
H	3.244261	-2.655613	0.835702
C	-2.878946	0.194131	1.337387
C	-0.315279	-0.084571	-2.375196
O	-0.509703	-0.160992	-3.524375
P	-2.504778	-0.263223	-0.389741
P	2.231034	-0.981655	-0.700035
Si	-1.473595	-0.386714	2.462561
Si	1.297939	-1.690433	2.137619
C	-2.124638	-1.582460	3.757601
H	-1.392302	-1.749385	4.555766
H	-3.029508	-1.175798	4.228058
H	-2.375472	-2.560594	3.334174
C	1.064109	-3.184275	3.238757
H	2.045038	-3.612507	3.487773
H	0.576741	-2.927781	4.186668
H	0.474370	-3.963068	2.734793
H	-2.842813	1.286157	1.338407
H	-3.872250	-0.088318	1.699591
P	0.355162	2.201997	-0.055626
C	1.595566	2.072076	1.285858
H	2.358999	1.410210	0.856950
H	2.101265	3.029217	1.454325
Si	1.155324	1.363803	2.989164
C	1.835086	2.565395	4.277398
H	2.903790	2.756779	4.117681

H	1.314357	3.530798	4.249941
H	1.721121	2.160385	5.290641
C	-0.678510	1.088761	3.318713
H	-1.229882	2.001266	3.063928
H	-0.784955	0.947504	4.404224
C	2.030007	-0.289076	3.158864
H	3.095305	-0.153660	2.933843
H	1.979428	-0.599574	4.212313
C	-0.319167	-4.969144	0.319336
O	-0.256005	-3.733508	0.030867
O	-0.436467	-5.494543	1.433050
H	-0.262848	-5.658465	-0.564147
H	-0.608536	-2.032945	0.990091
N	-3.012901	-1.880817	-0.498564
N	-3.560357	0.697895	-1.320698
N	2.606387	-1.858616	-2.113594
N	3.589469	0.020502	-0.308886
N	1.219474	3.134911	-1.210039
N	-0.821261	3.221195	0.701307
C	-2.607561	-2.595991	-1.708264
H	-2.177931	-1.899783	-2.432836
H	-1.854180	-3.355966	-1.479457
H	-3.472305	-3.058928	-2.198891
C	-3.109977	1.373468	-2.525470
H	-3.693046	2.288614	-2.682353
H	-2.067900	1.673814	-2.413318
H	-3.191085	0.756751	-3.430379
C	-0.440575	4.316654	1.585384
H	-0.410243	5.291258	1.075172
H	-1.146690	4.398614	2.419350
H	0.538337	4.147547	2.028916
C	1.104295	2.885740	-2.632495
H	0.794940	1.858104	-2.804546
H	0.381828	3.545417	-3.137050
H	2.073713	3.021658	-3.130526
C	3.962460	0.879161	-1.424482
H	3.068557	1.376613	-1.809346
H	4.651527	1.658490	-1.094754
H	4.441732	0.332071	-2.250356
C	2.429746	-1.222893	-3.407962
H	1.741891	-1.784298	-4.052269
H	2.018888	-0.221655	-3.280951
H	3.385895	-1.112037	-3.936973
C	-3.922827	-2.611155	0.400265

C	-3.276959	-3.871859	0.975427
C	-5.267970	-2.983111	-0.242566
H	-4.140157	-1.945533	1.237909
H	-2.307314	-3.670827	1.431307
H	-3.938869	-4.315653	1.728590
H	-3.109976	-4.626421	0.199360
H	-5.771768	-2.125606	-0.694328
H	-5.151299	-3.752324	-1.013737
H	-5.932494	-3.397853	0.523888
C	-5.010159	0.510696	-1.184868
C	-5.632219	-0.103746	-2.441529
C	-5.721604	1.801765	-0.775663
H	-5.151409	-0.199489	-0.365271
H	-5.091143	-1.006820	-2.743348
H	-6.677958	-0.373596	-2.257101
H	-5.618767	0.601880	-3.279866
H	-5.360709	2.141772	0.199293
H	-5.564868	2.605426	-1.504704
H	-6.801999	1.633754	-0.697880
C	-2.097614	3.461138	0.005656
C	-2.004768	4.440572	-1.169949
C	-3.187335	3.937526	0.971432
H	-2.414846	2.496569	-0.391392
H	-1.306729	4.085746	-1.931957
H	-2.987710	4.556578	-1.640959
H	-1.682449	5.434973	-0.839248
H	-3.255529	3.306635	1.864852
H	-3.023344	4.970209	1.298003
H	-4.154622	3.913381	0.462606
C	1.907723	4.388013	-0.846413
C	1.465908	5.587598	-1.690347
C	3.431635	4.239690	-0.890518
H	1.638191	4.619423	0.185309
H	0.379221	5.703100	-1.691616
H	1.903716	6.503660	-1.278873
H	1.803251	5.502317	-2.729296
H	3.769013	3.479893	-0.180388
H	3.777605	3.952883	-1.890203
H	3.914485	5.189634	-0.632576
C	4.713493	-0.414758	0.535551
C	5.382306	0.784423	1.216643
C	5.744467	-1.287706	-0.185263
H	4.279710	-1.010369	1.340010
H	4.632648	1.447138	1.663427

H	6.046155	0.432229	2.013921
H	5.994786	1.375516	0.526691
H	5.283527	-2.197800	-0.581056
H	6.213177	-0.752527	-1.019159
H	6.540518	-1.586946	0.506220
C	3.103244	-3.242793	-2.150489
C	4.331403	-3.401250	-3.052754
C	1.987772	-4.214445	-2.548659
H	3.415704	-3.498123	-1.135887
H	5.094348	-2.647803	-2.828880
H	4.775531	-4.391199	-2.900269
H	4.072012	-3.321116	-4.114345
H	1.125035	-4.087738	-1.886682
H	1.663270	-4.043369	-3.582226
H	2.337562	-5.251492	-2.478819

A7

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.041639	-0.337250	-0.679474
N	0.187936	-1.041366	1.554254
C	2.893088	0.065566	1.157004
H	3.906544	-0.141356	1.515976
H	2.811028	1.145587	0.992002
C	-2.513446	-1.822709	1.063317
C	0.080067	-0.148574	-2.425595
O	0.172908	-0.099525	-3.588320
P	-2.407477	-0.799732	-0.444692
P	2.484428	-0.620526	-0.479831
Si	-1.351116	-1.290689	2.431305
Si	1.571617	-0.363160	2.432871
C	-1.216067	-2.679087	3.687297
H	-0.656430	-2.378579	4.581051
H	-2.217153	-2.985627	4.019356
H	-0.724789	-3.542590	3.228452
C	2.237979	-1.575962	3.706840
H	3.220245	-1.252031	4.075249
H	1.571743	-1.638202	4.575074
H	2.342628	-2.589298	3.306265
H	-3.527011	-2.042147	1.409972
H	-2.051631	-2.773829	0.757621

P	-0.162742	2.025049	-0.232900
C	-1.161466	2.359802	1.249837
H	-1.366055	3.433023	1.330979
H	-2.112431	1.874184	0.998910
Si	-0.739716	1.753066	2.994604
C	-1.164774	3.185081	4.148212
H	-0.538409	4.065085	3.952405
H	-2.211649	3.492891	4.032849
H	-1.016542	2.904415	5.198101
C	-1.832123	0.276909	3.361734
H	-2.880778	0.540603	3.179889
H	-1.756428	0.053441	4.435368
C	1.029676	1.208153	3.312898
H	1.734747	2.017748	3.096002
H	1.095910	1.031579	4.396795
H	-0.329632	-2.075063	-0.923705
H	0.448678	-2.009529	-0.829350
C	-0.043422	-4.605846	0.043003
O	-0.517060	-4.388074	-1.085408
O	-0.057432	-3.856505	1.060185
H	0.460424	-5.596831	0.192225
H	0.397616	-2.016086	1.258802
N	2.844561	-2.293180	-0.339688
N	3.654215	0.092658	-1.498687
N	1.277062	2.921547	0.109673
N	-1.115999	2.867622	-1.413009
N	-3.065211	-1.785606	-1.662478
N	-3.566133	0.463726	-0.158268
C	-2.390832	-1.909465	-2.946799
H	-3.080027	-2.340136	-3.679127
H	-2.104343	-0.931146	-3.333099
H	-1.505061	-2.555475	-2.896355
C	-3.925959	1.119694	-1.409756
H	-4.454893	2.057153	-1.217289
H	-3.010702	1.365017	-1.952283
H	-4.556549	0.494045	-2.057894
C	-2.140085	3.845084	-1.082794
H	-1.749842	4.821039	-0.757702
H	-2.760137	4.027164	-1.965871
H	-2.810527	3.471423	-0.308459
C	2.262556	2.955283	-0.958575
H	3.277057	2.851018	-0.566926
H	2.095429	2.113835	-1.626429
H	2.221513	3.877135	-1.555157

C	3.365603	0.392134	-2.888805
H	3.666615	-0.410173	-3.576692
H	2.300492	0.554785	-3.028910
H	3.879363	1.312918	-3.196594
C	2.679060	-3.020262	-1.593511
H	3.578817	-2.982052	-2.226554
H	2.427110	-4.067379	-1.404950
H	1.852113	-2.598076	-2.172589
C	-4.154212	-2.744448	-1.422887
C	-3.698170	-4.196427	-1.589631
C	-5.383066	-2.450955	-2.290981
H	-4.453221	-2.617806	-0.380230
H	-2.754019	-4.374877	-1.068047
H	-4.467434	-4.879602	-1.209942
H	-3.533835	-4.440817	-2.645967
H	-5.714577	-1.414133	-2.182416
H	-5.180757	-2.632571	-3.352571
H	-6.212290	-3.108039	-2.002769
C	-4.627906	0.440629	0.863722
C	-5.957114	-0.167200	0.403809
C	-4.874254	1.843524	1.435173
H	-4.253003	-0.167692	1.687961
H	-5.845378	-1.213448	0.112484
H	-6.690167	-0.125325	1.217450
H	-6.377719	0.382055	-0.445941
H	-3.954272	2.289259	1.823602
H	-5.294071	2.526237	0.687705
H	-5.594345	1.786733	2.259140
C	-0.565745	3.021866	-2.772586
C	-0.109165	4.456984	-3.068990
C	-1.536084	2.551017	-3.860909
H	0.313325	2.376283	-2.828930
H	0.500511	4.861819	-2.257099
H	0.483141	4.482472	-3.990355
H	-0.963938	5.128465	-3.211444
H	-1.815720	1.505702	-3.719323
H	-2.450509	3.155518	-3.885444
H	-1.059942	2.638487	-4.844002
C	1.371350	4.048465	1.049480
C	0.920133	5.398823	0.483619
C	2.789252	4.176711	1.618686
H	0.718329	3.811536	1.891600
H	-0.109449	5.357893	0.121021
H	0.972667	6.169526	1.261464

H	1.561369	5.723196	-0.343842
H	3.178608	3.210933	1.957553
H	3.490802	4.586346	0.883492
H	2.780870	4.858621	2.475777
C	5.081810	0.072267	-1.144605
C	5.624036	1.479338	-0.874292
C	5.939169	-0.648689	-2.190182
H	5.168092	-0.488962	-0.210584
H	5.137674	1.924654	-0.000534
H	6.702068	1.442819	-0.677908
H	5.464753	2.142156	-1.732523
H	5.516891	-1.625231	-2.448081
H	6.032507	-0.063264	-3.111506
H	6.949957	-0.807227	-1.798763
C	3.748905	-2.929090	0.637590
C	5.134585	-3.298448	0.091011
C	3.111403	-4.180387	1.251276
H	3.891060	-2.206179	1.444355
H	5.682322	-2.440332	-0.301721
H	5.735066	-3.737199	0.896023
H	5.062410	-4.049297	-0.703756
H	2.078399	-3.999766	1.558041
H	3.098482	-5.009768	0.533976
H	3.702155	-4.510952	2.114025

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.024369	-0.266737	-0.589779
N	-0.013816	-0.931468	1.722882
C	2.844802	-0.684734	1.229077
H	3.721150	-1.252417	1.559033
H	3.185473	0.340568	1.056041
C	-2.795202	-1.123641	1.171041
C	-0.089902	-0.376416	-2.330448
O	-0.140856	-0.608841	-3.480094
P	-2.445456	-0.210603	-0.373486
P	2.137937	-1.197160	-0.391048
Si	-1.577221	-0.749837	2.541216
Si	1.504017	-0.564298	2.546508
C	-1.814331	-2.058296	3.873147

H	-1.100030	-1.941966	4.696913
H	-2.822390	-1.987514	4.302946
H	-1.698732	-3.064327	3.456035
C	1.851922	-1.779656	3.944153
H	2.897203	-1.709421	4.272203
H	1.223416	-1.573042	4.818456
H	1.663776	-2.817225	3.644460
H	-3.836835	-1.098295	1.502719
H	-2.551775	-2.174703	0.983168
P	0.500507	2.128871	-0.261946
C	-0.546894	2.719965	1.120577
H	-0.585318	3.811349	1.190024
H	-1.564176	2.389843	0.878538
Si	-0.235150	2.096720	2.887546
C	-0.304719	3.627688	3.991824
H	0.476788	4.351985	3.729442
H	-1.272063	4.136671	3.892831
H	-0.173367	3.369087	5.049739
C	-1.648407	0.944454	3.345020
H	-2.598970	1.434417	3.104079
H	-1.640665	0.799468	4.434792
C	1.378051	1.180227	3.221328
H	2.215505	1.754851	2.817203
H	1.506250	1.154403	4.313272
H	-0.894096	-3.102030	-0.778017
H	-0.549371	-1.808954	-0.650575
C	-1.581131	-4.683638	0.120182
O	-1.130204	-4.084375	-0.953360
O	-1.753079	-4.185972	1.215517
H	-1.801388	-5.742445	-0.086491
H	0.012530	-1.867698	1.308627
N	3.419247	-0.861405	-1.473594
N	2.079478	-2.911939	-0.255273
N	2.045993	2.769002	0.237817
N	-0.043223	3.122147	-1.568806
N	-3.266902	-1.162670	-1.553876
N	-3.404384	1.223882	-0.152704
C	-3.334438	-0.597829	-2.888236
H	-2.741912	0.316748	-2.933938
H	-2.925700	-1.275268	-3.646465
H	-4.363667	-0.333753	-3.180015
C	-3.148367	2.298372	-1.100353
H	-3.364001	3.274483	-0.646563
H	-2.096628	2.288029	-1.385063

H	-3.747894	2.222335	-2.019304
C	-0.565971	4.465594	-1.392312
H	0.197937	5.223031	-1.166582
H	-1.077572	4.782566	-2.306822
H	-1.315376	4.494583	-0.598527
C	3.185469	2.330422	-0.552096
H	4.112559	2.417722	0.028357
H	3.069562	1.285194	-0.828959
H	3.328688	2.903670	-1.479484
C	3.167680	-0.318793	-2.793755
H	3.116414	-1.089628	-3.575708
H	2.220365	0.216921	-2.788957
H	3.949752	0.400089	-3.072903
C	1.797928	-3.551056	-1.530948
H	1.312557	-4.520137	-1.388345
H	1.108392	-2.928930	-2.109534
H	2.704059	-3.703419	-2.136218
C	-4.059713	-2.374087	-1.329263
C	-3.876895	-3.387837	-2.465478
C	-5.554894	-2.109466	-1.105961
H	-3.676518	-2.847978	-0.423911
H	-2.818930	-3.535688	-2.693907
H	-4.299228	-4.353450	-2.164736
H	-4.396437	-3.075736	-3.378843
H	-5.724358	-1.487047	-0.222703
H	-6.006402	-1.609251	-1.970737
H	-6.088793	-3.055869	-0.956313
C	-4.794087	1.204932	0.335727
C	-5.848694	1.364081	-0.767284
C	-5.001874	2.263187	1.423564
H	-4.962207	0.232009	0.799171
H	-5.648419	0.696382	-1.609495
H	-6.840507	1.119919	-0.370422
H	-5.891310	2.391705	-1.145384
H	-4.322525	2.097708	2.264282
H	-4.827960	3.274918	1.039409
H	-6.029519	2.227380	1.804001
C	0.372999	2.780840	-2.938691
C	1.373101	3.770753	-3.545815
C	-0.822806	2.602748	-3.879136
H	0.872645	1.813888	-2.865112
H	2.286124	3.842036	-2.949258
H	1.659002	3.439640	-4.550693
H	0.945288	4.775908	-3.641886

H	-1.501893	1.836881	-3.502514
H	-1.386963	3.534720	-4.006317
H	-0.479719	2.287472	-4.870431
C	2.209875	4.149534	0.748939
C	2.774627	5.145009	-0.275969
C	3.088032	4.185131	2.006774
H	1.221121	4.513120	1.035233
H	2.260020	5.084960	-1.236959
H	2.658263	6.165362	0.106170
H	3.843829	4.982185	-0.452972
H	2.607915	3.693689	2.855429
H	4.054848	3.698430	1.833418
H	3.290751	5.223149	2.295617
C	4.788416	-1.309345	-1.200083
C	5.716203	-0.131939	-0.880465
C	5.367773	-2.173925	-2.322973
H	4.738904	-1.937216	-0.305608
H	5.383464	0.388805	0.022080
H	6.742034	-0.481600	-0.714807
H	5.739836	0.592662	-1.702663
H	4.691649	-2.994733	-2.581822
H	5.556512	-1.588597	-3.230077
H	6.323447	-2.606538	-2.006640
C	2.679789	-3.771043	0.769721
C	3.854609	-4.620840	0.267369
C	1.616042	-4.671261	1.408169
H	3.058509	-3.119514	1.560055
H	4.632844	-4.010965	-0.200915
H	4.308653	-5.162281	1.105069
H	3.524578	-5.365763	-0.465304
H	0.782214	-4.078812	1.795118
H	1.209784	-5.386575	0.682711
H	2.044762	-5.250692	2.234461

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.031925	-0.294461	-0.690918
N	0.174251	-1.063979	1.563458
C	2.886498	0.016020	1.163688
H	3.895381	-0.221087	1.517394

H	2.833280	1.099635	1.009996
C	-2.527439	-1.811415	1.046570
C	0.081392	-0.105703	-2.428924
O	0.184705	-0.069922	-3.595073
P	-2.389042	-0.776402	-0.458737
P	2.451275	-0.642503	-0.483382
Si	-1.372630	-1.287302	2.426129
Si	1.562240	-0.390097	2.439560
C	-1.286235	-2.646858	3.719804
H	-0.726270	-2.329084	4.607585
H	-2.300103	-2.905399	4.054663
H	-0.820654	-3.546083	3.307753
C	2.221747	-1.598806	3.722065
H	3.178685	-1.246357	4.129034
H	1.526623	-1.698159	4.563790
H	2.377760	-2.601938	3.312613
H	-3.548632	-2.003676	1.387377
H	-2.101912	-2.777697	0.746999
P	-0.141113	2.044640	-0.220769
C	-1.146445	2.394203	1.257517
H	-1.334956	3.469622	1.348232
H	-2.104050	1.923734	1.002236
Si	-0.736671	1.757595	2.992509
C	-1.146640	3.174936	4.170180
H	-0.500467	4.045308	3.997180
H	-2.185669	3.506463	4.049413
H	-1.015626	2.871268	5.215995
C	-1.853961	0.293006	3.332504
H	-2.893085	0.570596	3.119251
H	-1.813229	0.072544	4.408642
C	1.022790	1.183471	3.317560
H	1.739475	1.985540	3.110417
H	1.078266	1.002487	4.401538
H	-0.152195	-2.810413	-0.975683
H	-0.050972	-1.958434	-1.001718
C	-0.205803	-4.687456	0.131294
O	-0.268619	-4.222679	-1.047549
O	-0.170101	-4.046649	1.193885
H	-0.189464	-5.797293	0.188107
H	0.394649	-2.018004	1.233169
N	2.776227	-2.325034	-0.361972
N	3.655909	0.045198	-1.485563
N	1.306449	2.929453	0.138412
N	-1.074887	2.915041	-1.401200

N	-3.032813	-1.773407	-1.680684
N	-3.560851	0.479494	-0.171211
C	-2.397264	-1.813449	-2.988877
H	-2.156736	-0.809258	-3.339695
H	-1.480155	-2.416022	-2.998243
H	-3.090141	-2.240239	-3.719889
C	-3.889116	1.155212	-1.420266
H	-4.413680	2.095394	-1.228076
H	-2.960085	1.399108	-1.940202
H	-4.512871	0.543769	-2.089730
C	-2.091136	3.899670	-1.071977
H	-1.695072	4.868823	-0.732318
H	-2.700613	4.097946	-1.959226
H	-2.773943	3.525847	-0.308206
C	2.303308	2.946406	-0.918876
H	3.313256	2.839264	-0.515676
H	2.136726	2.098886	-1.579235
H	2.276542	3.862353	-1.526120
C	3.383707	0.397861	-2.865584
H	3.706451	-0.372986	-3.579431
H	2.317558	0.546817	-3.014641
H	3.887379	1.337726	-3.132150
C	2.610899	-3.000093	-1.643558
H	2.363956	-4.055152	-1.500028
H	1.777572	-2.551128	-2.190622
H	3.509710	-2.928163	-2.276057
C	-4.111276	-2.744810	-1.463261
C	-3.636676	-4.189149	-1.646039
C	-5.340356	-2.461190	-2.335993
H	-4.421190	-2.635954	-0.421633
H	-2.738476	-4.385470	-1.055772
H	-4.424544	-4.889696	-1.345018
H	-3.390624	-4.397357	-2.693816
H	-5.654812	-1.416838	-2.252163
H	-5.146587	-2.672651	-3.393607
H	-6.177492	-3.098460	-2.027202
C	-4.643942	0.448119	0.825477
C	-5.961322	-0.163634	0.336890
C	-4.905986	1.848124	1.397260
H	-4.285127	-0.160419	1.656985
H	-5.838266	-1.208035	0.042617
H	-6.710720	-0.129148	1.135993
H	-6.367296	0.387631	-0.518721
H	-3.991056	2.298295	1.792908

H	-5.323725	2.529665	0.647604
H	-5.632459	1.785430	2.215272
C	-0.515147	3.068469	-2.756178
C	-0.037212	4.498437	-3.043817
C	-1.485272	2.615903	-3.852641
H	0.354703	2.410346	-2.811034
H	0.581168	4.887782	-2.230997
H	0.553042	4.521342	-3.966697
H	-0.881561	5.184693	-3.178980
H	-1.776871	1.573094	-3.717614
H	-2.392345	3.231599	-3.878806
H	-1.003025	2.702409	-4.832914
C	1.408448	4.052985	1.079421
C	0.986669	5.411964	0.510557
C	2.822003	4.157339	1.665128
H	0.741983	3.826678	1.914133
H	-0.038106	5.387625	0.132958
H	1.040477	6.180803	1.290353
H	1.644702	5.727162	-0.307249
H	3.193927	3.182495	1.997980
H	3.536857	4.563257	0.940707
H	2.814848	4.831318	2.528619
C	5.076756	0.006545	-1.112141
C	5.616404	1.396048	-0.756365
C	5.953052	-0.652449	-2.182913
H	5.151481	-0.607330	-0.210538
H	5.112302	1.797024	0.128607
H	6.690304	1.346407	-0.540202
H	5.476165	2.102810	-1.582456
H	5.534197	-1.609253	-2.511547
H	6.066553	-0.010703	-3.063673
H	6.955170	-0.837762	-1.780875
C	3.688965	-2.993439	0.581970
C	5.040847	-3.415280	-0.010828
C	3.023731	-4.220588	1.212899
H	3.886377	-2.281174	1.387370
H	5.583650	-2.584062	-0.463630
H	5.671397	-3.833692	0.781948
H	4.918518	-4.193301	-0.772890
H	2.042301	-3.982127	1.625177
H	2.879127	-5.018881	0.474402
H	3.662433	-4.625094	2.007420

A2

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.160916	-0.168826	-0.514271
N	-0.121666	-0.641697	1.537033
C	2.799020	-0.980947	1.113469
H	3.396378	-1.845394	1.421658
H	3.462720	-0.111754	1.087656
C	-2.965377	-0.045197	1.467573
C	-0.253506	-0.174519	-2.260960
O	-0.329102	-0.213315	-3.434335
P	-2.523630	-0.437984	-0.248159
P	2.043575	-1.159030	-0.530431
Si	-1.463709	-0.372842	2.582086
Si	1.396758	-0.639062	2.348561
C	-1.892517	-1.763147	3.802767
H	-1.281923	-1.684034	4.709450
H	-2.940191	-1.675161	4.121693
H	-1.744110	-2.769679	3.402690
C	1.535057	-1.929005	3.734193
H	2.585998	-2.101063	4.002732
H	1.021966	-1.606504	4.648256
H	1.099129	-2.890285	3.437789
H	-3.126306	1.039979	1.463298
H	-3.890208	-0.511101	1.823215
P	0.298141	2.079839	-0.324770
C	-0.267923	2.808005	1.271581
H	-0.089474	3.891219	1.246570
H	-1.359402	2.690975	1.213283
Si	0.209679	2.179004	3.012007
C	0.489450	3.746539	4.035357
H	1.343078	4.326051	3.658910
H	-0.389263	4.404046	4.015416
H	0.696278	3.504361	5.085348
C	-1.231037	1.174893	3.670070
H	-2.154013	1.769139	3.709053
H	-1.006953	0.877188	4.704364
C	1.716681	1.058332	3.153450
H	2.626347	1.521624	2.756804
H	1.895051	0.922361	4.231210
C	-2.753491	-2.711581	-1.709085
H	-2.180622	-2.083419	-2.397164

H	-2.279457	-3.700222	-1.721895
H	-3.768633	-2.822814	-2.119566
C	-3.741195	0.224980	-2.589742
H	-2.715472	0.071784	-2.926052
H	-4.346698	-0.603193	-2.987742
H	-4.096285	1.152879	-3.050581
C	-0.031827	4.537885	-1.527027
H	1.049078	4.671684	-1.534837
H	-0.415598	5.002773	-2.439793
H	-0.444754	5.101601	-0.674652
C	2.594972	2.440628	-1.652657
H	1.958226	1.859294	-2.322397
H	2.766429	3.415686	-2.135741
H	3.550410	1.916532	-1.571865
C	0.560238	-3.257734	-1.397678
H	-0.306834	-2.644642	-1.152213
H	0.723011	-3.212938	-2.485348
H	0.291724	-4.286242	-1.140125
C	3.044477	-0.652370	-2.993070
H	2.038605	-0.257059	-3.125236
H	3.737084	0.048165	-3.476541
H	3.099379	-1.608848	-3.534992
N	-2.751887	-2.149703	-0.369866
N	-3.794428	0.317217	-1.135713
N	-0.371601	3.128421	-1.516134
N	1.943972	2.573051	-0.360178
N	1.709127	-2.835356	-0.614990
N	3.350763	-0.781131	-1.578515
C	-2.958402	-3.105974	0.724179
C	-1.682144	-3.900781	1.033446
C	-4.117042	-4.079406	0.466565
H	-3.215931	-2.526268	1.612799
H	-0.833935	-3.225532	1.182429
H	-1.818500	-4.511689	1.933770
H	-1.445671	-4.587530	0.213014
H	-5.050216	-3.565672	0.222256
H	-3.887542	-4.769533	-0.353008
H	-4.289025	-4.684685	1.363591
C	-5.161229	0.422091	-0.581177
C	-5.879743	-0.924992	-0.469959
C	-6.023350	1.419786	-1.357141
H	-5.056178	0.828977	0.427968
H	-5.361931	-1.578759	0.233432
H	-6.906802	-0.785894	-0.112635

H	-5.926826	-1.434769	-1.439450
H	-5.522723	2.385945	-1.465297
H	-6.294030	1.051008	-2.352598
H	-6.956135	1.585551	-0.807436
C	-1.638537	2.796053	-2.168323
C	-1.532447	2.916389	-3.691022
C	-2.817128	3.607541	-1.624801
H	-1.825482	1.751679	-1.928327
H	-0.687300	2.328075	-4.058005
H	-2.444546	2.539412	-4.167635
H	-1.401437	3.955500	-4.017157
H	-2.952896	3.435781	-0.551394
H	-2.680435	4.683346	-1.786804
H	-3.740299	3.316710	-2.134997
C	2.642288	3.386176	0.642203
C	2.656516	4.902342	0.395742
C	4.078977	2.898691	0.849952
H	2.125671	3.230036	1.586881
H	1.657840	5.340236	0.468928
H	3.284468	5.387575	1.152314
H	3.076704	5.152323	-0.585352
H	4.107295	1.814692	0.985054
H	4.725522	3.158442	0.003970
H	4.505912	3.365149	1.744501
C	2.702249	-3.876769	-0.323351
C	2.944222	-4.829713	-1.502059
C	2.310833	-4.659911	0.932737
H	3.651960	-3.372098	-0.121676
H	3.055679	-4.287078	-2.446102
H	3.857828	-5.409898	-1.331688
H	2.122672	-5.544535	-1.622782
H	2.246082	-3.992870	1.797189
H	1.331461	-5.136922	0.804608
H	3.043906	-5.445701	1.152550
C	4.762639	-1.088503	-1.279270
C	5.630949	0.172462	-1.332511
C	5.369264	-2.170558	-2.180546
H	4.800248	-1.460339	-0.252701
H	5.302004	0.905024	-0.592600
H	6.678392	-0.074859	-1.123061
H	5.595539	0.643447	-2.321707
H	4.753990	-3.072494	-2.210155
H	5.502192	-1.814150	-3.208215
H	6.358436	-2.450938	-1.801327

A1

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.177396	-0.250250	-0.673094
N	-0.008421	-0.866393	1.706251
C	2.787118	-0.660960	0.868724
H	3.753893	-1.138868	1.063471
H	2.975836	0.402014	0.684668
C	-2.858982	-0.170228	1.473008
C	-0.357610	-0.261129	-2.395858
O	-0.518548	-0.371524	-3.558804
P	-2.499886	-0.454078	-0.303793
P	1.964152	-1.107514	-0.709567
Si	-1.464527	-0.584914	2.667089
Si	1.630113	-0.701035	2.351490
C	-1.898768	-2.049627	3.766006
H	-1.093715	-2.240313	4.486815
H	-2.808087	-1.834329	4.342306
H	-2.067591	-2.978368	3.213585
C	2.043222	-2.091568	3.555448
H	3.113745	-2.093805	3.799023
H	1.499719	-1.951609	4.498605
H	1.783646	-3.083884	3.173587
H	-2.944044	0.922708	1.521710
H	-3.819542	-0.570615	1.814548
P	0.360441	2.029287	-0.257962
C	-0.251316	2.679758	1.375324
H	-0.083317	3.764652	1.401028
H	-1.339835	2.558808	1.284850
Si	0.202201	2.022960	3.103222
C	0.403286	3.545721	4.199845
H	1.221056	4.188889	3.849688
H	-0.511357	4.152168	4.205728
H	0.623047	3.268020	5.238071
C	-1.177304	0.921540	3.753236
H	-2.120799	1.475661	3.846653
H	-0.900884	0.604077	4.768642
C	1.726953	0.927299	3.284238
H	2.665015	1.435613	3.037796
H	1.782891	0.707769	4.360888

H	-0.470222	-1.816090	-0.714534
H	-0.100725	-1.699414	1.111410
C	-2.756934	-2.606304	-1.910066
H	-2.382009	-1.830729	-2.575438
H	-1.961105	-3.360979	-1.852845
H	-3.634923	-3.056296	-2.392110
C	-3.800258	0.465270	-2.463626
H	-2.805251	0.316923	-2.885441
H	-4.431313	-0.370448	-2.805240
H	-4.197829	1.387177	-2.899569
C	0.092622	4.568460	-1.329967
H	1.170240	4.689948	-1.234489
H	-0.200397	5.063055	-2.261148
H	-0.390064	5.114647	-0.502746
C	2.729367	2.606041	-1.445990
H	2.046234	2.369170	-2.263368
H	3.134452	3.606546	-1.656867
H	3.553385	1.885913	-1.470099
C	1.323726	-3.470675	-1.798881
H	1.082882	-2.742458	-2.577193
H	1.921711	-4.264817	-2.265610
H	0.368682	-3.899572	-1.464380
C	2.758026	-0.164143	-3.167237
H	1.832572	0.399832	-3.084855
H	3.522040	0.514047	-3.569409
H	2.599378	-0.967766	-3.901476
N	-3.112284	-2.053474	-0.610971
N	-3.725593	0.570349	-1.010014
N	-0.262718	3.165675	-1.387661
N	2.011545	2.580890	-0.181001
N	2.056640	-2.828346	-0.722605
N	3.150214	-0.644080	-1.856095
C	-3.399897	-3.068468	0.404104
C	-2.193652	-3.950426	0.758725
C	-4.577013	-3.963340	-0.008601
H	-3.702964	-2.541189	1.313238
H	-1.334995	-3.342642	1.046577
H	-2.440743	-4.624382	1.587638
H	-1.884448	-4.573992	-0.086447
H	-5.435569	-3.371372	-0.338116
H	-4.298797	-4.641736	-0.822940
H	-4.888967	-4.584458	0.838967
C	-5.050143	0.739491	-0.372145
C	-5.919640	-0.524676	-0.324267

C	-5.841432	1.887129	-1.007677
H	-4.860833	1.046532	0.659665
H	-5.492579	-1.279568	0.337972
H	-6.920855	-0.275702	0.047848
H	-6.031905	-0.976169	-1.316000
H	-5.234356	2.792311	-1.092286
H	-6.227911	1.629983	-1.999957
H	-6.705328	2.119631	-0.374809
C	-1.464730	2.859434	-2.163228
C	-1.204523	2.948429	-3.668799
C	-2.657845	3.723911	-1.749321
H	-1.708256	1.826777	-1.922382
H	-0.374374	2.294889	-3.950018
H	-2.091274	2.628739	-4.228952
H	-0.967368	3.971656	-3.986923
H	-2.885051	3.587175	-0.686687
H	-2.475937	4.789971	-1.930431
H	-3.543804	3.445235	-2.327545
C	2.666028	3.314725	0.909260
C	2.600284	4.849094	0.833174
C	4.133050	2.891541	1.070627
H	2.160676	3.034237	1.830246
H	1.574095	5.218889	0.899818
H	3.162112	5.280335	1.670326
H	3.047502	5.236684	-0.089442
H	4.242380	1.805964	1.143670
H	4.749048	3.236704	0.232773
H	4.547488	3.332503	1.984137
C	2.593677	-3.713082	0.306252
C	3.741324	-4.596296	-0.203670
C	1.507210	-4.581621	0.953504
H	3.008896	-3.076820	1.090432
H	4.545832	-3.991393	-0.632339
H	4.159638	-5.185302	0.621101
H	3.402360	-5.302688	-0.969880
H	0.685496	-3.962271	1.325707
H	1.089554	-5.303034	0.242272
H	1.920287	-5.150996	1.794101
C	4.497328	-1.220695	-1.765577
C	5.559039	-0.123767	-1.648512
C	4.813765	-2.196920	-2.902374
H	4.528724	-1.799853	-0.838364
H	5.364766	0.503600	-0.771868
H	6.559198	-0.561408	-1.543743

H	5.571301	0.522363	-2.534391
H	4.033402	-2.960690	-2.984297
H	4.899704	-1.685321	-3.867685
H	5.768543	-2.701459	-2.714241

$R^1=R^2=R^3=CF_3$

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.064284	-0.686837	-0.365874
N	-0.063013	-0.188929	1.717137
C	2.871794	-0.394223	1.468203
H	3.451421	-1.130921	2.032729
H	3.563355	0.398382	1.177314
C	-2.962099	0.159934	1.297832
C	-0.018762	-1.214866	-2.084655
O	0.034977	-1.612864	-3.166318
P	-2.345980	-0.720238	-0.155765
P	2.132743	-1.153514	-0.005746
Si	-1.511011	0.209301	2.558069
Si	1.401651	0.310523	2.475936
C	-1.994585	-0.937708	3.968837
H	-1.220771	-0.972384	4.743747
H	-2.924118	-0.598867	4.444672
H	-2.151481	-1.961878	3.612710
C	1.623026	-0.300324	4.244937
H	2.628589	-0.056749	4.612283
H	0.908907	0.161602	4.937951
H	1.495474	-1.387530	4.307869
H	-3.211365	1.181223	0.992225
H	-3.877340	-0.288521	1.697153
C	2.369697	-2.972544	0.454125
C	3.433384	-1.111275	-1.384388
C	-2.958111	-2.475980	0.217974
C	-3.587798	-0.327007	-1.540303
P	0.105501	1.545996	-0.832083
C	-0.670481	2.782397	0.265308
H	-0.560715	3.768483	-0.197585
H	-1.743360	2.559445	0.242151
Si	-0.169563	2.939763	2.119950
C	1.791492	2.396850	-1.129255

C	-0.604934	2.145664	-2.484753
C	-0.221396	4.791289	2.454572
H	0.528925	5.325894	1.859229
H	-1.203834	5.217487	2.215878
H	-0.018562	5.002519	3.511588
C	-1.419604	2.002663	3.168582
H	-2.409308	2.477699	3.153579
H	-1.075504	2.035961	4.212819
C	1.517531	2.209288	2.499217
H	2.281647	2.594039	1.815696
H	1.807144	2.546642	3.505025
H	-0.239250	-2.161117	0.556500
H	-0.222264	-2.427753	-0.189095
F	1.769085	-3.204342	1.635904
F	3.660863	-3.306726	0.593486
F	1.828196	-3.804069	-0.444183
F	4.669011	-0.869621	-0.932415
F	3.129494	-0.160581	-2.276116
F	3.455196	-2.278647	-2.044985
F	-4.250304	-2.542054	0.555123
F	-2.270302	-2.993259	1.252385
F	-2.763190	-3.272861	-0.842315
F	-4.687473	-1.090402	-1.528940
F	-3.011052	-0.477319	-2.737551
F	-3.995603	0.945831	-1.423448
F	-0.192086	1.395629	-3.509608
F	-1.943047	2.081810	-2.440696
F	-0.288077	3.423799	-2.757483
F	2.157524	2.325026	-2.412391
F	2.767835	1.810177	-0.410116
F	1.793578	3.692036	-0.780634

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.103749	-0.640648	-0.194090
N	-0.218211	0.054386	1.896078
C	2.356485	-1.139729	2.048726
H	1.923070	-2.013421	2.552243
H	3.420885	-1.110747	2.295400
C	-2.904805	0.821334	1.054066

C	-0.134799	-1.577587	-1.719615
O	-0.154622	-2.226984	-2.673588
P	-2.365899	-0.567301	0.019157
P	2.050302	-1.317500	0.260342
Si	-1.562807	1.010604	2.418075
Si	1.326352	0.358428	2.609351
C	-2.353567	0.504430	4.046785
H	-1.621371	0.517696	4.862479
H	-3.154558	1.206429	4.312848
H	-2.786261	-0.499817	4.003121
C	1.327524	0.375713	4.491262
H	2.354322	0.430273	4.875601
H	0.790216	1.243788	4.892708
H	0.863402	-0.527783	4.903291
H	-2.913104	1.709116	0.412132
H	-3.914006	0.689194	1.456576
C	2.258328	-3.181975	-0.053764
C	3.766221	-0.850758	-0.403157
C	-3.026283	-2.040768	1.014854
C	-3.638244	-0.708421	-1.402340
P	0.128422	1.369969	-1.185040
C	-0.024883	2.962715	-0.293089
H	0.431179	3.749786	-0.903741
H	-1.098958	3.191671	-0.273572
Si	0.541302	3.156146	1.524365
C	1.694460	1.721321	-2.183145
C	-1.067731	1.763596	-2.601701
C	1.062627	4.957266	1.682750
H	1.962491	5.164379	1.090490
H	0.274409	5.641764	1.346038
H	1.291070	5.204729	2.726861
C	-0.989252	2.807906	2.568307
H	-1.790148	3.509609	2.296882
H	-0.762510	3.008338	3.626042
C	1.971584	2.021695	1.997300
H	2.636058	1.912285	1.133601
H	2.567087	2.507516	2.782582
H	-0.291397	-2.047377	0.741215
H	-0.319631	-1.351493	1.362997
F	-2.830322	-3.185820	0.350692
F	-2.391867	-2.149051	2.194943
F	-4.333898	-1.934238	1.294681
F	-4.465524	0.344584	-1.415542
F	-4.397691	-1.808828	-1.317020

F	-3.010506	-0.764477	-2.580633
F	-2.323120	1.777112	-2.098170
F	-1.013367	0.841862	-3.565281
F	-0.888756	2.961127	-3.172734
F	1.934544	0.731640	-3.048730
F	2.737442	1.815357	-1.340557
F	1.670656	2.866513	-2.880436
F	2.655745	-3.386849	-1.318871
F	1.107664	-3.842152	0.120839
F	3.156742	-3.748891	0.762294
F	4.695012	-1.768734	-0.090796
F	3.775106	-0.711421	-1.729191
F	4.172107	0.302822	0.150869

A6

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.034502	-0.529973	-0.424801
N	-0.034815	-0.555194	1.850515
C	2.873551	-0.220744	1.525743
H	3.509956	-0.965731	2.013716
H	3.496824	0.661287	1.369803
C	-2.797040	-1.219902	1.352905
C	0.200133	-0.820476	-2.196801
O	0.347615	-1.096787	-3.304864
P	-2.301499	-0.839455	-0.361080
P	2.263226	-0.854454	-0.082758
Si	-1.650214	-0.352111	2.582584
Si	1.375249	0.197722	2.626918
C	-1.801569	-1.289427	4.197928
H	-1.298883	-0.785218	5.030367
H	-2.859355	-1.395410	4.471142
H	-1.379233	-2.294816	4.095367
C	1.706098	-0.548506	4.314230
H	2.689242	-0.234137	4.687242
H	0.962323	-0.238407	5.056375
H	1.699326	-1.644232	4.270250
H	-3.861772	-1.044389	1.530540
H	-2.606554	-2.287043	1.514757
C	2.889184	-2.632668	0.071160
C	3.535005	-0.330494	-1.398348

C	-2.900757	-2.362875	-1.353665
C	-3.750528	0.284547	-0.851183
P	0.112689	1.754532	-0.680600
C	-0.870077	2.847998	0.394740
H	-0.712547	3.891484	0.111104
H	-1.915234	2.618821	0.178669
Si	-0.663147	2.664033	2.276523
C	1.719263	2.816657	-0.720134
C	-0.503462	2.384010	-2.359515
C	-0.950353	4.373640	2.997549
H	-0.172317	5.075359	2.673025
H	-1.918444	4.780208	2.680046
H	-0.943017	4.352538	4.094015
C	-2.001114	1.471442	2.850803
H	-2.942762	1.755493	2.363432
H	-2.162008	1.616668	3.928301
C	1.048609	2.044674	2.778857
H	1.815854	2.626150	2.254461
H	1.170012	2.300821	3.841773
C	-0.289952	-3.500303	0.597768
O	-0.182021	-2.613864	-0.310552
O	-0.370295	-3.323385	1.823199
H	-0.313020	-4.535317	0.211345
H	0.063051	-1.592632	1.887752
F	3.007367	0.595858	-2.209549
F	3.870993	-1.371798	-2.171813
F	4.658100	0.175106	-0.875964
F	2.527777	-3.409175	-0.946461
F	4.232943	-2.673279	0.162145
F	2.414063	-3.170789	1.206221
F	2.721320	2.192800	-0.066574
F	1.574879	4.007908	-0.115040
F	2.147913	3.058601	-1.959889
F	-0.445464	3.723098	-2.463723
F	0.184882	1.867329	-3.380526
F	-1.788226	2.032912	-2.513203
F	-4.939067	-0.165461	-0.423410
F	-3.828194	0.440500	-2.173943
F	-3.601066	1.504856	-0.293998
F	-2.155837	-2.538962	-2.444598
F	-4.175566	-2.246245	-1.762529
F	-2.843184	-3.476962	-0.612633

A7

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.041026	-0.375363	-0.593167
N	-0.170163	-1.041647	1.548357
C	2.753881	-0.880519	1.466339
H	3.222715	-1.833858	1.734200
H	3.512843	-0.109214	1.615842
C	-2.909300	-1.325424	0.788125
C	0.235917	-0.144298	-2.371644
O	0.362915	-0.079644	-3.513946
P	-2.302659	-0.454633	-0.682064
P	2.222839	-0.927421	-0.282585
Si	-1.809999	-0.908039	2.266551
Si	1.221085	-0.600092	2.572006
C	-2.130541	-2.203825	3.578622
H	-1.644954	-1.959752	4.529909
H	-3.209109	-2.276256	3.769832
H	-1.764082	-3.181794	3.253243
C	1.377298	-1.763951	4.028893
H	2.365651	-1.669275	4.496564
H	0.630076	-1.556612	4.803197
H	1.245065	-2.800608	3.699131
H	-3.983057	-1.200474	0.949137
H	-2.700491	-2.390630	0.601117
C	2.687143	-2.699099	-0.754646
C	3.580909	-0.090131	-1.320757
C	-2.920522	-1.480442	-2.162380
C	-3.675089	0.852163	-0.811498
P	0.293645	1.888892	-0.216757
C	-0.771642	2.694444	1.008736
H	-0.595997	3.773464	1.015587
H	-1.801270	2.540283	0.675967
Si	-0.646706	2.021114	2.793245
C	1.936899	2.793640	0.224429
C	-0.054366	2.959809	-1.740776
C	-0.852681	3.509196	3.917109
H	-0.037553	4.228829	3.773398
H	-1.797998	4.030298	3.723359
H	-0.849805	3.211492	4.972678
C	-2.049352	0.795591	3.025920
H	-2.983990	1.249542	2.675704

H	-2.178924	0.635164	4.105770
C	0.997250	1.170815	3.173046
H	1.839096	1.810570	2.890800
H	1.041044	1.118579	4.271642
H	-0.452745	-2.238704	-0.627189
H	0.059505	-1.983594	-1.187893
C	-0.741228	-4.358601	0.833763
O	-1.338269	-3.807542	-0.121977
O	-0.053661	-3.801475	1.725127
H	-0.833700	-5.465409	0.905060
H	-0.079454	-2.092928	1.458445
F	-4.030474	-2.167664	-1.880304
F	-1.998772	-2.344683	-2.582874
F	-3.192285	-0.653113	-3.188233
F	-4.881447	0.274700	-0.905740
F	-3.552252	1.686818	-1.837302
F	-3.692390	1.592497	0.319310
F	-0.022753	4.272224	-1.459968
F	-1.277578	2.678614	-2.202657
F	0.815071	2.729972	-2.727856
F	1.762754	3.723308	1.178441
F	2.850063	1.928005	0.706708
F	2.491384	3.410681	-0.818174
F	4.688194	0.169937	-0.619285
F	3.127500	1.067366	-1.822351
F	3.921528	-0.851615	-2.366848
F	4.009906	-2.912936	-0.660883
F	2.307665	-2.982113	-2.005432
F	2.084840	-3.556971	0.067644

A8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.089136	0.237985	-0.529983
N	-0.134482	0.860048	1.692518
C	-2.885136	-0.097235	1.430441
H	-3.697017	0.562957	1.751395
H	-3.291463	-1.110154	1.419190
C	2.375543	1.950091	0.953950
C	-0.267729	0.210866	-2.299940
O	-0.445207	0.299287	-3.439738

P	2.000487	1.019206	-0.573148
P	-2.288932	0.334506	-0.249230
Si	1.487528	1.111060	2.395856
Si	-1.396688	0.001877	2.610586
C	1.473889	2.287764	3.854454
H	1.035804	1.827738	4.747578
H	2.504220	2.569453	4.108574
H	0.917564	3.202111	3.627975
C	-1.919800	0.987095	4.116909
H	-2.831662	0.565624	4.558469
H	-1.149079	0.987329	4.895628
H	-2.128308	2.031154	3.854357
H	3.444708	2.118626	1.101857
H	1.890859	2.929936	0.861688
C	-3.091294	2.041608	-0.367747
C	-3.502395	-0.497218	-1.453023
C	2.355586	2.285458	-1.943953
C	3.689706	0.148979	-0.785466
P	0.234122	-1.972349	-0.336817
C	1.328810	-2.678001	0.946175
H	1.290262	-3.769935	0.926807
H	2.344541	-2.397441	0.656965
Si	1.089977	-2.056909	2.722120
C	-1.167152	-3.287542	-0.229442
C	1.037887	-2.790251	-1.847870
C	1.686735	-3.441359	3.842608
H	1.078128	-4.344767	3.715382
H	2.727513	-3.706724	3.619637
H	1.638131	-3.152604	4.899593
C	2.185069	-0.538919	2.948802
H	3.144018	-0.741058	2.455490
H	2.411875	-0.439441	4.019660
C	-0.720629	-1.677854	3.113009
H	-1.342431	-2.481415	2.699441
H	-0.833169	-1.755031	4.204292
H	-0.438548	3.468985	-0.681547
H	-0.172499	1.823198	-0.662683
C	-0.524089	4.713602	0.735277
O	-0.622863	4.429272	-0.544731
O	-0.236847	3.930976	1.618025
H	-0.733004	5.775267	0.918682
H	-0.457469	1.814562	1.491658
F	3.595265	2.798020	-1.871969
F	1.509714	3.322702	-1.875444

F	2.217988	1.726097	-3.151270
F	4.740643	0.908091	-0.432202
F	3.890553	-0.235979	-2.049695
F	3.755492	-0.949266	-0.003146
F	2.270145	-2.288871	-2.021059
F	0.351496	-2.571941	-2.973196
F	1.173591	-4.122185	-1.707280
F	-0.839177	-4.369108	0.498180
F	-1.542292	-3.727230	-1.434339
F	-2.265307	-2.770973	0.361690
F	-4.433294	2.001391	-0.321027
F	-2.744019	2.705167	-1.470753
F	-2.692342	2.772497	0.697770
F	-3.802467	0.341266	-2.457056
F	-4.650430	-0.867936	-0.869685
F	-2.956719	-1.586402	-2.003256

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.044376	-0.369454	-0.578201
N	-0.158207	-1.028399	1.569132
C	2.760959	-0.837729	1.477229
H	3.242750	-1.781642	1.755379
H	3.510937	-0.055294	1.614009
C	-2.888161	-1.355693	0.793442
C	0.240897	-0.184362	-2.356569
O	0.370013	-0.154802	-3.501004
P	-2.285922	-0.478826	-0.680122
P	2.221526	-0.907273	-0.270560
Si	-1.801869	-0.909347	2.276086
Si	1.230002	-0.557150	2.584069
C	-2.119367	-2.194848	3.599658
H	-1.624325	-1.946951	4.545020
H	-3.196934	-2.256839	3.800335
H	-1.765207	-3.179913	3.282343
C	1.395907	-1.701748	4.055952
H	2.383806	-1.595280	4.521993
H	0.648059	-1.488317	4.828068
H	1.271217	-2.744701	3.743357
H	-3.963596	-1.239754	0.950865

H	-2.680233	-2.420102	0.612549
C	2.701250	-2.680170	-0.721431
C	3.575821	-0.073175	-1.317671
C	-2.900391	-1.512145	-2.157704
C	-3.678050	0.809374	-0.805581
P	0.274220	1.890290	-0.235455
C	-0.796477	2.704514	0.982224
H	-0.625097	3.784257	0.982972
H	-1.824685	2.544272	0.648167
Si	-0.672541	2.042273	2.769904
C	1.910407	2.815037	0.193607
C	-0.083455	2.941016	-1.771504
C	-0.904882	3.532424	3.885889
H	-0.096465	4.260471	3.746483
H	-1.853766	4.042553	3.680644
H	-0.908780	3.239868	4.942910
C	-2.060195	0.799442	3.014133
H	-3.000788	1.238837	2.661876
H	-2.185411	0.650037	4.096167
C	0.981727	1.216916	3.163386
H	1.814840	1.864290	2.872624
H	1.025574	1.179412	4.262557
H	-0.462537	-2.460989	-0.599280
H	0.025393	-1.984506	-1.074265
C	-0.701485	-4.358529	0.841364
O	-1.195170	-3.808927	-0.184392
O	-0.042687	-3.810695	1.748767
H	-0.891252	-5.447724	0.938216
H	-0.049142	-2.070462	1.475326
F	-4.005736	-2.207210	-1.870434
F	-1.975822	-2.372238	-2.578749
F	-3.181777	-0.689498	-3.184184
F	-4.878408	0.217774	-0.895540
F	-3.568934	1.644358	-1.832715
F	-3.702264	1.551910	0.323854
F	-0.056258	4.257769	-1.508286
F	-1.307127	2.650172	-2.226900
F	0.783531	2.701740	-2.758726
F	1.731522	3.755391	1.137078
F	2.830843	1.962184	0.686157
F	2.461010	3.423505	-0.856439
F	4.679726	0.208622	-0.618155
F	3.113166	1.072449	-1.837637
F	3.927544	-0.846768	-2.351523

F	4.026364	-2.882253	-0.620289
F	2.328863	-2.986483	-1.967213
F	2.106398	-3.533274	0.113982

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.044372	-0.456437	-0.338900
N	0.027580	-0.324173	1.664307
C	2.958047	-0.451102	1.337771
H	3.573080	-1.217465	1.819033
H	3.615563	0.375199	1.056658
C	-2.908762	-0.085269	1.456577
C	-0.088631	-1.059953	-2.028799
O	-0.097672	-1.485624	-3.103869
P	-2.262138	-0.713240	-0.105166
P	2.109878	-1.076232	-0.132552
Si	-1.394108	-0.022446	2.624894
Si	1.515655	0.168787	2.431146
C	-1.713024	-1.300747	3.964015
H	-0.920698	-1.328796	4.718930
H	-2.658113	-1.094973	4.482644
H	-1.785455	-2.301652	3.521531
C	1.776317	-0.543555	4.153566
H	2.795722	-0.328342	4.499077
H	1.089983	-0.115442	4.893898
H	1.642279	-1.631469	4.157296
H	-3.267767	0.934067	1.276635
H	-3.747931	-0.672300	1.841626
C	2.093126	-2.932284	0.235957
C	3.371464	-1.125511	-1.534526
C	-2.494893	-2.583987	0.055195
C	-3.649560	-0.396495	-1.349022
P	0.030335	1.688839	-0.795918
C	-0.705621	2.815026	0.442747
H	-0.628049	3.843455	0.072998
H	-1.776896	2.575155	0.446172
Si	-0.134286	2.793865	2.283136
C	1.686407	2.563530	-1.138615
C	-0.820104	2.348643	-2.352389
C	-0.188584	4.600541	2.806256

H	0.535543	5.198711	2.239379
H	-1.181048	5.040708	2.647361
H	0.052813	4.709332	3.870654
C	-1.316526	1.741813	3.308532
H	-2.320012	2.184581	3.360758
H	-0.929786	1.736587	4.338666
C	1.576487	2.061006	2.539713
H	2.297544	2.487368	1.834791
H	1.915978	2.356252	3.543133
F	3.314742	-3.487268	0.192398
F	1.316294	-3.591856	-0.631719
F	1.604781	-3.144077	1.467138
F	4.623516	-1.325897	-1.104946
F	3.355330	0.029253	-2.210291
F	3.063667	-2.105816	-2.395473
F	1.680234	3.865580	-0.814913
F	2.020563	2.465299	-2.430203
F	2.684300	2.000584	-0.428294
F	-0.564117	3.646836	-2.590741
F	-0.470657	1.658009	-3.440431
F	-2.149567	2.230765	-2.200954
F	-4.682459	-1.238671	-1.195521
F	-3.213679	-0.507222	-2.605615
F	-4.125005	0.846498	-1.176295
F	-2.505232	-3.154285	-1.157165
F	-1.458777	-3.098511	0.738843
F	-3.611130	-2.950240	0.695992

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.065031	-0.476142	-0.473572
N	-0.099817	-0.490815	1.840510
C	2.800855	-0.706930	1.370325
H	3.385254	-1.509412	1.830933
H	3.503617	0.086151	1.101837
C	-2.937434	0.104288	1.242101
C	-0.031616	-0.868783	-2.204657
O	0.011485	-1.223528	-3.305837
P	-2.232301	-0.658600	-0.263143
P	1.951728	-1.260936	-0.156084

Si	-1.624772	0.064827	2.609875
Si	1.482090	0.002868	2.532975
C	-2.130164	-1.151651	3.939810
H	-1.365723	-1.240244	4.720481
H	-3.061797	-0.830214	4.421328
H	-2.300808	-2.149284	3.519532
C	1.679923	-0.751323	4.238618
H	2.692154	-0.579556	4.625628
H	0.977681	-0.316130	4.960210
H	1.513806	-1.835130	4.217146
H	-3.147265	1.151347	0.997475
H	-3.883948	-0.354267	1.546877
C	2.006672	-3.120420	0.196426
C	3.324676	-1.259571	-1.460219
C	-2.826606	-2.438952	0.011642
C	-3.509045	-0.171503	-1.587194
P	0.172851	1.691678	-0.715871
C	-0.537978	2.893686	0.480059
H	-0.347007	3.915799	0.137117
H	-1.624248	2.748213	0.420062
Si	-0.053847	2.780305	2.319313
C	1.887768	2.505874	-0.966680
C	-0.548219	2.484690	-2.284218
C	0.046055	4.544022	2.952961
H	0.849159	5.097495	2.451274
H	-0.892096	5.083864	2.775700
H	0.245638	4.569199	4.030980
C	-1.357882	1.798714	3.260565
H	-2.319623	2.328896	3.267130
H	-1.029355	1.746324	4.309056
C	1.566922	1.875479	2.624108
H	2.355221	2.259701	1.970057
H	1.871329	2.131465	3.649501
H	-0.288753	-1.998249	-0.276056
H	-0.131699	-1.513110	1.836972
F	3.254723	-3.593949	0.358800
F	1.416828	-3.857287	-0.742221
F	1.354451	-3.344685	1.365002
F	4.551856	-1.419694	-0.942029
F	3.322113	-0.102984	-2.132833
F	3.122091	-2.245590	-2.346927
F	1.947259	3.794761	-0.584654
F	2.268961	2.448670	-2.248154
F	2.837194	1.865154	-0.250627

F	-0.161611	3.764784	-2.454639
F	-0.220580	1.816979	-3.392886
F	-1.888226	2.498230	-2.197840
F	-4.610200	-0.936000	-1.613236
F	-2.958358	-0.224666	-2.804289
F	-3.917872	1.090790	-1.371811
F	-2.629666	-3.189843	-1.076089
F	-2.125676	-2.986268	1.029029
F	-4.119429	-2.550092	0.356905

$R^1=R^2=R^3=CHF_2$

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.176303	-0.922305	-0.356081
N	-0.067883	0.080550	1.533009
C	2.798288	-0.642762	1.419402
H	3.195991	-1.337020	2.166547
H	3.642794	-0.081910	1.013830
C	-2.862726	0.787981	0.908070
C	-0.262091	-1.801188	-1.898618
O	-0.312895	-2.375938	-2.907858
P	-2.423970	-0.577864	-0.196564
P	1.964647	-1.564079	0.090430
Si	-1.420662	0.934128	2.168017
Si	1.475818	0.526544	2.154577
C	-2.087987	0.321068	3.819631
H	-1.314765	0.332596	4.596202
H	-2.913741	0.957216	4.164856
H	-2.464218	-0.704409	3.740261
C	1.625978	0.396018	4.031714
H	2.659360	0.584515	4.351196
H	0.991465	1.125081	4.550849
H	1.342499	-0.603781	4.382030
H	-2.932875	1.705009	0.312104
H	-3.838858	0.630723	1.378043
C	1.983579	-3.291057	0.822553
C	3.225234	-1.939727	-1.266602
C	-3.289934	-2.036463	0.620785
C	-3.560913	-0.468992	-1.682092
P	0.303379	1.068058	-1.370331

C	-0.199573	2.678496	-0.666531
H	0.103174	3.457744	-1.373711
H	-1.295041	2.678915	-0.669461
Si	0.357564	3.206828	1.092436
C	2.075297	1.452222	-1.913725
C	-0.402735	1.263359	-3.106208
C	0.633195	5.066237	0.958419
H	1.442894	5.295963	0.254643
H	-0.269954	5.582232	0.608835
H	0.905296	5.496477	1.929842
C	-1.018161	2.785647	2.303478
H	-1.916055	3.393969	2.130524
H	-0.671725	3.026492	3.319306
C	1.904955	2.315973	1.666985
H	2.678034	2.350438	0.892053
H	2.309102	2.852255	2.537420
H	-0.495976	-2.097234	0.931572
H	-0.586003	-2.521937	0.269501
F	1.378045	-3.263624	2.041741
F	3.265787	-3.717642	1.017825
F	4.442188	-1.420436	-0.979127
F	2.805662	-1.392808	-2.446679
F	-4.596959	-1.764006	0.866368
F	-2.701557	-2.291832	1.826411
F	-3.570048	-1.701823	-2.277569
F	-4.836514	-0.165001	-1.329620
F	-1.717259	1.631975	-2.996414
F	0.221185	2.254892	-3.800890
F	2.969905	0.949874	-1.012628
F	2.304808	2.789705	-1.974820
H	-3.232908	-2.944478	0.014133
H	-3.224723	0.262013	-2.416177
H	3.343429	-3.014084	-1.436590
H	1.472700	-4.030879	0.196540
H	2.308225	1.017379	-2.887556
H	-0.352772	0.346936	-3.701366

TSA5-1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.061338	-0.799387	-0.439792

N	-0.036425	-0.252143	1.694847
C	2.672996	-1.130823	1.507737
H	2.426683	-2.086489	1.986945
H	3.745177	-0.958952	1.630007
C	-2.874818	0.275151	1.157079
C	-0.123755	-1.594088	-2.019367
O	-0.128915	-2.129009	-3.052186
P	-2.295447	-0.946262	-0.057162
P	2.183395	-1.249826	-0.245643
Si	-1.417623	0.534255	2.377859
Si	1.535095	0.189086	2.264077
C	-1.971605	-0.129306	4.049496
H	-1.171938	-0.067842	4.796938
H	-2.824068	0.448505	4.429866
H	-2.280955	-1.177065	3.977271
C	1.732509	0.109415	4.136676
H	2.783583	0.257936	4.416109
H	1.151943	0.888133	4.646987
H	1.414790	-0.862194	4.532853
H	-3.073028	1.202559	0.609923
H	-3.803639	-0.029979	1.649815
C	2.584692	-3.035821	-0.726752
C	3.686643	-0.486724	-1.101117
C	-2.728857	-2.564139	0.794529
C	-3.644333	-1.143934	-1.371483
P	-0.116555	1.277099	-1.331824
C	-0.264913	2.835904	-0.374485
H	0.178331	3.643601	-0.968783
H	-1.338242	3.061653	-0.327192
Si	0.369913	2.949048	1.420145
C	1.300068	1.716573	-2.483378
C	-1.516252	1.558346	-2.558403
C	0.715555	4.781751	1.689207
H	1.543260	5.126922	1.057260
H	-0.163208	5.396033	1.455577
H	0.989658	4.982507	2.732418
C	-1.025594	2.379722	2.555061
H	-1.919760	2.994923	2.382531
H	-0.727870	2.571156	3.597031
C	1.939503	1.943142	1.697466
H	2.513395	1.936270	0.764020
H	2.568981	2.447441	2.443527
H	-0.040580	-2.281066	0.421528
H	-0.068553	-1.627485	1.087830

F	-2.095423	-2.669732	1.992848
F	-4.071600	-2.625631	1.049000
F	-4.612154	-0.207541	-1.223715
F	-3.107272	-1.013815	-2.617305
F	-2.677308	1.522210	-1.829243
F	-1.481853	2.779452	-3.147089
F	2.406741	1.934552	-1.708673
F	1.104640	2.855212	-3.193616
F	1.513230	-3.843152	-0.503221
F	3.604664	-3.514392	0.032721
F	4.699664	-1.395599	-1.196731
F	4.152328	0.545513	-0.352332
H	-2.455138	-3.431806	0.185213
H	-4.121449	-2.126546	-1.329713
H	2.862603	-3.128958	-1.780744
H	3.474826	-0.123829	-2.108640
H	1.522161	0.908131	-3.189405
H	-1.573449	0.794868	-3.337895

A6

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.055792	-0.649066	-0.593356
N	0.141008	-0.528466	1.665607
C	3.023793	-0.242242	1.129561
H	3.648931	-0.994572	1.621502
H	3.670409	0.603126	0.885317
C	-2.658799	-1.182708	1.362561
C	0.070003	-1.040694	-2.327648
O	0.103417	-1.372039	-3.438990
P	-2.246234	-0.845607	-0.383620
P	2.295659	-0.931750	-0.404555
Si	-1.430379	-0.270474	2.475580
Si	1.597589	0.292849	2.271751
C	-1.475305	-1.117320	4.148286
H	-0.890078	-0.587516	4.907947
H	-2.507989	-1.180377	4.514872
H	-1.085326	-2.137490	4.062653
C	2.024270	-0.287444	4.005116
H	3.030248	0.048934	4.286517
H	1.327689	0.101453	4.756332

H	2.008473	-1.382296	4.067416
H	-3.711696	-0.980378	1.580530
H	-2.480207	-2.247952	1.551130
C	2.847693	-2.720388	-0.277300
C	3.438495	-0.491377	-1.841902
C	-2.846275	-2.327916	-1.369006
C	-3.673947	0.290801	-0.841087
P	0.108395	1.593997	-1.033462
C	-0.826839	2.768357	-0.003809
H	-0.687551	3.785827	-0.378634
H	-1.882806	2.519253	-0.136491
Si	-0.475334	2.720108	1.863218
C	1.699508	2.599763	-1.307971
C	-0.557198	2.004871	-2.740940
C	-0.710459	4.477809	2.486181
H	0.035523	5.153230	2.049436
H	-1.703260	4.863324	2.223282
H	-0.611216	4.533645	3.577145
C	-1.734176	1.572585	2.666990
H	-2.731960	1.832546	2.293026
H	-1.745667	1.785407	3.745657
C	1.279683	2.147543	2.263553
H	1.984071	2.656431	1.596519
H	1.506498	2.518702	3.273701
C	-0.205112	-3.576699	0.650536
O	-0.118865	-2.771965	-0.334244
O	-0.205159	-3.305999	1.858711
H	-0.292071	-4.641433	0.352260
H	0.254656	-1.556736	1.768785
F	2.793059	0.352845	-2.704777
F	4.568418	0.128432	-1.426940
F	4.197927	-2.825216	-0.479594
F	2.601621	-3.168910	0.981774
F	2.730287	2.080016	-0.577063
F	1.560436	3.890627	-0.902053
F	-0.552397	3.350666	-2.960008
F	-1.851351	1.585561	-2.840075
F	-4.860521	-0.329537	-0.605627
F	-3.647238	1.392469	-0.024931
F	-3.199370	-1.870236	-2.610064
F	-3.935276	-2.920744	-0.815825
H	-2.057503	-3.072243	-1.481105
H	-3.660461	0.627804	-1.875595
H	0.015797	1.530020	-3.543198

H	2.011659	2.608764	-2.353757
H	2.340446	-3.372674	-0.991815
H	3.720477	-1.376611	-2.417767

A7

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.320397	0.231773	-0.755221
N	-0.554184	0.503346	1.479111
C	-2.372508	-1.808637	1.123454
H	-3.392629	-1.908501	1.508528
H	-1.980248	-2.808117	0.920127
C	1.206199	2.713590	0.907684
C	-0.373105	0.097356	-2.533981
O	-0.427010	0.003292	-3.686539
P	1.338963	1.843421	-0.676065
P	-2.326083	-0.855725	-0.424392
Si	0.788974	1.431825	2.225468
Si	-1.223165	-0.911885	2.352407
C	0.202221	2.322331	3.763025
H	0.058571	1.646753	4.613736
H	0.936911	3.079277	4.065059
H	-0.744131	2.833562	3.555497
C	-2.205130	-0.359061	3.849875
H	-2.810750	-1.189554	4.233973
H	-1.551083	-0.028413	4.664144
H	-2.881517	0.466739	3.607747
H	2.069346	3.345328	1.128210
H	0.297798	3.330278	0.849976
C	-3.750797	0.342549	-0.113354
C	-3.184706	-1.906633	-1.708624
C	1.122832	3.172860	-1.981747
C	3.202585	1.653548	-0.882300
P	1.124767	-1.547418	-0.741969
C	2.292910	-2.040648	0.581163
H	2.433583	-3.125531	0.525169
H	3.265600	-1.605916	0.339846
Si	1.928920	-1.562982	2.378099
C	0.425981	-3.244651	-1.131690
C	2.230772	-1.558129	-2.289092
C	3.169788	-2.540482	3.399085

H	3.034288	-3.620557	3.264573
H	4.201157	-2.295477	3.116859
H	3.060311	-2.324056	4.468836
C	2.217878	0.280657	2.621717
H	3.105792	0.569955	2.046295
H	2.475793	0.440816	3.678198
C	0.181243	-2.040948	2.883426
H	-0.011632	-3.063995	2.537259
H	0.163282	-2.084948	3.982077
H	-1.376134	1.534211	-1.231554
H	-1.267782	1.765051	-0.475229
C	-2.620311	3.640148	0.355626
O	-3.332616	3.275563	-0.591173
O	-1.832140	2.937813	1.061144
H	-2.653771	4.721791	0.631403
H	-1.292646	1.235547	1.403298
F	2.081061	4.133417	-1.860086
F	-0.084871	3.763241	-1.805240
F	3.867713	2.632512	-0.220049
F	3.604839	0.469064	-0.331511
F	3.434873	-2.122202	-2.038374
F	2.466252	-0.288811	-2.740845
F	1.421432	-4.123963	-1.440616
F	-0.200211	-3.737139	-0.021748
F	-2.417689	-2.994503	-2.012447
F	-3.310897	-1.156792	-2.834265
F	-4.945400	-0.285116	-0.340681
F	-3.725781	0.663493	1.212165
H	1.171123	2.768726	-2.998330
H	3.520090	1.668457	-1.925869
H	1.758506	-2.102598	-3.112066
H	-0.285332	-3.231083	-1.957480
H	-3.699529	1.276247	-0.681815
H	-4.169538	-2.268562	-1.408720

A8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.228078	0.148175	-0.772370
N	-0.502198	0.567297	1.473034
C	-2.453803	-1.617246	1.141458

H	-3.495594	-1.569858	1.474476
H	-2.189331	-2.671860	1.028737
C	1.302911	2.676560	0.811567
C	-0.339975	0.090178	-2.527192
O	-0.466628	0.105345	-3.685910
P	1.347748	1.732145	-0.748650
P	-2.226465	-0.804573	-0.480485
Si	0.884415	1.445835	2.176695
Si	-1.254111	-0.788878	2.356279
C	0.399559	2.365807	3.737101
H	0.284104	1.687636	4.590888
H	1.175855	3.094378	4.003592
H	-0.540123	2.909621	3.596864
C	-2.236110	-0.147781	3.820534
H	-2.818236	-0.958199	4.277283
H	-1.592082	0.275067	4.599349
H	-2.939915	0.632384	3.508154
H	2.212104	3.258442	0.978778
H	0.451933	3.365177	0.752943
C	-3.659000	0.405456	-0.420120
C	-2.983847	-1.993595	-1.721412
C	1.168912	3.042774	-2.081543
C	3.212797	1.506445	-0.978286
P	1.114474	-1.637718	-0.712936
C	2.241907	-2.171396	0.639803
H	2.330123	-3.263186	0.622764
H	3.239479	-1.791450	0.402117
Si	1.872458	-1.597077	2.403750
C	0.354401	-3.317737	-1.081699
C	2.248220	-1.774050	-2.237962
C	3.043750	-2.581521	3.501550
H	2.868343	-3.660071	3.405283
H	4.091051	-2.388645	3.238154
H	2.915892	-2.319755	4.559162
C	2.266512	0.239395	2.561080
H	3.137326	0.448299	1.928579
H	2.584790	0.432836	3.595043
C	0.095643	-1.969026	2.915489
H	-0.147277	-2.988405	2.588943
H	0.073326	-1.991244	4.014912
H	-1.864923	2.768226	-0.778508
H	-1.068162	1.499696	-0.880545
C	-2.577231	3.833549	0.614599
O	-2.547491	3.484454	-0.654851

O	-1.868323	3.388848	1.493091
H	-3.338677	4.605186	0.791484
H	-1.211929	1.294584	1.325500
F	2.223179	3.909433	-2.070596
F	0.046250	3.773612	-1.847271
F	3.929580	2.482900	-0.358585
F	3.597605	0.325681	-0.400512
F	2.513495	-0.547980	-2.779160
F	3.443383	-2.344347	-1.940264
F	1.293806	-4.294426	-1.241141
F	-0.439304	-3.705799	-0.036797
F	-4.867199	-0.210908	-0.344152
F	-3.516737	1.126874	0.740248
F	-3.416245	-1.254340	-2.785051
F	-4.047290	-2.669039	-1.216138
H	1.095422	2.607063	-3.082918
H	3.512687	1.479470	-2.027152
H	1.778449	-2.368014	-3.028800
H	-0.256004	-3.303424	-1.991290
H	-3.671051	1.104490	-1.258664
H	-2.268312	-2.731027	-2.093857

TSA7-8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.281583	0.151218	-0.811135
N	-0.557026	0.844762	1.316205
C	-2.508608	-1.386351	1.263451
H	-3.544530	-1.415795	1.616881
H	-2.125099	-2.409178	1.240662
C	1.378356	2.750958	0.436860
C	-0.322924	-0.231054	-2.550422
O	-0.384325	-0.464142	-3.683326
P	1.545350	1.559509	-0.923010
P	-2.380120	-0.700022	-0.418126
Si	0.843131	1.763952	1.954449
Si	-1.381565	-0.329439	2.382479
C	0.331395	2.932550	3.323080
H	0.108736	2.405683	4.258332
H	1.137898	3.645891	3.535873
H	-0.555561	3.495505	3.015071

C	-2.405614	0.574117	3.666520
H	-3.142379	-0.098024	4.123541
H	-1.774641	0.966819	4.471750
H	-2.943291	1.417708	3.222600
H	2.263735	3.375519	0.572680
H	0.517690	3.390395	0.198792
C	-3.856649	0.471233	-0.356795
C	-3.214910	-1.922232	-1.566754
C	1.583792	2.625598	-2.467514
C	3.398951	1.194400	-0.930648
P	0.975286	-1.730150	-0.444723
C	2.029247	-2.091756	1.016916
H	2.015680	-3.174282	1.184354
H	3.061679	-1.855384	0.748900
Si	1.692980	-1.234136	2.670248
C	0.212830	-3.439928	-0.616203
C	2.158991	-2.059377	-1.900669
C	2.813188	-2.111207	3.901732
H	2.569035	-3.177451	3.982803
H	3.866760	-2.032363	3.606325
H	2.717643	-1.673080	4.902910
C	2.165630	0.584038	2.573152
H	3.080623	0.673917	1.976413
H	2.433402	0.911247	3.587599
C	-0.099230	-1.426693	3.210100
H	-0.386734	-2.481078	3.105137
H	-0.129136	-1.213159	4.288698
H	-1.503097	1.863506	-1.108454
H	-0.724879	1.702103	-1.283354
C	-2.522326	3.659859	-0.016362
O	-2.711181	3.014054	-1.079485
O	-1.807559	3.335443	0.958744
H	-3.052628	4.634904	0.057521
H	-1.217263	1.633283	1.117767
F	2.636388	3.492494	-2.414585
F	0.448005	3.361281	-2.531082
F	4.092939	2.170660	-0.292478
F	3.658204	0.034492	-0.259549
F	3.318251	-2.625813	-1.491625
F	2.486521	-0.906025	-2.560190
F	1.184896	-4.396632	-0.673906
F	-0.539895	-3.717732	0.489675
F	-2.401659	-2.982948	-1.832654
F	-3.439363	-1.272232	-2.740841

F	-5.015452	-0.260033	-0.328536
F	-3.798346	1.147103	0.821956
H	1.673224	2.036793	-3.386075
H	3.798254	1.094767	-1.941990
H	1.695049	-2.720694	-2.638825
H	-0.411536	-3.542060	-1.501940
H	-3.902332	1.191607	-1.171446
H	-4.161549	-2.315556	-1.191961

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.054203	-0.622994	-0.564749
N	-0.057878	-0.545921	1.431415
C	2.870051	-0.808835	1.207025
H	3.340356	-1.678041	1.677750
H	3.646204	-0.058846	1.039573
C	-2.987084	-0.247451	1.164174
C	-0.111325	-1.194961	-2.239909
O	-0.168735	-1.605381	-3.331577
P	-2.305198	-0.733246	-0.439810
P	2.089025	-1.256706	-0.371013
Si	-1.495068	-0.197501	2.347287
Si	1.424655	-0.108153	2.233952
C	-1.865432	-1.448770	3.702318
H	-1.098153	-1.475711	4.482463
H	-2.824552	-1.226403	4.187489
H	-1.934891	-2.455237	3.270788
C	1.617558	-0.800157	3.977009
H	2.638683	-0.618037	4.337418
H	0.935891	-0.333903	4.698325
H	1.443889	-1.882523	3.996964
H	-3.423656	0.751466	1.058421
H	-3.782180	-0.924841	1.489688
P	0.182741	1.522171	-1.014705
C	-0.640358	2.653004	0.160182
H	-0.524835	3.683565	-0.191710
H	-1.710196	2.417387	0.091475
Si	-0.137086	2.583972	2.019853
C	-0.138799	4.384376	2.574735
H	0.619260	4.966526	2.036448

H	-1.112292	4.859587	2.399508
H	0.079037	4.466403	3.646773
C	-1.385848	1.575556	3.011702
H	-2.376392	2.048919	3.027736
H	-1.029482	1.573232	4.053101
C	1.538047	1.785133	2.332135
H	2.294471	2.178840	1.646633
H	1.856100	2.077478	3.343600
C	-2.696509	-2.566738	-0.569972
H	-2.802080	-2.896197	-1.608366
C	-3.555153	-0.095013	-1.681301
H	-3.207668	-0.140038	-2.716275
C	-0.396971	2.144139	-2.684906
H	0.131950	1.647460	-3.506068
C	1.887475	2.325808	-1.208029
H	2.206612	2.370499	-2.252254
C	2.122557	-3.127338	-0.295917
H	1.653774	-3.595252	-1.167779
C	3.367236	-1.067246	-1.746378
H	3.534532	-1.997735	-2.296850
F	-1.656924	-3.256376	-0.009841
F	-3.819219	-2.915626	0.107167
F	-4.723423	-0.792247	-1.592128
F	-3.828826	1.200787	-1.365034
F	-1.728148	1.905053	-2.830839
F	-0.210187	3.490391	-2.813853
F	1.899501	3.591691	-0.708619
F	2.842633	1.628627	-0.524349
F	1.462399	-3.532381	0.820294
F	3.405936	-3.590559	-0.204351
F	4.557776	-0.644125	-1.256669
F	2.932874	-0.137239	-2.648779

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.182175	-0.734407	-0.560366
N	-0.157943	-0.220536	1.688255
C	2.666115	-1.052300	1.329834
H	3.033916	-1.868160	1.959880
H	3.539287	-0.496561	0.979249

C	-2.844949	0.782304	0.898207
C	-0.274891	-1.407055	-2.180640
O	-0.348958	-1.903619	-3.234425
P	-2.353357	-0.466993	-0.343973
P	1.745557	-1.698454	-0.120721
Si	-1.527555	0.793319	2.263427
Si	1.510002	0.121393	2.259699
C	-2.229935	0.080758	3.847985
H	-1.457006	-0.016899	4.619544
H	-3.013364	0.738078	4.245357
H	-2.674456	-0.906022	3.684836
C	1.616998	-0.223490	4.101986
H	2.654772	-0.153183	4.451684
H	1.026518	0.491798	4.687651
H	1.255588	-1.231493	4.339093
H	-2.853385	1.758535	0.399196
H	-3.852853	0.603686	1.287339
P	0.425030	1.281426	-1.257136
C	0.016386	2.853868	-0.396262
H	0.424806	3.696074	-0.963640
H	-1.075101	2.948596	-0.448090
Si	0.526944	3.037165	1.424091
C	0.996126	4.838146	1.681217
H	1.876414	5.102162	1.082350
H	0.180780	5.511388	1.389148
H	1.234170	5.042233	2.732340
C	-0.915099	2.544794	2.527849
H	-1.760690	3.233219	2.394928
H	-0.589504	2.654855	3.572619
C	1.952069	1.911996	1.906634
H	2.739844	1.959341	1.148684
H	2.386799	2.321579	2.830168
H	-0.641285	-2.156957	-0.053717
H	-0.381249	-1.193693	1.912308
C	-3.207471	-1.982658	0.364124
H	-3.057959	-2.870835	-0.253380
C	-3.528631	-0.187497	-1.779330
H	-3.146731	0.548947	-2.487705
C	-0.237234	1.736356	-2.957577
H	-0.143022	0.929477	-3.690337
C	2.231811	1.624712	-1.729143
H	2.458852	1.290342	-2.744315
C	1.531915	-3.463881	0.469091
H	0.913032	-4.068005	-0.200151

C	3.049975	-2.075542	-1.436515
H	2.956373	-3.094422	-1.825325
F	-2.671942	-2.231737	1.604298
F	-4.542027	-1.793171	0.551889
F	-3.665628	-1.380535	-2.434036
F	-4.765507	0.208981	-1.375196
F	-1.567381	2.044872	-2.831607
F	0.371414	2.844796	-3.469730
F	2.560532	2.944003	-1.633391
F	3.080795	0.963276	-0.882530
F	0.932598	-3.428006	1.699415
F	2.733519	-4.094974	0.637572
F	4.312062	-1.915536	-0.960860
F	2.898018	-1.227551	-2.494858

$R^1=R^2=R^3=Ph$

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.009007	0.482118	-0.291201
N	-0.359141	0.847931	1.805003
C	-3.031731	-0.205837	1.202454
H	-4.053395	0.117757	1.429237
H	-3.052498	-1.297501	1.102373
C	2.559384	1.290037	1.832738
C	0.202248	0.296963	-2.025987
O	0.327313	0.220099	-3.189618
P	2.190322	1.184192	0.047321
P	-2.387562	0.431967	-0.375957
Si	0.924323	1.347226	2.819333
Si	-1.771776	0.241834	2.559943
C	0.715162	3.077747	3.553334
H	-0.069495	3.078185	4.319659
H	1.634091	3.444872	4.029172
H	0.411716	3.799307	2.784982
C	-2.567887	1.446387	3.788406
H	-3.576412	1.120244	4.076590
H	-1.978199	1.501886	4.713052
H	-2.637437	2.463332	3.385446
H	3.054573	0.352249	2.105955
H	3.263830	2.090716	2.082588

P	0.486254	-1.746938	0.265263
C	1.254606	-2.046123	1.913834
H	1.512786	-3.110677	1.976548
H	2.217604	-1.522752	1.887432
Si	0.458313	-1.567189	3.592535
C	0.950818	-2.978481	4.751693
H	0.481517	-3.927935	4.462734
H	2.037399	-3.134739	4.756995
H	0.644869	-2.761855	5.782702
C	1.164271	0.069102	4.207669
H	2.219396	-0.015100	4.499753
H	0.609929	0.351528	5.114665
C	-1.402145	-1.351196	3.534176
H	-1.895907	-2.222379	3.088812
H	-1.771208	-1.268486	4.566683
H	-0.338947	2.225498	-0.025857
H	-0.233202	2.197238	-0.800009
C	2.347475	2.916633	-0.566461
C	2.339663	4.021854	0.286669
C	2.360886	3.137201	-1.949219
C	2.351142	5.317573	-0.228499
H	2.313883	3.888163	1.362815
C	2.378066	4.428428	-2.463430
H	2.354665	2.295362	-2.635954
C	2.371339	5.525435	-1.603058
H	2.343073	6.163438	0.453100
H	2.394186	4.578456	-3.539119
H	2.380368	6.534384	-2.004900
C	3.682965	0.416026	-0.707737
C	3.602634	-0.133790	-1.991405
C	4.916492	0.403103	-0.047970
C	4.728105	-0.675189	-2.604040
H	2.654622	-0.159498	-2.515405
C	6.039656	-0.153205	-0.654410
H	5.012037	0.836645	0.943061
C	5.948542	-0.690975	-1.935512
H	4.640973	-1.104763	-3.597127
H	6.989422	-0.158339	-0.126961
H	6.825209	-1.124309	-2.408441
C	1.688096	-2.617384	-0.854004
C	2.926174	-3.097909	-0.417195
C	1.352772	-2.793465	-2.202337
C	3.795346	-3.743362	-1.293843
H	3.239320	-2.967362	0.612277

C	2.215860	-3.442187	-3.078449
H	0.411061	-2.415662	-2.585188
C	3.441761	-3.924750	-2.625744
H	4.754205	-4.100291	-0.928891
H	1.928997	-3.569088	-4.118555
H	4.117946	-4.430502	-3.309061
C	-0.880031	-2.990877	0.222877
C	-1.748931	-2.964142	-0.871580
C	-1.081393	-3.968578	1.202239
C	-2.796858	-3.871846	-0.986172
H	-1.617456	-2.210572	-1.639697
C	-2.134551	-4.874403	1.098019
H	-0.423144	-4.035157	2.061675
C	-2.996270	-4.828714	0.005260
H	-3.461679	-3.816906	-1.843133
H	-2.277509	-5.620628	1.874444
H	-3.816386	-5.536584	-0.072476
C	-3.465998	-0.323294	-1.671723
C	-4.738578	-0.813123	-1.362410
C	-3.029859	-0.386670	-2.999498
C	-5.552417	-1.357352	-2.352069
H	-5.102760	-0.778626	-0.340665
C	-3.842920	-0.930175	-3.990978
H	-2.042674	-0.025649	-3.266615
C	-5.106453	-1.418929	-3.670113
H	-6.536856	-1.735286	-2.091011
H	-3.483163	-0.974744	-5.014978
H	-5.740746	-1.844907	-4.442175
C	-3.008385	2.166079	-0.482828
C	-2.734087	2.890636	-1.650289
C	-3.697371	2.800180	0.550627
C	-3.143279	4.211376	-1.780887
H	-2.186670	2.420105	-2.464059
C	-4.099899	4.130271	0.425952
H	-3.922662	2.269719	1.469031
C	-3.825486	4.838443	-0.738002
H	-2.923582	4.755288	-2.695137
H	-4.627833	4.608946	1.245960
H	-4.138062	5.874089	-0.835731

TSA5-1

Coordinates (Angstroms)

	X	Y	Z
Mn	-0.180605	-0.546774	-0.224138
N	-0.271359	-1.309174	1.888129
C	2.207628	-2.486961	1.173331
H	1.662277	-3.420964	0.984177
H	3.250510	-2.760321	1.360150
C	-2.781318	0.179360	1.811737
C	-0.232358	-0.372517	-1.969088
O	-0.270005	-0.310123	-3.137706
P	-2.484915	-0.346074	0.085835
P	1.987314	-1.466020	-0.342363
Si	-1.543549	-0.762543	2.913610
Si	1.283469	-1.617594	2.568436
C	-2.458082	-2.151548	3.801461
H	-1.798230	-2.659364	4.515662
H	-3.324445	-1.775730	4.361393
H	-2.815606	-2.905202	3.090113
C	1.251805	-2.748743	4.080170
H	2.271279	-3.012835	4.390590
H	0.765336	-2.273788	4.941507
H	0.716745	-3.681601	3.865830
H	-2.533960	1.246194	1.850112
H	-3.821887	0.086247	2.140594
P	0.231668	1.710841	0.210372
C	0.189003	2.291912	1.970995
H	0.696780	3.262511	2.020987
H	-0.865437	2.508370	2.182668
Si	0.741091	1.273988	3.481705
C	1.389373	2.545900	4.718967
H	2.289211	3.049595	4.343180
H	0.639805	3.318519	4.932526
H	1.652164	2.069523	5.671693
C	-0.797557	0.431519	4.181476
H	-1.529421	1.189806	4.493782
H	-0.522776	-0.120917	5.091941
C	2.082289	0.015539	3.081151
H	2.699159	0.420077	2.269203
H	2.744814	-0.123981	3.946400
H	-0.508536	-2.232250	-0.269474
H	-0.496031	-2.036887	0.662859
C	-3.622154	0.670792	-0.943541
C	-3.729755	0.378204	-2.308487
C	-4.383150	1.715545	-0.417674

C	-4.584840	1.108932	-3.124801
H	-3.137083	-0.422952	-2.741397
C	-5.233125	2.455098	-1.237415
H	-4.312709	1.969466	0.635141
C	-5.339638	2.152035	-2.590561
H	-4.658390	0.867369	-4.181359
H	-5.810034	3.272091	-0.813680
H	-6.003098	2.728591	-3.228699
C	-3.360199	-1.967709	-0.058481
C	-4.413501	-2.345015	0.779202
C	-2.992119	-2.831967	-1.096096
C	-5.065638	-3.563273	0.598676
H	-4.735312	-1.695848	1.587238
C	-3.651350	-4.041292	-1.288591
H	-2.174535	-2.556915	-1.755249
C	-4.686555	-4.414529	-0.434897
H	-5.872596	-3.844993	1.269103
H	-3.348675	-4.696688	-2.100342
H	-5.194982	-5.364043	-0.575291
C	2.249249	-2.745799	-1.659821
C	3.533040	-3.237406	-1.933387
C	1.164254	-3.315857	-2.330716
C	3.723829	-4.259011	-2.857520
H	4.396292	-2.816640	-1.426366
C	1.353545	-4.339710	-3.256925
H	0.161600	-2.960129	-2.126909
C	2.633246	-4.814034	-3.524083
H	4.727908	-4.623500	-3.055738
H	0.494700	-4.764342	-3.769080
H	2.781979	-5.609292	-4.249050
C	3.576325	-0.555206	-0.506135
C	4.552425	-0.502635	0.491945
C	3.843581	0.055582	-1.737370
C	5.773336	0.129849	0.260095
H	4.381262	-0.963786	1.458995
C	5.065837	0.670168	-1.974524
H	3.093957	0.031620	-2.524103
C	6.037703	0.706917	-0.976176
H	6.521525	0.156746	1.047297
H	5.255918	1.131862	-2.938604
H	6.992451	1.190816	-1.161106
C	1.806880	2.480136	-0.390118
C	1.937890	2.789812	-1.749116
C	2.859393	2.809096	0.467571

C	3.059801	3.457862	-2.224727
H	1.148690	2.526615	-2.446340
C	3.992884	3.463440	-0.010176
H	2.803254	2.571263	1.525210
C	4.089334	3.806219	-1.354069
H	3.130132	3.703799	-3.280592
H	4.798197	3.708417	0.676240
H	4.967523	4.327072	-1.724672
C	-0.919356	2.957159	-0.561680
C	-1.257987	4.161867	0.066732
C	-1.400908	2.739770	-1.857251
C	-2.055421	5.107900	-0.572172
H	-0.893233	4.388578	1.062184
C	-2.177312	3.693169	-2.508287
H	-1.177462	1.812910	-2.369667
C	-2.514721	4.879414	-1.865061
H	-2.305130	6.032032	-0.058193
H	-2.535947	3.493508	-3.513151
H	-3.132082	5.618898	-2.367055

A6

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.028125	0.384498	-0.340590
N	-0.293909	1.048410	1.854492
C	-2.978387	-0.107306	1.233743
H	-4.000834	0.216213	1.458029
H	-2.992437	-1.203638	1.197358
C	2.699119	1.067743	1.740443
C	0.212764	0.066891	-2.056273
O	0.319176	-0.046843	-3.216107
P	2.283616	0.972191	-0.046843
P	-2.373141	0.417387	-0.411948
Si	1.170515	1.315891	2.833782
Si	-1.761277	0.381085	2.602305
C	1.143853	3.039682	3.571092
H	0.368933	3.116188	4.343723
H	2.104251	3.288274	4.039823
H	0.911974	3.785203	2.803806
C	-2.505497	1.687543	3.735132
H	-3.539806	1.449289	4.013313

H	-1.929801	1.767878	4.665946
H	-2.495606	2.674731	3.259171
H	3.118789	0.092912	2.009871
H	3.483681	1.801972	1.954359
P	0.408030	-1.866434	0.332943
C	1.200361	-2.171855	1.973771
H	1.390874	-3.247748	2.068657
H	2.192828	-1.710740	1.916087
Si	0.456447	-1.596364	3.634130
C	0.803735	-2.981814	4.863791
H	0.270339	-3.905491	4.605921
H	1.874712	-3.217284	4.902484
H	0.492318	-2.693577	5.875284
C	1.282556	0.000807	4.173367
H	2.338672	-0.154684	4.430477
H	0.782507	0.345587	5.089262
C	-1.369944	-1.181419	3.580482
H	-1.961416	-2.020149	3.197513
H	-1.683379	-1.027353	4.623087
C	2.667378	2.661348	-0.674766
C	2.820529	3.764378	0.165663
C	2.738083	2.855944	-2.058822
C	3.047319	5.034705	-0.363587
H	2.742917	3.657088	1.242100
C	2.970932	4.118817	-2.587127
H	2.593964	2.017260	-2.733663
C	3.125458	5.215486	-1.739093
H	3.155154	5.881875	0.307681
H	3.023871	4.250210	-3.664041
H	3.300400	6.204529	-2.152673
C	3.705229	0.044401	-0.768645
C	3.570669	-0.526070	-2.038612
C	4.939465	-0.057037	-0.117935
C	4.642433	-1.171517	-2.646716
H	2.620302	-0.483362	-2.556799
C	6.008185	-0.716957	-0.718960
H	5.082432	0.392369	0.860167
C	5.863247	-1.273270	-1.986939
H	4.512392	-1.613009	-3.629969
H	6.959086	-0.787696	-0.198153
H	6.698604	-1.784087	-2.457371
C	1.544967	-2.838843	-0.773891
C	2.753408	-3.385804	-0.332452
C	1.184118	-3.038973	-2.112238

C	3.566669	-4.120115	-1.192457
H	3.089447	-3.241072	0.687657
C	1.990542	-3.777265	-2.971305
H	0.268280	-2.610497	-2.502816
C	3.185934	-4.325628	-2.513102
H	4.504009	-4.526118	-0.823154
H	1.683682	-3.919974	-4.003558
H	3.818186	-4.901097	-3.183098
C	-1.000703	-3.070033	0.378862
C	-1.857442	-3.103657	-0.724465
C	-1.245972	-3.962890	1.427619
C	-2.932740	-3.983966	-0.782056
H	-1.695311	-2.420044	-1.548429
C	-2.327412	-4.840305	1.381646
H	-0.596947	-3.990572	2.295949
C	-3.175615	-4.853176	0.277542
H	-3.583985	-3.973877	-1.651054
H	-2.501402	-5.520362	2.210773
H	-4.017142	-5.539004	0.243238
C	-3.469644	-0.487081	-1.592989
C	-4.740472	-0.930707	-1.215901
C	-3.050811	-0.696538	-2.910865
C	-5.567268	-1.581027	-2.127102
H	-5.094593	-0.777307	-0.201457
C	-3.876731	-1.347451	-3.824348
H	-2.067194	-0.365970	-3.227931
C	-5.136457	-1.794736	-3.434250
H	-6.549680	-1.922777	-1.813439
H	-3.531309	-1.506326	-4.841925
H	-5.779962	-2.305136	-4.145077
C	-3.099354	2.092885	-0.650378
C	-2.963933	2.697430	-1.906416
C	-3.757868	2.789838	0.361092
C	-3.478773	3.965298	-2.140760
H	-2.431053	2.181903	-2.699981
C	-4.272537	4.064934	0.129128
H	-3.873316	2.353801	1.347206
C	-4.133729	4.655693	-1.120212
H	-3.360224	4.422152	-3.119054
H	-4.776201	4.593971	0.933164
H	-4.531539	5.650062	-1.301677
C	-0.358215	3.474619	-0.308085
O	-0.165942	2.394601	-0.931938
O	-0.562374	3.625040	0.913951

H	-0.341528	4.383860	-0.940546
H	-0.522469	2.014164	1.508748

A7

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.065775	-0.466345	-0.363188
N	0.395492	-1.133824	1.789580
C	2.844070	0.478947	1.363813
H	3.889487	0.312860	1.643553
H	2.695202	1.563555	1.315373
C	-2.138356	-2.392344	1.298195
C	-0.119272	-0.283714	-2.108172
O	-0.241816	-0.272530	-3.267541
P	-2.121378	-1.334444	-0.193669
P	2.414227	-0.159908	-0.293500
Si	-1.063251	-1.681717	2.666596
Si	1.651080	-0.229252	2.660834
C	-0.642647	-3.062688	3.866705
H	-0.167992	-2.684416	4.779972
H	-1.551879	-3.599745	4.166503
H	0.044241	-3.771481	3.393078
C	2.593096	-1.391135	3.794955
H	3.537231	-0.947328	4.135356
H	2.009796	-1.645726	4.687944
H	2.806718	-2.328059	3.267334
H	-3.139243	-2.726083	1.592585
H	-1.570873	-3.283253	0.975259
P	-0.517547	1.815852	0.136213
C	-1.539492	2.047438	1.639483
H	-1.776050	3.110445	1.761057
H	-2.493881	1.547760	1.433851
Si	-1.000026	1.405326	3.347284
C	-1.658597	2.675476	4.576180
H	-1.175950	3.653486	4.451997
H	-2.738885	2.822873	4.453948
H	-1.482661	2.352672	5.609562
C	-1.819198	-0.254351	3.636266
H	-2.894537	-0.163853	3.444266
H	-1.718852	-0.498271	4.703404
C	0.847624	1.172887	3.625626

H	1.398099	2.106252	3.461977
H	0.951659	0.944692	4.697223
H	0.156494	-2.265022	-0.414776
H	0.794176	-1.962171	-0.775177
C	-2.676343	-2.495877	-1.521814
C	-4.036839	-2.780658	-1.698175
C	-1.745678	-3.162851	-2.323413
C	-4.454933	-3.695433	-2.658414
H	-4.782593	-2.282811	-1.085908
C	-2.164303	-4.078953	-3.284711
H	-0.685188	-2.995276	-2.190792
C	-3.518176	-4.344303	-3.459207
H	-5.514872	-3.898935	-2.781693
H	-1.424027	-4.588073	-3.894797
H	-3.843175	-5.057536	-4.211286
C	-3.610903	-0.267139	-0.091601
C	-3.934073	0.509373	-1.210388
C	-4.463619	-0.238760	1.015281
C	-5.085529	1.288284	-1.223807
H	-3.285372	0.500341	-2.082326
C	-5.604156	0.562498	1.012981
H	-4.252029	-0.852841	1.883686
C	-5.920029	1.323604	-0.108764
H	-5.320714	1.878386	-2.103978
H	-6.254551	0.574781	1.883001
H	-6.816583	1.936818	-0.116649
C	-1.490166	2.734884	-1.150624
C	-2.617085	3.501308	-0.841405
C	-1.043496	2.726662	-2.477301
C	-3.281039	4.227985	-1.826672
H	-3.011845	3.524858	0.167464
C	-1.706374	3.448336	-3.464528
H	-0.169226	2.151677	-2.756754
C	-2.831708	4.202294	-3.142670
H	-4.160291	4.807921	-1.560361
H	-1.340148	3.417773	-4.486515
H	-3.352725	4.764888	-3.911957
C	0.782458	3.122480	0.376546
C	1.687448	3.370196	-0.660405
C	0.874937	3.913855	1.526717
C	2.671672	4.346082	-0.543228
H	1.636130	2.794347	-1.576249
C	1.864225	4.886733	1.653332
H	0.170861	3.795928	2.341707

C	2.772293	5.101351	0.621553
H	3.365402	4.502859	-1.363354
H	1.916054	5.479991	2.561848
H	3.544097	5.859161	0.719161
C	3.419740	0.831571	-1.474979
C	4.589380	1.483646	-1.076062
C	3.038738	0.894071	-2.819037
C	5.354518	2.193797	-1.996721
H	4.907362	1.451721	-0.038693
C	3.802492	1.605444	-3.740729
H	2.134552	0.397081	-3.153882
C	4.961116	2.260444	-3.331190
H	6.258528	2.698637	-1.668512
H	3.488738	1.648553	-4.779695
H	5.556300	2.818085	-4.048386
C	3.311490	-1.760388	-0.461058
C	3.050603	-2.521614	-1.607109
C	4.235094	-2.238723	0.466582
C	3.689320	-3.737234	-1.814439
H	2.332020	-2.167858	-2.343484
C	4.876007	-3.458523	0.260882
H	4.449756	-1.684433	1.374225
C	4.604261	-4.210961	-0.875744
H	3.466447	-4.317759	-2.704786
H	5.581038	-3.824674	1.001459
H	5.097981	-5.166010	-1.029566
C	1.128520	-4.446003	0.726293
O	0.082931	-4.370223	0.049676
O	1.595867	-3.599771	1.535917
H	1.730803	-5.380479	0.616533
H	0.854980	-2.062170	1.568682

A8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.059222	-0.368326	-0.362032
N	0.481790	-1.017372	1.864068
C	2.783417	0.736955	1.339181
H	3.841886	0.655044	1.608543
H	2.562629	1.805915	1.239851
C	-1.942221	-2.458382	1.347880

C	-0.088923	-0.249243	-2.093810
O	-0.171550	-0.284869	-3.265003
P	-1.947928	-1.428893	-0.186658
P	2.353408	-0.007989	-0.285159
Si	-0.940853	-1.654831	2.721468
Si	1.658234	0.027013	2.684425
C	-0.455023	-2.978712	3.966016
H	0.052136	-2.548534	4.837973
H	-1.346755	-3.503318	4.333407
H	0.218534	-3.717010	3.519145
C	2.674538	-0.999180	3.891403
H	3.574224	-0.464033	4.220856
H	2.096760	-1.250758	4.788897
H	2.985863	-1.943315	3.429702
H	-2.939437	-2.803507	1.643161
H	-1.380498	-3.361692	1.072673
P	-0.674589	1.808445	0.105250
C	-1.725375	2.017309	1.599543
H	-2.050158	3.059952	1.694791
H	-2.634656	1.435143	1.402895
Si	-1.132591	1.454920	3.310499
C	-1.884439	2.676262	4.535390
H	-1.478511	3.686775	4.397373
H	-2.973367	2.738442	4.417058
H	-1.678736	2.380362	5.571460
C	-1.809113	-0.265589	3.642704
H	-2.887296	-0.269627	3.442675
H	-1.698046	-0.469354	4.717276
C	0.730851	1.390797	3.585110
H	1.191961	2.361060	3.367068
H	0.861328	1.229646	4.665830
H	0.681519	-3.256694	-0.470705
H	0.454233	-1.910169	-0.602961
C	-2.399531	-2.726869	-1.432482
C	-3.664831	-3.327983	-1.374428
C	-1.492530	-3.178619	-2.392410
C	-4.011471	-4.350510	-2.249180
H	-4.392877	-2.988949	-0.642354
C	-1.840200	-4.200722	-3.274690
H	-0.507215	-2.734473	-2.452201
C	-3.097366	-4.790067	-3.205645
H	-4.996634	-4.804077	-2.185474
H	-1.120001	-4.534322	-4.016293
H	-3.367958	-5.585999	-3.893807

C	-3.570040	-0.550260	-0.143662
C	-3.950042	0.129432	-1.307335
C	-4.433006	-0.525147	0.955173
C	-5.164497	0.802143	-1.375035
H	-3.287173	0.134697	-2.169187
C	-5.642187	0.167262	0.897092
H	-4.175890	-1.055455	1.866251
C	-6.012549	0.829171	-0.269588
H	-5.437379	1.321565	-2.288333
H	-6.299348	0.176245	1.762412
H	-6.959118	1.359669	-0.319376
C	-1.724095	2.625289	-1.196670
C	-2.933698	3.265474	-0.914099
C	-1.261688	2.651969	-2.518256
C	-3.657678	3.908057	-1.916213
H	-3.346806	3.252160	0.087803
C	-1.982001	3.291244	-3.521430
H	-0.331027	2.163748	-2.779786
C	-3.186457	3.924005	-3.224464
H	-4.599513	4.390119	-1.668867
H	-1.598382	3.291189	-4.537682
H	-3.751525	4.423087	-4.006620
C	0.514773	3.227090	0.313281
C	1.448594	3.456144	-0.702582
C	0.519029	4.095352	1.410154
C	2.369814	4.494698	-0.620072
H	1.469369	2.806631	-1.569712
C	1.445524	5.132738	1.503956
H	-0.205257	3.983837	2.209386
C	2.378583	5.333321	0.491569
H	3.088649	4.634368	-1.421823
H	1.429869	5.788019	2.370578
H	3.102920	6.139399	0.564772
C	3.344839	0.972785	-1.499208
C	4.471747	1.707467	-1.119296
C	2.981232	0.956623	-2.850078
C	5.208653	2.419545	-2.061747
H	4.777163	1.742040	-0.078420
C	3.717359	1.668325	-3.794008
H	2.108984	0.398867	-3.172110
C	4.831587	2.405754	-3.402460
H	6.077690	2.989809	-1.745605
H	3.414777	1.647441	-4.837162
H	5.403806	2.965258	-4.136916

C	3.366624	-1.552204	-0.350755
C	3.218756	-2.363709	-1.482059
C	4.280414	-1.938977	0.630810
C	3.959367	-3.529817	-1.626741
H	2.499454	-2.087467	-2.248376
C	5.012569	-3.118015	0.496822
H	4.427261	-1.337743	1.521933
C	4.854598	-3.916956	-0.629971
H	3.824343	-4.145862	-2.511053
H	5.706355	-3.410208	1.280038
H	5.424629	-4.835767	-0.734895
C	1.558876	-4.496087	0.681253
O	0.903612	-4.247116	-0.426967
O	1.742231	-3.716094	1.596549
H	1.925924	-5.531566	0.706838
H	0.986733	-1.858080	1.550018

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.064347	-0.409568	-0.369071
N	0.441472	-1.087550	1.804349
C	2.842102	0.572329	1.336610
H	3.890836	0.432041	1.618308
H	2.674634	1.652444	1.258036
C	-2.074796	-2.391131	1.322495
C	-0.108745	-0.192657	-2.102656
O	-0.215673	-0.149738	-3.266090
P	-2.064031	-1.355982	-0.196465
P	2.404518	-0.124859	-0.299353
Si	-1.006531	-1.654190	2.683894
Si	1.665788	-0.115780	2.654389
C	-0.575389	-3.018410	3.901479
H	-0.078156	-2.625072	4.796179
H	-1.486304	-3.533645	4.233202
H	0.093392	-3.751876	3.440424
C	2.632039	-1.213781	3.833147
H	3.549401	-0.720261	4.178271
H	2.043721	-1.471195	4.722001
H	2.903015	-2.153265	3.338194
H	-3.077882	-2.706895	1.630358

H	-1.536382	-3.300904	1.018423
P	-0.577228	1.824872	0.130042
C	-1.618679	2.047923	1.622624
H	-1.907049	3.100434	1.723645
H	-2.547594	1.499561	1.424038
Si	-1.039587	1.449348	3.329152
C	-1.723583	2.701349	4.562138
H	-1.272772	3.692755	4.424824
H	-2.809391	2.814541	4.453861
H	-1.523064	2.391744	5.595121
C	-1.795486	-0.238104	3.640035
H	-2.874828	-0.188561	3.453358
H	-1.681261	-0.468418	4.708846
C	0.819292	1.285932	3.580831
H	1.331358	2.233060	3.375336
H	0.950914	1.098231	4.657220
H	0.417997	-2.740921	-0.437771
H	0.526581	-1.963514	-0.805013
C	-2.583385	-2.592448	-1.470139
C	-3.879563	-3.123985	-1.425299
C	-1.700890	-3.063171	-2.443172
C	-4.282424	-4.096855	-2.331719
H	-4.586498	-2.769317	-0.679988
C	-2.105652	-4.034791	-3.356827
H	-0.688614	-2.683227	-2.489401
C	-3.394064	-4.553842	-3.304133
H	-5.290479	-4.498515	-2.279914
H	-1.404085	-4.386896	-4.107494
H	-3.707939	-5.311665	-4.016310
C	-3.614033	-0.369273	-0.136287
C	-3.974463	0.329278	-1.294542
C	-4.462907	-0.313865	0.972230
C	-5.160376	1.052525	-1.346454
H	-3.323835	0.306271	-2.165176
C	-5.641242	0.430080	0.929081
H	-4.219766	-0.861691	1.876475
C	-5.994880	1.110810	-0.232185
H	-5.422053	1.584147	-2.255973
H	-6.289011	0.462309	1.800669
H	-6.919780	1.679035	-0.271024
C	-1.574575	2.708189	-1.165916
C	-2.784206	3.349633	-0.887350
C	-1.070358	2.793191	-2.469835
C	-3.469104	4.050055	-1.878308

H	-3.227076	3.292630	0.100164
C	-1.752866	3.488458	-3.461623
H	-0.135277	2.311221	-2.728227
C	-2.958120	4.122016	-3.169443
H	-4.411698	4.532778	-1.635821
H	-1.337805	3.534215	-4.464202
H	-3.493282	4.665513	-3.942852
C	0.686343	3.168484	0.365607
C	1.642379	3.366488	-0.635552
C	0.710278	4.026916	1.470167
C	2.603164	4.366913	-0.531427
H	1.650514	2.725551	-1.508804
C	1.676401	5.024497	1.585226
H	-0.027947	3.939316	2.259115
C	2.629400	5.196401	0.586228
H	3.336489	4.484997	-1.323202
H	1.674725	5.672580	2.457188
H	3.382544	5.973900	0.674753
C	3.421468	0.828278	-1.507122
C	4.561850	1.538501	-1.122369
C	3.067694	0.807535	-2.860354
C	5.323812	2.222981	-2.065404
H	4.857898	1.574478	-0.078666
C	3.828293	1.492688	-3.804144
H	2.186918	0.263933	-3.184682
C	4.956936	2.206090	-3.408892
H	6.204729	2.773604	-1.747647
H	3.535333	1.468819	-4.849874
H	5.549052	2.744101	-4.143517
C	3.317782	-1.722379	-0.402844
C	3.058921	-2.534579	-1.512578
C	4.269495	-2.141802	0.527164
C	3.725951	-3.740544	-1.683269
H	2.312615	-2.230159	-2.241219
C	4.933897	-3.355369	0.362274
H	4.492257	-1.542403	1.403987
C	4.662740	-4.158408	-0.739734
H	3.502588	-4.361150	-2.546146
H	5.658864	-3.675321	1.105123
H	5.176038	-5.107550	-0.864528
C	1.245303	-4.408277	0.770547
O	0.420076	-4.136169	-0.156924
O	1.688836	-3.635127	1.634945
H	1.582278	-5.464933	0.796426

H	0.931470	-1.981490	1.577504

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.146812	0.309941	-0.202762
N	0.119090	1.005520	1.720707
C	-2.791378	1.216689	1.278525
H	-3.468135	2.061158	1.448789
H	-3.373150	0.288411	1.332932
C	2.940016	0.113376	1.708124
C	0.283352	0.192437	-1.950429
O	0.415917	0.182495	-3.116499
P	2.442590	0.267194	-0.035832
P	-1.990021	1.256190	-0.360786
Si	1.536733	0.922452	2.707263
Si	-1.391811	1.104223	2.559947
C	2.165615	2.606093	3.281553
H	1.423408	3.150314	3.876844
H	3.074213	2.506202	3.889328
H	2.415594	3.229137	2.412616
C	-1.525700	2.592983	3.717959
H	-2.526869	2.648648	4.165154
H	-0.806642	2.531619	4.544492
H	-1.346014	3.536623	3.188457
H	2.962662	-0.947615	1.976242
H	3.931418	0.529290	1.917271
P	-0.270593	-1.877372	0.304670
C	0.300524	-2.389621	1.992323
H	0.029348	-3.442750	2.141080
H	1.395748	-2.398697	1.912843
Si	-0.118427	-1.486180	3.635046
C	-0.250698	-2.882631	4.902937
H	-1.081066	-3.564460	4.677358
H	0.668700	-3.481190	4.938654
H	-0.420143	-2.478523	5.908700
C	1.232676	-0.272211	4.146693
H	2.164194	-0.774780	4.438395
H	0.864013	0.249837	5.042007
C	-1.686311	-0.457639	3.601042
H	-2.549186	-1.019709	3.228871

H	-1.916346	-0.178279	4.639670
C	3.547762	-0.838920	-0.998482
C	3.757765	-0.576891	-2.357925
C	4.111984	-1.987685	-0.439329
C	4.515032	-1.445112	-3.137094
H	3.324674	0.309940	-2.812025
C	4.870397	-2.857199	-1.219165
H	3.961400	-2.218830	0.610664
C	5.073811	-2.588999	-2.569021
H	4.670000	-1.227028	-4.189825
H	5.299710	-3.747389	-0.768753
H	5.665611	-3.266706	-3.177527
C	3.103428	1.923092	-0.494071
C	4.443077	2.263056	-0.266044
C	2.254886	2.873128	-1.064875
C	4.914725	3.530446	-0.586655
H	5.125623	1.529094	0.155318
C	2.724078	4.146567	-1.383558
H	1.216718	2.625236	-1.265346
C	4.052842	4.477164	-1.141585
H	5.955929	3.781051	-0.404969
H	2.043469	4.874062	-1.816032
H	4.421984	5.468759	-1.387947
C	0.424614	-3.268236	-0.705765
C	0.182434	-4.604568	-0.356961
C	1.173939	-3.006894	-1.852031
C	0.697159	-5.644926	-1.120527
H	-0.433147	-4.839800	0.507630
C	1.689418	-4.047740	-2.623680
H	1.362422	-1.985521	-2.151927
C	1.457611	-5.367810	-2.257137
H	0.497606	-6.674264	-0.835866
H	2.276054	-3.815615	-3.507366
H	1.858538	-6.181141	-2.855589
C	-2.036863	-2.401604	0.263767
C	-2.701235	-2.253052	-0.958526
C	-2.735947	-2.949064	1.341706
C	-4.036484	-2.612173	-1.095465
H	-2.166056	-1.842276	-1.809883
C	-4.078685	-3.303477	1.211037
H	-2.242023	-3.112108	2.293954
C	-4.733057	-3.129506	-0.004835
H	-4.534106	-2.468973	-2.050030
H	-4.608587	-3.720782	2.062732

H	-5.780232	-3.400344	-0.105182
C	-3.321196	0.858316	-1.562170
C	-4.669608	0.866735	-1.193689
C	-2.988846	0.548049	-2.886065
C	-5.661463	0.559618	-2.121683
H	-4.956057	1.107776	-0.175172
C	-3.979186	0.243574	-3.814949
H	-1.949874	0.537249	-3.197157
C	-5.319658	0.245208	-3.434013
H	-6.703972	0.565752	-1.816397
H	-3.701634	0.002709	-4.837074
H	-6.092946	0.003898	-4.157659
C	-1.738656	3.065745	-0.669343
C	-2.419695	3.761864	-1.673948
C	-0.816368	3.766332	0.120860
C	-2.187333	5.119966	-1.880435
H	-3.138620	3.249990	-2.305042
C	-0.594396	5.125703	-0.079081
H	-0.252492	3.233300	0.881566
C	-1.277245	5.808014	-1.083220
H	-2.724079	5.639967	-2.669046
H	0.127053	5.646010	0.544772
H	-1.099357	6.867317	-1.245411

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.096774	0.535204	-0.282600
N	-0.600756	0.966685	1.992666
C	-2.881559	-0.690978	1.167458
H	-3.951790	-0.690158	1.399058
H	-2.603017	-1.723316	0.929465
C	1.924474	2.350522	1.670444
C	0.026340	0.580808	-2.018572
O	0.072245	0.711328	-3.185852
P	1.889989	1.522123	0.012087
P	-2.390355	0.325364	-0.283232
Si	0.810762	1.504048	2.927018
Si	-1.850456	-0.119577	2.643302
C	0.277194	2.791675	4.192392
H	-0.330873	2.350382	4.991135

H	1.146837	3.265336	4.665831
H	-0.316317	3.586140	3.722953
C	-2.945680	0.813174	3.855260
H	-3.803214	0.201579	4.164213
H	-2.399115	1.095593	4.763169
H	-3.339182	1.732235	3.404334
H	2.940162	2.544215	2.033814
H	1.469335	3.335298	1.499025
P	0.596004	-1.649533	-0.004608
C	1.496930	-2.069500	1.550145
H	1.754601	-3.135336	1.557798
H	2.452502	-1.534487	1.468318
Si	0.862408	-1.646716	3.280649
C	1.548790	-2.986703	4.415929
H	1.111944	-3.967815	4.190220
H	2.637155	-3.078027	4.311837
H	1.333805	-2.766253	5.468850
C	1.555347	0.022699	3.805952
H	2.646697	0.012473	3.695160
H	1.361834	0.141612	4.881758
C	-1.006907	-1.570656	3.481524
H	-1.466274	-2.504734	3.135701
H	-1.201266	-1.512501	4.562518
H	-0.372345	2.102300	-0.321699
H	-1.042898	1.809146	1.616401
C	3.507394	0.630821	-0.077171
C	3.958340	0.240573	-1.345608
C	4.278442	0.287372	1.035360
C	5.154351	-0.448981	-1.496166
H	3.368957	0.482424	-2.226427
C	5.470726	-0.423201	0.888882
H	3.962650	0.579546	2.032480
C	5.914528	-0.787657	-0.377373
H	5.484146	-0.738566	-2.489243
H	6.055698	-0.678680	1.768432
H	6.847554	-1.331326	-0.495056
C	2.342085	2.968418	-1.061798
C	3.604134	3.564558	-0.933275
C	1.431026	3.527198	-1.959470
C	3.944171	4.686403	-1.681054
H	4.333354	3.144972	-0.245167
C	1.773311	4.645510	-2.718501
H	0.448786	3.083677	-2.063532
C	3.027928	5.229190	-2.580744

H	4.926272	5.136171	-1.564123
H	1.053125	5.057221	-3.420304
H	3.293669	6.102001	-3.170850
C	1.799141	-2.324888	-1.260896
C	2.949797	-3.040093	-0.914394
C	1.526792	-2.149020	-2.623032
C	3.800690	-3.553829	-1.890103
H	3.218579	-3.192634	0.123794
C	2.375159	-2.658997	-3.600448
H	0.648444	-1.600008	-2.936115
C	3.519584	-3.364704	-3.238441
H	4.693401	-4.094688	-1.588189
H	2.138974	-2.499210	-4.648734
H	4.185992	-3.760062	-3.999980
C	-0.633584	-3.037846	-0.113909
C	-1.465815	-3.070869	-1.238979
C	-0.790467	-4.037955	0.850555
C	-2.416927	-4.072195	-1.401122
H	-1.382578	-2.292488	-1.992076
C	-1.757486	-5.031736	0.702649
H	-0.159954	-4.058426	1.733485
C	-2.572764	-5.053594	-0.424530
H	-3.048524	-4.071084	-2.284412
H	-1.865577	-5.793711	1.469806
H	-3.323622	-5.829718	-0.542179
C	-3.405742	-0.319763	-1.678146
C	-4.381005	-1.307254	-1.521162
C	-3.209149	0.238162	-2.946717
C	-5.139550	-1.732831	-2.609745
H	-4.547728	-1.763129	-0.550479
C	-3.966547	-0.185703	-4.033764
H	-2.457085	1.007955	-3.087169
C	-4.933864	-1.174853	-3.868225
H	-5.892193	-2.504346	-2.471789
H	-3.799556	0.258118	-5.010956
H	-5.525331	-1.507787	-4.716379
C	-3.341412	1.901828	0.008377
C	-2.873184	3.096588	-0.548939
C	-4.553099	1.932118	0.709981
C	-3.578170	4.287270	-0.392768
H	-1.933667	3.090072	-1.090436
C	-5.254155	3.123461	0.879774
H	-4.968378	1.023962	1.134611
C	-4.766520	4.306817	0.331588

H	-3.190688	5.201642	-0.833394
H	-6.186389	3.123752	1.437770
H	-5.311291	5.237102	0.465326

$R^1=R^2=R^3$=iPr

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.133784	-0.852570	0.206191
N	-0.364909	0.468057	-1.507862
C	-2.992925	1.028675	-0.342050
H	-4.001585	1.121705	-0.759196
H	-2.975734	1.633189	0.571588
C	2.511205	-0.142770	-1.895438
C	-0.028796	-1.970417	1.559537
O	0.054433	-2.724171	2.453788
P	2.082921	-1.328383	-0.562648
P	-2.556483	-0.680468	0.140647
Si	0.963916	0.752784	-2.542988
Si	-1.635528	1.615718	-1.539466
C	0.713616	0.174452	-4.328628
H	-0.148593	0.661796	-4.799687
H	1.594322	0.383335	-4.950577
H	0.532495	-0.908570	-4.362378
C	-2.416252	1.840157	-3.253457
H	-3.329206	2.448942	-3.205941
H	-1.726307	2.347942	-3.940085
H	-2.676720	0.876944	-3.708884
H	3.173316	0.618813	-1.468137
H	3.079191	-0.616214	-2.704209
P	0.535845	0.984268	1.536942
C	1.534723	2.241211	0.612234
H	1.947126	2.956351	1.332971
H	2.404127	1.704503	0.213154
Si	0.845391	3.285445	-0.846153
C	1.541504	5.021911	-0.559920
H	1.139274	5.474801	0.355729
H	2.635555	5.010915	-0.470890
H	1.285762	5.687210	-1.394177
C	1.433263	2.596583	-2.500478
H	2.510297	2.737787	-2.661884

H	0.921282	3.163946	-3.291991
C	-1.027130	3.344978	-1.004209
H	-1.521008	3.718449	-0.099355
H	-1.254879	4.074518	-1.795992
H	-0.388093	-1.840436	-1.227717
H	-0.574013	-2.335702	-0.642537
C	-0.747970	2.094713	2.335485
C	-0.230991	3.352753	3.039285
C	-1.737127	1.348385	3.242309
H	-1.305961	2.429062	1.457431
H	0.368983	3.990382	2.383194
H	-1.080945	3.954344	3.386173
H	0.372024	3.105422	3.919811
H	-1.835713	0.295004	2.969430
H	-1.429038	1.386369	4.290750
H	-2.729169	1.812539	3.183491
C	1.699372	0.464493	2.935755
C	0.976632	0.064432	4.226572
C	2.860237	1.409212	3.258618
H	2.127496	-0.458171	2.539172
H	0.113516	-0.579628	4.042644
H	1.668085	-0.495026	4.868623
H	0.644330	0.940926	4.791799
H	3.496188	1.607871	2.390359
H	2.512296	2.373801	3.645016
H	3.494699	0.955801	4.030871
C	3.609781	-1.287834	0.528483
C	4.976257	-1.212244	-0.162980
C	3.609095	-2.396378	1.586857
H	3.476215	-0.327325	1.041815
H	5.015418	-0.440912	-0.937468
H	5.742190	-0.965590	0.583228
H	5.262921	-2.162588	-0.619669
H	2.625256	-2.557305	2.037576
H	3.936897	-3.347203	1.151862
H	4.311873	-2.149931	2.392353
C	2.091740	-2.968810	-1.484269
C	1.568660	-4.146870	-0.652889
C	3.405502	-3.373229	-2.160817
H	1.358630	-2.770433	-2.279871
H	0.601130	-3.946565	-0.187697
H	1.454934	-5.028619	-1.295840
H	2.265522	-4.415301	0.146794
H	3.890121	-2.549430	-2.692834

H	4.118012	-3.773220	-1.431755
H	3.211638	-4.167950	-2.891637
C	-3.093943	-1.696725	-1.351351
C	-4.359487	-1.278021	-2.106746
C	-3.140498	-3.193989	-1.022537
H	-2.257009	-1.521969	-2.038085
H	-4.343211	-0.224149	-2.397682
H	-4.429017	-1.863901	-3.032513
H	-5.274567	-1.460060	-1.537709
H	-2.278498	-3.525989	-0.432728
H	-4.043924	-3.448399	-0.457604
H	-3.158896	-3.782373	-1.948077
C	-3.776057	-1.043186	1.519290
C	-3.389600	-2.258178	2.367034
C	-5.250659	-1.101981	1.111457
H	-3.666151	-0.156800	2.153495
H	-2.391906	-2.152740	2.799628
H	-4.102244	-2.376677	3.193210
H	-3.402843	-3.187437	1.787773
H	-5.542862	-0.251817	0.486351
H	-5.486909	-2.024783	0.572061
H	-5.880682	-1.082692	2.009921

TSA5-1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.040830	-0.798244	0.084494
N	0.213859	0.481246	-1.781895
C	-2.457856	-0.357212	-2.209809
H	-2.041427	-1.035194	-2.965491
H	-3.492647	-0.154687	-2.499453
C	2.936508	0.784852	-0.773347
C	-0.016281	-2.148670	1.194627
O	-0.038746	-3.093601	1.890747
P	2.396884	-0.864756	-0.157301
P	-2.302689	-1.175201	-0.562985
Si	1.647465	1.403178	-2.026643
Si	-1.307259	1.131123	-2.257112
C	2.394269	1.212333	-3.752030
H	1.700993	1.569488	-4.523615
H	3.324934	1.786217	-3.852187

H	2.623529	0.163289	-3.978429
C	-1.342921	1.816194	-4.020611
H	-2.366799	2.091566	-4.307097
H	-0.724659	2.714841	-4.137419
H	-0.987609	1.070106	-4.742001
H	2.956346	1.456546	0.093623
H	3.949593	0.780554	-1.190062
P	0.012920	0.928554	1.722566
C	0.437082	2.639962	1.137800
H	0.187295	3.351170	1.931479
H	1.531868	2.670288	1.065756
Si	-0.193611	3.385018	-0.489337
C	-0.527741	5.213702	-0.145462
H	-1.333867	5.348874	0.587145
H	0.365696	5.716898	0.245527
H	-0.825488	5.737768	-1.062501
C	1.222376	3.227231	-1.730662
H	2.092646	3.783388	-1.354107
H	0.946298	3.699729	-2.683928
C	-1.773511	2.550533	-1.101068
H	-2.329639	2.191803	-0.224191
H	-2.418983	3.276976	-1.612621
H	0.091405	-1.821821	-1.307648
H	0.184871	-0.938461	-1.673322
C	1.308943	0.847765	3.098749
C	1.407492	-0.495553	3.831343
C	1.315571	1.995127	4.116123
H	2.225870	0.961047	2.503192
H	1.298818	-1.349257	3.160843
H	2.383851	-0.577679	4.326576
H	0.646869	-0.587696	4.611280
H	1.372361	2.980251	3.645559
H	0.433017	1.976359	4.762995
H	2.193044	1.897282	4.768223
C	-1.634835	1.196458	2.595992
C	-2.011802	2.628668	2.984006
C	-1.792710	0.261335	3.800123
H	-2.349487	0.873046	1.835451
H	-2.081504	3.290150	2.114212
H	-2.997380	2.624537	3.467092
H	-1.303795	3.071786	3.692472
H	-1.460254	-0.758992	3.584891
H	-1.226574	0.624835	4.663135
H	-2.844864	0.212700	4.103278

C	-3.885271	-0.611077	0.277909
C	-4.001371	-1.115324	1.724607
C	-5.204553	-0.875565	-0.455613
H	-3.742180	0.478525	0.304477
H	-3.028942	-1.284887	2.189439
H	-4.552485	-0.393873	2.339335
H	-4.550372	-2.060281	1.767713
H	-5.208753	-0.515738	-1.488288
H	-5.445021	-1.943506	-0.465456
H	-6.021669	-0.365057	0.070367
C	-2.522823	-3.008659	-0.943448
C	-3.388148	-3.356573	-2.159211
C	-2.971528	-3.829558	0.271079
H	-1.493281	-3.307321	-1.174073
H	-3.027807	-2.891107	-3.080601
H	-3.368453	-4.442629	-2.316681
H	-4.434275	-3.065803	-2.023009
H	-2.435354	-3.563514	1.185099
H	-4.045404	-3.714830	0.452574
H	-2.787186	-4.893908	0.081120
C	2.832997	-1.984827	-1.602817
C	2.374803	-3.437970	-1.411921
C	4.280384	-1.953859	-2.100493
H	2.201865	-1.557543	-2.393105
H	1.393069	-3.502796	-0.936060
H	2.307518	-3.933384	-2.388480
H	3.083377	-4.011327	-0.807113
H	4.658992	-0.939328	-2.258419
H	4.953619	-2.467762	-1.406100
H	4.348193	-2.479345	-3.061624
C	3.603551	-1.247003	1.223805
C	5.028846	-0.711554	1.054945
C	3.612890	-2.729920	1.608496
H	3.166442	-0.709373	2.067666
H	5.046357	0.370823	0.894091
H	5.602870	-0.916536	1.967809
H	5.558335	-1.184033	0.222687
H	2.606344	-3.156016	1.660572
H	4.199695	-3.321766	0.898143
H	4.077186	-2.853661	2.594619

A6

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.007500	-0.633276	-0.510622
N	-0.284923	-0.258224	1.737851
C	2.660805	-0.598291	1.793115
H	2.896713	-1.468717	2.417629
H	3.529838	0.066729	1.852708
C	-3.050854	0.439059	0.839290
C	0.208777	-1.229423	-2.151410
O	0.348018	-1.742133	-3.194905
P	-2.458360	-0.628509	-0.538362
P	2.356041	-1.156260	0.045777
Si	-1.855556	0.359378	2.299099
Si	1.187588	0.302882	2.546138
C	-2.535541	-0.806630	3.603947
H	-1.916785	-0.798894	4.509104
H	-3.557910	-0.535652	3.895168
H	-2.543774	-1.838056	3.232138
C	1.119042	-0.115343	4.381579
H	2.080309	0.092267	4.869388
H	0.351629	0.462667	4.911530
H	0.897217	-1.179756	4.523845
H	-3.075759	1.468687	0.468315
H	-4.074666	0.205312	1.149389
P	0.205769	1.761913	-1.081618
C	-0.664720	2.936826	0.067890
H	-0.506491	3.956873	-0.296686
H	-1.739094	2.757075	-0.051071
Si	-0.276173	3.004558	1.930419
C	-0.252738	4.826607	2.418273
H	0.522623	5.391715	1.886620
H	-1.217007	5.304435	2.203636
H	-0.063249	4.939994	3.493008
C	-1.608598	2.113568	2.920023
H	-2.562955	2.654241	2.863777
H	-1.308107	2.114311	3.977574
C	1.351773	2.170151	2.367139
H	2.137975	2.433805	1.651859
H	1.683115	2.561758	3.339863
C	-0.297431	-3.406196	1.032545
O	-0.264533	-2.694562	-0.006220
O	-0.232045	-3.031333	2.222009
H	-0.404955	-4.496511	0.844426

H	-0.295297	-1.285909	1.918157
C	3.792426	-0.423141	-0.917939
C	3.864132	-1.000991	-2.335899
C	5.193234	-0.389991	-0.296427
H	3.483100	0.616384	-1.012422
H	2.879712	-1.100489	-2.802442
H	4.475805	-0.351190	-2.974097
H	4.337927	-1.988131	-2.334213
H	5.202407	-0.011850	0.730404
H	5.675711	-1.369393	-0.298096
H	5.825158	0.281139	-0.892878
C	2.735090	-2.991186	0.198002
C	4.161648	-3.347352	0.630181
C	2.341292	-3.810662	-1.037123
H	2.072119	-3.282155	1.018930
H	4.543217	-2.709387	1.434346
H	4.180839	-4.381842	0.995677
H	4.859924	-3.292327	-0.211670
H	1.305496	-3.627551	-1.321933
H	2.987256	-3.591090	-1.892053
H	2.450412	-4.879969	-0.813891
C	-0.639730	2.267178	-2.698827
C	-0.118337	1.583886	-3.972297
C	-0.788762	3.767271	-2.977518
H	-1.644488	1.870587	-2.523740
H	0.208442	0.556951	-3.813576
H	-0.916099	1.563884	-4.724403
H	0.716920	2.136263	-4.411004
H	-1.291950	4.310857	-2.173402
H	0.181435	4.240866	-3.160224
H	-1.388642	3.905978	-3.885929
C	1.914545	2.570375	-1.150590
C	2.026565	4.058625	-0.799330
C	2.618442	2.317542	-2.489741
H	2.462136	2.027309	-0.372216
H	1.745702	4.272705	0.235139
H	3.071221	4.374062	-0.916925
H	1.419720	4.693662	-1.451457
H	2.445487	1.312404	-2.883808
H	2.280377	3.037893	-3.241381
H	3.701171	2.455251	-2.377947
C	-3.478847	0.019667	-1.972669
C	-4.998833	-0.112804	-1.856488
C	-2.994293	-0.497257	-3.329369

H	-3.255273	1.094324	-1.926670
H	-5.377270	0.221342	-0.884809
H	-5.480519	0.501544	-2.627852
H	-5.323093	-1.145605	-2.018604
H	-1.916402	-0.383781	-3.451758
H	-3.230012	-1.557023	-3.466952
H	-3.487968	0.055400	-4.138902
C	-3.164563	-2.296876	-0.051998
C	-3.027646	-3.303552	-1.198622
C	-4.559466	-2.362996	0.579113
H	-2.468305	-2.601549	0.731884
H	-2.036678	-3.254244	-1.657070
H	-3.168858	-4.322792	-0.817976
H	-3.789159	-3.136810	-1.969915
H	-4.635983	-1.763325	1.491441
H	-5.359737	-2.059252	-0.099046
H	-4.757444	-3.402740	0.869360

A7

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.162489	-0.083146	-0.817217
N	0.331599	-1.066248	1.258672
C	2.754520	0.616789	1.422964
H	3.749296	0.325246	1.774439
H	2.679267	1.697260	1.591944
C	-1.950257	-2.471484	0.240303
C	0.263347	0.366183	-2.517778
O	0.381118	0.568737	-3.661756
P	-1.972335	-1.182023	-1.058791
P	2.540946	0.302660	-0.379191
Si	-1.195342	-1.798095	1.822134
Si	1.398387	-0.247524	2.421996
C	-0.861986	-3.234966	2.986799
H	-0.642519	-2.903635	4.008694
H	-1.735643	-3.897647	3.038028
H	-0.009076	-3.817178	2.622946
C	2.197019	-1.510819	3.558777
H	3.058143	-1.081063	4.086279
H	1.497669	-1.882318	4.316476
H	2.535591	-2.373998	2.973451

H	-2.912757	-2.971423	0.384810
H	-1.219170	-3.233522	-0.085566
P	-0.705150	2.093326	-0.146618
C	-1.713540	2.194094	1.406696
H	-1.764004	3.241032	1.721566
H	-2.744977	1.943301	1.124404
Si	-1.407954	1.175304	2.965461
C	-2.300395	2.112208	4.339141
H	-1.849085	3.098098	4.509612
H	-3.358331	2.270369	4.094011
H	-2.260406	1.563202	5.287964
C	-2.212974	-0.508792	2.743699
H	-3.187684	-0.345836	2.267154
H	-2.432314	-0.923716	3.737475
C	0.410894	1.014620	3.411231
H	0.884117	2.003399	3.341778
H	0.464117	0.732256	4.472547
H	0.415742	-1.844538	-1.084656
H	1.028447	-1.489855	-1.423675
C	1.396718	-4.401804	0.129697
O	0.417262	-4.428968	-0.635588
O	1.757785	-3.476940	0.912202
H	2.051831	-5.308617	0.139803
H	0.868787	-1.925999	0.985318
C	3.592287	1.658275	-1.135152
C	3.467449	1.782033	-2.657155
C	5.068297	1.649290	-0.726115
H	3.145974	2.558818	-0.699968
H	2.432133	1.754054	-3.000487
H	3.903130	2.734569	-2.983605
H	4.005931	0.983157	-3.175588
H	5.208409	1.540948	0.353987
H	5.613834	0.843064	-1.226317
H	5.537086	2.594211	-1.028025
C	3.440828	-1.319487	-0.640250
C	4.695285	-1.606185	0.189700
C	3.695409	-1.576746	-2.130079
H	2.708195	-2.055215	-0.296450
H	4.489438	-1.589832	1.263961
H	5.037108	-2.621632	-0.044496
H	5.523750	-0.922676	-0.015821
H	2.841154	-1.302092	-2.760339
H	4.570200	-1.023411	-2.489910
H	3.892008	-2.642929	-2.291077

C	-1.976724	2.934905	-1.269931
C	-1.680416	2.926748	-2.770980
C	-2.423833	4.337866	-0.837344
H	-2.841847	2.279718	-1.125627
H	-1.532293	1.919611	-3.158357
H	-2.535538	3.360882	-3.304471
H	-0.799932	3.518320	-3.035188
H	-2.700599	4.394314	0.218659
H	-1.654949	5.091986	-1.029606
H	-3.308708	4.626113	-1.418330
C	0.629569	3.389540	0.156879
C	0.370321	4.468789	1.211832
C	1.102372	4.020742	-1.157245
H	1.453643	2.781981	0.536530
H	0.203612	4.043654	2.206595
H	1.252754	5.117299	1.282477
H	-0.482964	5.107461	0.965242
H	1.245600	3.275887	-1.944567
H	0.391342	4.767056	-1.523342
H	2.058942	4.535812	-1.006716
C	-3.622215	-0.304110	-0.809849
C	-4.727228	-1.087478	-0.091944
C	-4.162856	0.285431	-2.119174
H	-3.357376	0.528473	-0.151658
H	-4.423718	-1.426463	0.901784
H	-5.602382	-0.438021	0.036262
H	-5.052702	-1.967289	-0.654006
H	-3.390769	0.778455	-2.716693
H	-4.617316	-0.490820	-2.743821
H	-4.941710	1.026658	-1.903569
C	-2.211604	-2.112376	-2.672627
C	-3.340366	-3.147179	-2.625149
C	-0.923554	-2.784085	-3.166152
H	-2.477599	-1.334752	-3.399924
H	-4.314046	-2.707192	-2.395755
H	-3.429965	-3.639255	-3.601203
H	-3.130960	-3.927410	-1.884972
H	-0.151181	-2.054415	-3.418754
H	-0.513283	-3.483521	-2.429731
H	-1.145571	-3.347655	-4.081090

A8

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.100211	-0.241319	-0.734158
N	0.174214	-0.849609	1.523242
C	2.788984	0.432474	1.079684
H	3.803514	0.263192	1.458622
H	2.701276	1.498968	0.857500
C	-2.390672	-1.890535	0.832880
C	0.169117	-0.225873	-2.476222
O	0.235721	-0.333999	-3.644735
P	-2.252730	-0.847762	-0.692364
P	2.397710	-0.436697	-0.504917
Si	-1.426250	-1.108590	2.241037
Si	1.480656	-0.013407	2.371335
C	-1.334347	-2.321682	3.678021
H	-0.851425	-1.873440	4.555316
H	-2.340618	-2.634730	3.986462
H	-0.767462	-3.217308	3.401966
C	2.280325	-1.169658	3.623234
H	3.122336	-0.685529	4.134455
H	1.569220	-1.500143	4.389173
H	2.664884	-2.069630	3.127398
H	-3.424270	-2.123725	1.107922
H	-1.896122	-2.847437	0.639015
P	-0.048753	2.167911	-0.510430
C	-1.232061	2.638176	0.835314
H	-1.363207	3.727609	0.871511
H	-2.203990	2.227046	0.536562
Si	-1.005406	2.015512	2.620774
C	-1.601842	3.424399	3.727809
H	-0.983256	4.323690	3.614588
H	-2.635754	3.702994	3.487305
H	-1.574792	3.137109	4.786169
C	-2.116750	0.518539	2.887575
H	-3.117201	0.720133	2.486068
H	-2.250675	0.399935	3.972475
C	0.704383	1.473727	3.221733
H	1.407154	2.311329	3.273427
H	0.527004	1.179252	4.268947
H	-0.076154	-3.154446	-0.682166
H	0.049696	-1.875682	-0.864544
C	0.243446	-4.587479	0.573273
O	-0.202624	-4.179772	-0.587423

O	0.692408	-3.886159	1.463126
H	0.161827	-5.679726	0.675957
H	0.488479	-1.795268	1.278260
C	3.538363	0.337124	-1.772034
C	3.711496	-0.521885	-3.029720
C	4.898400	0.826929	-1.267879
H	2.953640	1.209915	-2.074248
H	2.770140	-0.961709	-3.370291
H	4.100195	0.100332	-3.845485
H	4.433802	-1.328160	-2.866622
H	4.819879	1.461967	-0.380403
H	5.563028	-0.005940	-1.017703
H	5.392112	1.416655	-2.050962
C	3.040604	-2.165324	-0.168413
C	4.487677	-2.287751	0.317246
C	2.793255	-3.146466	-1.323303
H	2.390582	-2.487371	0.653813
H	4.715319	-1.628780	1.160739
H	4.677349	-3.316869	0.648037
H	5.200252	-2.071318	-0.485956
H	1.850671	-2.950675	-1.840360
H	3.599002	-3.109603	-2.061993
H	2.760778	-4.172513	-0.936174
C	1.165884	3.637890	-0.315644
C	2.468879	3.552213	-1.116259
C	1.521602	4.067358	1.110940
H	0.582097	4.463792	-0.739404
H	2.335007	3.183561	-2.133050
H	2.919881	4.550236	-1.186799
H	3.199282	2.908600	-0.619519
H	0.648684	4.238137	1.745775
H	2.173319	3.343814	1.607933
H	2.074274	5.014590	1.068844
C	-0.927537	2.804840	-2.062878
C	0.021637	3.003975	-3.251820
C	-1.790456	4.060573	-1.902112
H	-1.575111	1.962511	-2.320675
H	0.737314	2.186399	-3.365982
H	-0.562077	3.053613	-4.179058
H	0.574369	3.946524	-3.168077
H	-2.541822	3.977266	-1.112035
H	-1.185660	4.950150	-1.688286
H	-2.324871	4.255863	-2.840372
C	-3.885167	0.098924	-0.472796

C	-5.168784	-0.742317	-0.486073
C	-4.083142	1.301992	-1.396818
H	-3.771458	0.496929	0.544112
H	-5.108988	-1.650262	0.119671
H	-6.000749	-0.143369	-0.093928
H	-5.437587	-1.035882	-1.505875
H	-3.276082	2.024829	-1.306010
H	-4.156669	1.014153	-2.449367
H	-5.015272	1.819573	-1.135398
C	-2.557501	-2.025113	-2.130027
C	-3.057013	-1.289819	-3.378702
C	-3.399112	-3.272757	-1.849937
H	-1.540785	-2.364875	-2.347279
H	-2.498071	-0.368050	-3.568462
H	-2.931306	-1.932279	-4.258503
H	-4.121436	-1.041664	-3.305241
H	-3.014534	-3.846093	-1.001909
H	-4.450332	-3.040883	-1.657373
H	-3.364872	-3.933452	-2.725834

TSA7-8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.106733	-0.242559	-0.737259
N	0.163636	-0.918605	1.470743
C	2.788026	0.371440	1.093571
H	3.798462	0.185338	1.475165
H	2.706828	1.445003	0.905753
C	-2.419472	-1.912736	0.767742
C	0.170968	-0.133909	-2.485156
O	0.233487	-0.165922	-3.654627
P	-2.301049	-0.823181	-0.719714
P	2.417840	-0.447136	-0.518511
Si	-1.440375	-1.182027	2.192178
Si	1.466986	-0.114987	2.360356
C	-1.344557	-2.439065	3.587662
H	-0.859817	-2.021682	4.478957
H	-2.349401	-2.765117	3.886885
H	-0.774591	-3.319528	3.271889
C	2.246695	-1.319600	3.576479
H	3.125866	-0.883409	4.067553

H	1.542128	-1.622024	4.359799
H	2.566126	-2.233461	3.060909
H	-3.449765	-2.161228	1.041978
H	-1.917284	-2.856741	0.528021
P	-0.028186	2.179570	-0.446563
C	-1.221812	2.597178	0.902876
H	-1.355758	3.684681	0.968943
H	-2.189626	2.193185	0.581845
Si	-1.003961	1.924807	2.672932
C	-1.588965	3.309503	3.815428
H	-0.959676	4.204587	3.730966
H	-2.618760	3.606683	3.579902
H	-1.568796	2.990843	4.864887
C	-2.124984	0.428996	2.887710
H	-3.123521	0.646816	2.489781
H	-2.262506	0.275295	3.967735
C	0.700175	1.351147	3.255699
H	1.409160	2.180305	3.342483
H	0.515683	1.019446	4.290522
H	-0.056381	-2.788404	-0.760357
H	0.080875	-1.910170	-0.974729
C	0.258163	-4.490816	0.500381
O	-0.256949	-4.077801	-0.593579
O	0.760956	-3.805516	1.400183
H	0.226715	-5.591034	0.623811
H	0.477392	-1.884981	1.277293
C	3.540770	0.380730	-1.763879
C	3.710987	-0.435825	-3.049977
C	4.901695	0.860139	-1.251272
H	2.948837	1.260397	-2.031920
H	2.770119	-0.867080	-3.402723
H	4.096417	0.213770	-3.845554
H	4.434318	-1.246145	-2.914930
H	4.829634	1.431029	-0.320690
H	5.583398	0.023379	-1.069748
H	5.370964	1.510033	-2.000825
C	3.058140	-2.182550	-0.245546
C	4.511928	-2.308865	0.218405
C	2.800117	-3.132041	-1.425058
H	2.416955	-2.533935	0.571295
H	4.744046	-1.676734	1.081341
H	4.711271	-3.347030	0.512308
H	5.213769	-2.060663	-0.585127
H	1.846872	-2.938389	-1.921941

H	3.594702	-3.070626	-2.174601
H	2.777331	-4.166241	-1.060855
C	1.191092	3.633863	-0.193891
C	2.501602	3.573935	-0.984371
C	1.533210	4.014735	1.249546
H	0.611675	4.474069	-0.595280
H	2.376028	3.263101	-2.021370
H	2.962271	4.569732	-0.995451
H	3.219875	2.897951	-0.514359
H	0.654610	4.162408	1.881955
H	2.183561	3.277121	1.727019
H	2.083290	4.964136	1.242745
C	-0.895457	2.864365	-1.983414
C	0.062780	3.118173	-3.154777
C	-1.766373	4.108131	-1.779308
H	-1.537108	2.029267	-2.278802
H	0.790280	2.315277	-3.295372
H	-0.513023	3.196944	-4.084629
H	0.603713	4.062698	-3.029235
H	-2.528343	3.986697	-1.004647
H	-1.168094	4.989406	-1.518051
H	-2.288426	4.342413	-2.715430
C	-3.913683	0.137741	-0.482744
C	-5.201105	-0.696468	-0.506977
C	-4.099849	1.353421	-1.392395
H	-3.793514	0.519861	0.539263
H	-5.146681	-1.608584	0.092862
H	-6.030544	-0.095567	-0.113093
H	-5.466618	-0.980786	-1.530158
H	-3.268584	2.050942	-1.321729
H	-4.212773	1.074186	-2.443621
H	-5.008167	1.895890	-1.100478
C	-2.584483	-1.961439	-2.189424
C	-3.070146	-1.191714	-3.422454
C	-3.430751	-3.213434	-1.947317
H	-1.567291	-2.302664	-2.403710
H	-2.517115	-0.259724	-3.577281
H	-2.928763	-1.806290	-4.319284
H	-4.137357	-0.953629	-3.354708
H	-3.030049	-3.823924	-1.133882
H	-4.476806	-2.982815	-1.726428
H	-3.416215	-3.834275	-2.852354

A2

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.139107	-0.527449	-0.505179
N	-0.249996	-0.055416	1.519032
C	2.524146	-1.089183	1.638646
H	2.830909	-1.876218	2.337970
H	3.425275	-0.516758	1.387650
C	-2.911298	0.989542	0.851425
C	-0.222618	-1.266460	-2.093066
O	-0.305984	-1.755316	-3.159572
P	-2.530093	-0.283283	-0.400065
P	1.808448	-1.763322	0.088424
Si	-1.555501	0.862108	2.173217
Si	1.239195	0.104237	2.371457
C	-2.379398	0.092328	3.696177
H	-1.685645	-0.011818	4.537808
H	-3.220209	0.711141	4.037416
H	-2.775001	-0.907906	3.476253
C	1.127909	-0.259641	4.229038
H	2.133080	-0.318472	4.667695
H	0.586726	0.523475	4.774634
H	0.622116	-1.213172	4.424280
H	-2.849772	1.964525	0.351970
H	-3.915927	0.902988	1.280535
P	0.695636	1.478056	-1.290159
C	0.188649	2.937547	-0.276473
H	0.604112	3.846575	-0.728581
H	-0.901426	3.019533	-0.388313
Si	0.553958	3.042179	1.600282
C	1.047914	4.842878	1.905546
H	1.965258	5.116887	1.368688
H	0.258811	5.535190	1.584895
H	1.227717	5.022123	2.973173
C	-0.991029	2.625363	2.592312
H	-1.799813	3.345838	2.409024
H	-0.737308	2.706695	3.659850
C	1.905876	1.881133	2.208597
H	2.790024	1.916001	1.561307
H	2.239319	2.241442	3.193340
C	-3.017617	-1.872953	0.469917
C	-2.540972	-3.125764	-0.274111

C	-4.480253	-2.021415	0.893789
H	-2.417647	-1.801369	1.384930
H	-1.485221	-3.057733	-0.552531
H	-2.665755	-4.008082	0.365622
H	-3.108794	-3.301583	-1.192736
H	-4.871676	-1.124830	1.384943
H	-5.124382	-2.255241	0.039348
H	-4.572253	-2.851308	1.605947
C	-3.784922	0.024857	-1.758831
C	-5.190798	0.439110	-1.310680
C	-3.848752	-1.120723	-2.773771
H	-3.361754	0.893516	-2.270018
H	-5.172990	1.297789	-0.632799
H	-5.775743	0.730470	-2.192584
H	-5.730254	-0.372470	-0.815888
H	-2.856120	-1.468200	-3.076314
H	-4.400903	-1.976192	-2.369141
H	-4.377787	-0.790971	-3.676351
C	0.239525	2.017016	-3.037279
C	0.664604	3.426750	-3.456571
C	-1.252902	1.833824	-3.294116
H	0.759570	1.294364	-3.677285
H	1.738027	3.599961	-3.355645
H	0.409709	3.588412	-4.511384
H	0.141335	4.195466	-2.876444
H	-1.539337	0.789489	-3.169322
H	-1.857545	2.453400	-2.619442
H	-1.500883	2.130381	-4.320974
C	2.579541	1.604985	-1.330332
C	3.219873	2.967353	-1.040957
C	3.141034	1.030062	-2.638442
H	2.879020	0.934708	-0.516207
H	2.913128	3.382486	-0.078042
H	4.311368	2.854916	-1.010809
H	2.991338	3.712816	-1.807571
H	2.646510	0.099436	-2.936018
H	3.032598	1.742990	-3.462804
H	4.213199	0.823665	-2.532241
C	1.202190	-3.474919	0.572265
C	0.267540	-3.391400	1.786023
C	2.275558	-4.532603	0.842758
H	0.612422	-3.798336	-0.295577
H	-0.456971	-2.578912	1.708997
H	-0.270385	-4.339353	1.906128

H	0.843025	-3.222642	2.704685
H	2.814012	-4.826276	-0.061400
H	3.005832	-4.186904	1.583670
H	1.803127	-5.436934	1.246872
C	3.296447	-2.025224	-1.017760
C	2.938965	-2.803191	-2.287298
C	4.583534	-2.562931	-0.379118
H	3.516118	-0.997736	-1.320173
H	2.070600	-2.381188	-2.798970
H	3.782319	-2.785634	-2.988856
H	2.718373	-3.854680	-2.069905
H	4.816063	-2.074405	0.572189
H	4.547983	-3.640015	-0.202751
H	5.424550	-2.373802	-1.058421

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.169198	-0.638224	-0.603832
N	-0.280427	-0.050273	1.704186
C	2.498312	-1.081829	1.559416
H	2.916952	-1.821177	2.253240
H	3.346582	-0.491364	1.194771
C	-2.805118	1.128907	0.689446
C	-0.100031	-1.200878	-2.244068
O	-0.043428	-1.579503	-3.360422
P	-2.497758	-0.304524	-0.437663
P	1.666420	-1.860554	0.090982
Si	-1.620085	1.036903	2.151857
Si	1.336398	0.123828	2.424264
C	-2.468304	0.314694	3.670010
H	-1.799860	0.354525	4.538871
H	-3.381134	0.863979	3.931428
H	-2.743944	-0.736160	3.519724
C	1.249789	-0.257951	4.269162
H	2.255283	-0.308813	4.706284
H	0.698803	0.519691	4.813212
H	0.754704	-1.216131	4.468699
H	-2.562182	2.026902	0.107754
H	-3.844725	1.237517	1.019726
P	0.736593	1.421888	-1.261193

C	0.356590	2.980323	-0.318430
H	0.884141	3.824918	-0.777536
H	-0.712342	3.178212	-0.478604
Si	0.660551	3.103325	1.546127
C	1.221810	4.869904	1.895195
H	2.172248	5.095433	1.395225
H	0.482215	5.598779	1.540745
H	1.366202	5.039020	2.969479
C	-0.918003	2.737963	2.506961
H	-1.687276	3.489828	2.284709
H	-0.689081	2.832072	3.578294
C	1.940514	1.890108	2.203559
H	2.844938	1.895207	1.585403
H	2.250745	2.259377	3.192063
H	-0.755189	-2.039915	-0.176048
H	-0.587929	-1.012677	1.845932
C	-3.271462	-1.718131	0.549703
C	-3.390069	-2.990979	-0.293695
C	-4.572159	-1.475734	1.324925
H	-2.488350	-1.906344	1.294759
H	-2.490428	-3.160039	-0.893429
H	-3.534868	-3.862961	0.356744
H	-4.256075	-2.940744	-0.963228
H	-4.564537	-0.550002	1.906538
H	-5.448325	-1.453486	0.672721
H	-4.723350	-2.299177	2.035350
C	-3.707044	0.049162	-1.833112
C	-5.191109	0.154330	-1.471266
C	-3.524722	-0.886643	-3.035389
H	-3.389746	1.050897	-2.141475
H	-5.369425	0.755841	-0.574259
H	-5.734397	0.628144	-2.299221
H	-5.639741	-0.832316	-1.318393
H	-2.475067	-1.062200	-3.281021
H	-3.984410	-1.863402	-2.854077
H	-4.012171	-0.456477	-3.919479
C	0.286120	1.995973	-3.007400
C	0.796813	3.371460	-3.446918
C	-1.218843	1.925947	-3.236812
H	0.736286	1.237623	-3.657589
H	1.876390	3.492106	-3.340836
H	0.559110	3.525990	-4.507055
H	0.310829	4.180113	-2.888488
H	-1.573648	0.906852	-3.103621

H	-1.766911	2.583975	-2.549582
H	-1.465659	2.241431	-4.258581
C	2.636777	1.478649	-1.365614
C	3.358873	2.798806	-1.069997
C	3.135158	0.909350	-2.703230
H	2.937415	0.772814	-0.583611
H	3.123175	3.202752	-0.081933
H	4.443996	2.633376	-1.098877
H	3.132806	3.578869	-1.802223
H	2.564704	0.033984	-3.029651
H	3.074031	1.656182	-3.501798
H	4.188375	0.612991	-2.619510
C	1.238967	-3.564265	0.789854
C	0.269455	-3.470737	1.972364
C	2.419443	-4.451760	1.198506
H	0.701133	-4.047408	-0.035814
H	-0.664200	-2.981571	1.684384
H	0.010781	-4.477073	2.323984
H	0.714783	-2.941440	2.825075
H	3.049384	-4.737328	0.354513
H	3.056843	-3.971425	1.950554
H	2.042028	-5.380755	1.644400
C	3.080973	-2.220439	-1.097396
C	2.692142	-3.306416	-2.108138
C	4.486471	-2.449183	-0.531842
H	3.124522	-1.284225	-1.655406
H	1.715532	-3.112450	-2.559305
H	3.430980	-3.337441	-2.918665
H	2.664499	-4.303473	-1.656076
H	4.800840	-1.642449	0.137915
H	4.584432	-3.390331	0.014837
H	5.206655	-2.477811	-1.360201

$R^1=R^2=R^3=Cy$

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.094010	-0.415300	-0.195238
N	0.106888	-0.889112	1.920574
C	3.005332	-0.701029	1.398367
H	3.837660	-1.370235	1.635913

H	3.429548	0.308451	1.364938
C	-2.793242	-0.323430	1.849513
C	-0.223130	-0.243148	-1.940437
O	-0.329282	-0.211478	-3.108325
P	-2.432927	-0.592440	0.075434
P	2.238561	-1.056322	-0.224986
Si	-1.305780	-0.917076	2.882971
Si	1.622807	-0.754880	2.702697
C	-1.751822	-2.620871	3.582483
H	-0.988432	-2.969910	4.289110
H	-2.712186	-2.604802	4.114671
H	-1.822209	-3.376633	2.789219
C	1.996200	-2.190892	3.882450
H	3.023342	-2.141751	4.267958
H	1.325221	-2.183591	4.751586
H	1.868019	-3.159496	3.382222
H	-2.888197	0.757202	2.000364
H	-3.739400	-0.766366	2.179305
P	0.049355	1.929179	0.372378
C	-0.505318	2.409582	2.082449
H	-0.350431	3.489559	2.180707
H	-1.596420	2.289401	2.070918
Si	0.060793	1.662955	3.746233
C	0.041833	3.127947	4.945065
H	0.779800	3.889489	4.660656
H	-0.941500	3.614638	4.975663
H	0.280339	2.804988	5.966121
C	-1.150132	0.332563	4.305231
H	-2.128693	0.751726	4.575579
H	-0.746268	-0.139093	5.213050
C	1.752642	0.857690	3.708511
H	2.510758	1.532240	3.290577
H	2.058499	0.645818	4.743349
H	-0.280033	-2.128741	0.113185
H	-0.207101	-2.107018	-0.670368
C	1.786778	2.648462	0.292204
C	2.207377	2.956046	-1.155688
C	2.128556	3.823121	1.225076
H	2.402321	1.804881	0.624511
C	3.680090	3.370725	-1.251005
H	1.599996	3.777838	-1.551669
H	2.009875	2.087555	-1.794772
C	3.609679	4.203363	1.118203
H	1.521321	4.701266	0.979258

H	1.901691	3.563155	2.263601
C	3.995736	4.543331	-0.321695
H	3.923377	3.625751	-2.289621
H	4.324411	2.523871	-0.976735
H	3.823034	5.048319	1.783679
H	4.226778	3.362420	1.467787
H	5.060009	4.799675	-0.383481
H	3.434506	5.430913	-0.647534
C	-1.060024	3.154292	-0.552099
C	-0.820904	4.653194	-0.287146
C	-1.185996	2.895716	-2.061157
H	-2.042819	2.919510	-0.112193
C	-1.909612	5.524399	-0.922803
H	0.145594	4.954924	-0.707715
H	-0.777246	4.859669	0.786326
C	-2.257121	3.789140	-2.696533
H	-0.224686	3.071088	-2.559561
H	-1.436964	1.849441	-2.241117
C	-2.008293	5.272254	-2.426987
H	-1.698580	6.581769	-0.721863
H	-2.877851	5.299620	-0.452076
H	-2.311253	3.592574	-3.773961
H	-3.237033	3.520009	-2.276130
H	-2.807661	5.880327	-2.867101
H	-1.069924	5.581112	-2.909522
C	-3.677080	0.452695	-0.855156
C	-3.913283	-0.053639	-2.287906
C	-5.019426	0.705639	-0.151097
H	-3.174203	1.424474	-0.938304
C	-4.781822	0.912051	-3.098924
H	-4.435440	-1.016862	-2.242045
H	-2.959895	-0.227692	-2.798495
C	-5.879327	1.684287	-0.960207
H	-5.563484	-0.239458	-0.029460
H	-4.857682	1.107760	0.854558
C	-6.109282	1.188415	-2.389848
H	-4.962399	0.492064	-4.095685
H	-4.242118	1.855284	-3.247915
H	-6.838831	1.842707	-0.453326
H	-5.373883	2.660945	-0.992610
H	-6.700071	1.918671	-2.955503
H	-6.699100	0.260836	-2.356509
C	-2.947685	-2.388602	-0.134322
C	-4.392553	-2.762481	0.234980

C	-2.596654	-3.039831	-1.486366
H	-2.299207	-2.866449	0.616532
C	-4.545080	-4.286256	0.333796
H	-5.078322	-2.381999	-0.533776
H	-4.692346	-2.305716	1.183481
C	-2.704340	-4.564487	-1.381051
H	-3.292111	-2.694927	-2.258628
H	-1.599036	-2.753609	-1.829112
C	-4.114310	-4.986611	-0.958363
H	-5.584529	-4.541118	0.573821
H	-3.928926	-4.650186	1.168229
H	-2.442101	-5.025870	-2.340496
H	-1.974747	-4.928058	-0.642326
H	-4.168501	-6.074717	-0.834490
H	-4.819060	-4.723653	-1.760286
C	2.263943	-2.935465	-0.266617
C	1.938055	-3.472645	-1.669231
C	3.459289	-3.699487	0.325880
H	1.415790	-3.178746	0.388347
C	1.624350	-4.970589	-1.628852
H	2.804037	-3.309949	-2.324910
H	1.102145	-2.921767	-2.117137
C	3.154479	-5.203464	0.369538
H	4.364852	-3.532124	-0.267376
H	3.673023	-3.356842	1.343199
C	2.783005	-5.755469	-1.008899
H	1.412681	-5.337636	-2.640235
H	0.712694	-5.130412	-1.034932
H	4.019148	-5.743159	0.774147
H	2.320713	-5.376317	1.065369
H	2.528300	-6.819437	-0.934356
H	3.656753	-5.684946	-1.672761
C	3.524679	-0.427498	-1.421851
C	4.912744	-1.076839	-1.327440
C	3.074547	-0.346312	-2.888036
H	3.633720	0.607917	-1.070582
C	5.939136	-0.295183	-2.154687
H	4.859512	-2.101722	-1.717386
H	5.241474	-1.145671	-0.284098
C	4.100966	0.415796	-3.734705
H	2.948020	-1.355697	-3.299784
H	2.101347	0.142815	-2.963463
C	5.501792	-0.190076	-3.617700
H	6.921251	-0.778265	-2.083833

H	6.050771	0.713997	-1.732599
H	3.778527	0.429076	-4.782748
H	4.132343	1.462558	-3.400924
H	6.222379	0.406852	-4.189554
H	5.498647	-1.195064	-4.063976

TSA5-1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.142052	-0.401501	-0.077381
N	-0.266793	-0.973267	2.119420
C	2.205192	-2.244993	1.608008
H	1.640121	-3.184790	1.637155
H	3.231768	-2.484539	1.897724
C	-2.867271	0.312679	1.874142
C	-0.212776	-0.417565	-1.827544
O	-0.290046	-0.482196	-2.996448
P	-2.504911	-0.332580	0.185296
P	2.071520	-1.537145	-0.095138
Si	-1.573758	-0.392939	3.073720
Si	1.289511	-1.146117	2.827226
C	-2.436410	-1.726672	4.097924
H	-1.743921	-2.192233	4.810090
H	-3.271849	-1.307867	4.674493
H	-2.840074	-2.524937	3.462012
C	1.300260	-2.050665	4.490132
H	2.329575	-2.219174	4.833783
H	0.784612	-1.493548	5.281971
H	0.816655	-3.031659	4.403635
H	-2.772813	1.403987	1.823450
H	-3.889479	0.101189	2.206950
P	0.245269	1.933174	0.161987
C	-0.037803	2.601808	1.872405
H	0.291857	3.644468	1.906128
H	-1.127459	2.645770	1.991866
Si	0.612934	1.774564	3.451100
C	1.222355	3.163512	4.579624
H	2.081694	3.691722	4.146894
H	0.434806	3.904919	4.765970
H	1.537785	2.767789	5.553399
C	-0.884045	0.932580	4.241400

H	-1.637761	1.696980	4.478701
H	-0.606526	0.469621	5.198993
C	2.027047	0.569002	3.104123
H	2.556424	0.915540	2.205579
H	2.754206	0.571790	3.926999
H	-0.426878	-2.098960	0.068490
H	-0.421223	-1.807105	0.967256
C	1.865848	-3.051867	-1.199591
C	2.224735	-2.801222	-2.673087
C	2.480974	-4.385398	-0.743086
H	0.776665	-3.183095	-1.161959
C	1.690964	-3.934102	-3.556052
H	3.316739	-2.762376	-2.781168
H	1.828454	-1.841888	-3.017888
C	1.958780	-5.534098	-1.616574
H	3.574478	-4.346139	-0.816103
H	2.243326	-4.595979	0.303826
C	2.235957	-5.290687	-3.102395
H	1.956011	-3.748544	-4.603817
H	0.593021	-3.940407	-3.502762
H	2.411874	-6.480166	-1.295837
H	0.874671	-5.633291	-1.461509
H	1.803717	-6.097974	-3.705918
H	3.322173	-5.315054	-3.272990
C	3.834530	-0.936739	-0.332790
C	4.933281	-2.004952	-0.183773
C	4.079259	-0.159917	-1.635508
H	3.947651	-0.223215	0.501304
C	6.326012	-1.367851	-0.156360
H	4.881368	-2.690723	-1.039289
H	4.790838	-2.612814	0.714029
C	5.471224	0.485265	-1.634550
H	4.017288	-0.842771	-2.488866
H	3.300139	0.590931	-1.788639
C	6.577514	-0.550272	-1.423406
H	7.089689	-2.147500	-0.047345
H	6.409222	-0.715415	0.724749
H	5.635012	1.017612	-2.578982
H	5.523849	1.235414	-0.832017
H	7.555125	-0.056250	-1.375025
H	6.605703	-1.228771	-2.287867
C	1.980216	2.574010	-0.241583
C	2.113091	2.955418	-1.728373
C	2.519762	3.697606	0.659157

H	2.612116	1.692990	-0.065472
C	3.514306	3.437954	-2.115460
H	1.420007	3.770472	-1.952332
H	1.815317	2.110647	-2.361572
C	3.938728	4.115374	0.262227
H	1.866033	4.577411	0.603557
H	2.524076	3.372118	1.704778
C	3.999512	4.560201	-1.198617
H	3.501586	3.772714	-3.159992
H	4.225697	2.610310	-2.060769
H	4.283368	4.918142	0.925245
H	4.622573	3.266893	0.411660
H	5.021168	4.854318	-1.467210
H	3.366244	5.449365	-1.332931
C	-0.959354	3.102450	-0.718688
C	-0.749731	4.613079	-0.491481
C	-1.197706	2.799948	-2.209255
H	-1.896330	2.844458	-0.198805
C	-1.892496	5.443771	-1.085310
H	0.187898	4.940212	-0.955520
H	-0.664771	4.834712	0.576199
C	-2.321673	3.663405	-2.793739
H	-0.288033	2.980320	-2.789262
H	-1.434333	1.741894	-2.342914
C	-2.071400	5.154692	-2.574985
H	-1.696498	6.509904	-0.918789
H	-2.827903	5.207694	-0.556705
H	-2.436114	3.442295	-3.861815
H	-3.273747	3.398514	-2.312935
H	-2.899980	5.744811	-2.984369
H	-1.164074	5.459142	-3.116436
C	-3.708902	0.590939	-0.911307
C	-3.924753	-0.100789	-2.267102
C	-5.058825	0.969778	-0.279997
H	-3.184588	1.531771	-1.110253
C	-4.753797	0.765476	-3.219856
H	-4.467575	-1.039566	-2.104745
H	-2.964320	-0.360206	-2.725771
C	-5.889312	1.835054	-1.235562
H	-5.626047	0.065182	-0.029382
H	-4.903841	1.514063	0.657382
C	-6.093563	1.151314	-2.589300
H	-4.917360	0.224913	-4.159843
H	-4.192670	1.673683	-3.472355

H	-6.857513	2.066816	-0.775569
H	-5.375597	2.795100	-1.389369
H	-6.660680	1.804319	-3.263312
H	-6.697034	0.243256	-2.444915
C	-3.111477	-2.105890	0.307957
C	-4.560534	-2.352640	0.751895
C	-2.800555	-2.981133	-0.921671
H	-2.466296	-2.480779	1.116729
C	-4.764401	-3.833441	1.100050
H	-5.248119	-2.077449	-0.059028
H	-4.822912	-1.735897	1.618459
C	-2.968637	-4.462690	-0.571748
H	-3.488572	-2.739144	-1.738948
H	-1.789969	-2.788554	-1.290977
C	-4.385767	-4.750223	-0.067020
H	-5.806326	-4.007866	1.394692
H	-4.142786	-4.081511	1.972670
H	-2.746613	-5.081532	-1.449797
H	-2.236924	-4.735262	0.202832
H	-4.482012	-5.801130	0.231539
H	-5.095787	-4.590057	-0.891407

A6

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.104119	-0.541722	-0.262838
N	0.274661	-1.219280	1.949564
C	2.889179	0.168984	1.702994
H	3.885205	-0.119700	2.052570
H	2.883582	1.263434	1.698774
C	-2.279269	-2.421055	1.262121
C	0.119128	-0.424361	-2.018318
O	0.135395	-0.501182	-3.185395
P	-2.242021	-1.324897	-0.215801
P	2.535999	-0.424193	-0.010626
Si	-1.280947	-1.670724	2.678283
Si	1.544979	-0.422608	2.894863
C	-1.055244	-3.008001	3.982293
H	-0.600827	-2.621494	4.902274
H	-2.022525	-3.449360	4.255677
H	-0.415998	-3.807592	3.592019

C	2.315187	-1.652819	4.093500
H	3.225189	-1.244181	4.551172
H	1.631120	-1.923603	4.905562
H	2.586812	-2.580690	3.575092
H	-3.288705	-2.722938	1.559500
H	-1.736634	-3.338726	1.005879
P	-0.378652	1.856834	0.165146
C	-1.297595	2.247283	1.736294
H	-1.267126	3.326405	1.912017
H	-2.355044	2.039828	1.529361
Si	-1.002429	1.421024	3.409332
C	-1.669758	2.647891	4.680187
H	-1.103083	3.587732	4.672524
H	-2.720468	2.892435	4.477967
H	-1.615624	2.239602	5.697027
C	-2.032913	-0.151079	3.496923
H	-3.022607	0.084518	3.088512
H	-2.198861	-0.395723	4.555695
C	0.796485	1.041638	3.810643
H	1.409906	1.938067	3.649809
H	0.842959	0.837279	4.890371
C	0.540424	-3.748603	-0.025049
O	0.395382	-2.649526	-0.622127
O	0.758021	-3.936242	1.190984
H	0.474852	-4.646454	-0.676875
H	0.639013	-2.145673	1.652838
C	3.316035	-2.125732	0.010564
C	3.455224	-2.686742	-1.415228
C	4.604891	-2.369199	0.816865
H	2.549599	-2.718555	0.516548
C	3.804828	-4.177960	-1.394654
H	4.256614	-2.151232	-1.942624
H	2.526565	-2.524248	-1.971350
C	4.939786	-3.867425	0.833241
H	5.452305	-1.818882	0.394710
H	4.486168	-2.030394	1.851466
C	5.073715	-4.437495	-0.580560
H	3.925616	-4.545885	-2.420837
H	2.972367	-4.739858	-0.950669
H	5.865639	-4.031814	1.398521
H	4.140760	-4.404635	1.363193
H	5.286474	-5.512455	-0.536322
H	5.930550	-3.963571	-1.082037
C	3.640099	0.674892	-1.048423

C	5.151977	0.550742	-0.807477
C	3.327053	0.620199	-2.552685
H	3.350373	1.674786	-0.704939
C	5.924522	1.634845	-1.567457
H	5.500382	-0.428676	-1.156973
H	5.378692	0.609835	0.263657
C	4.116682	1.681462	-3.327226
H	3.570052	-0.370958	-2.953169
H	2.257325	0.764856	-2.719596
C	5.620883	1.580257	-3.066123
H	7.000448	1.514515	-1.392125
H	5.648700	2.623840	-1.175046
H	3.909219	1.582400	-4.399423
H	3.767090	2.679445	-3.029039
H	6.152861	2.382198	-3.592219
H	5.995962	0.630180	-3.473547
C	-1.587116	2.726562	-1.006382
C	-1.858009	4.218220	-0.723511
C	-1.331848	2.476165	-2.501332
H	-2.518837	2.200857	-0.770669
C	-2.958255	4.786598	-1.627784
H	-0.948384	4.806855	-0.883275
H	-2.144603	4.364655	0.322911
C	-2.434552	3.075094	-3.382179
H	-0.368941	2.898833	-2.808890
H	-1.271048	1.403375	-2.685442
C	-2.639275	4.563559	-3.105366
H	-3.087311	5.855335	-1.417415
H	-3.914802	4.300325	-1.391859
H	-2.187800	2.907508	-4.437252
H	-3.380736	2.547656	-3.193315
H	-3.442915	4.963767	-3.734951
H	-1.724104	5.114132	-3.368056
C	1.097501	3.042077	0.295272
C	1.565687	3.565196	-1.075376
C	0.998249	4.192258	1.313491
H	1.894599	2.390086	0.659746
C	2.858924	4.382209	-0.975196
H	0.798216	4.210861	-1.512464
H	1.698364	2.729936	-1.771297
C	2.306380	4.986409	1.393727
H	0.181817	4.874656	1.047223
H	0.770185	3.797477	2.308903
C	2.723125	5.527526	0.027291

H	3.125070	4.767379	-1.966823
H	3.686826	3.733907	-0.658060
H	2.196023	5.803359	2.116928
H	3.101730	4.330185	1.777438
H	3.667692	6.078456	0.105654
H	1.965610	6.240405	-0.328926
C	-2.903244	-2.360186	-1.642166
C	-1.904596	-3.363922	-2.239228
C	-4.222590	-3.093351	-1.341670
H	-3.096160	-1.608371	-2.421805
C	-2.466824	-4.019476	-3.504365
H	-1.700250	-4.148116	-1.498053
H	-0.950399	-2.884011	-2.448899
C	-4.795507	-3.768391	-2.593836
H	-4.039365	-3.853489	-0.569091
H	-4.974515	-2.412158	-0.940089
C	-3.792171	-4.730262	-3.229850
H	-1.730904	-4.727018	-3.905482
H	-2.616515	-3.249616	-4.275409
H	-5.722971	-4.294920	-2.336955
H	-5.065452	-2.991960	-3.324468
H	-4.204175	-5.155833	-4.153023
H	-3.614127	-5.570600	-2.543333
C	-3.689513	-0.153553	0.107054
C	-4.299196	0.397846	-1.194603
C	-4.816878	-0.589226	1.063299
H	-3.196682	0.688899	0.601828
C	-5.245088	1.568115	-0.909822
H	-4.869372	-0.391079	-1.700332
H	-3.512770	0.703029	-1.893862
C	-5.763831	0.582463	1.349409
H	-5.395052	-1.415339	0.635755
H	-4.408832	-0.959968	2.007113
C	-6.354353	1.159668	0.061193
H	-5.673072	1.941724	-1.848001
H	-4.676699	2.399246	-0.469311
H	-6.563663	0.255364	2.024269
H	-5.209734	1.373439	1.877469
H	-6.996669	2.018590	0.288699
H	-6.992523	0.401985	-0.415202

A7

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.089197	-0.405858	-0.277935
N	0.351680	-1.198654	1.885138
C	2.985804	0.115611	1.606803
H	3.964673	-0.284566	1.887634
H	3.081451	1.206172	1.651219
C	-2.185380	-2.354048	1.326703
C	0.131308	-0.077219	-2.007407
O	0.243406	0.054442	-3.163137
P	-2.191854	-1.267948	-0.158633
P	2.521002	-0.344195	-0.114757
Si	-1.164182	-1.642248	2.718857
Si	1.652014	-0.437064	2.825468
C	-0.882410	-2.982351	4.006825
H	-0.449257	-2.589125	4.934155
H	-1.837171	-3.457603	4.267971
H	-0.210806	-3.749910	3.608119
C	2.410285	-1.692751	4.000180
H	3.381683	-1.347876	4.377003
H	1.771713	-1.890731	4.868188
H	2.556250	-2.647151	3.479602
H	-3.180056	-2.688527	1.634006
H	-1.622159	-3.247353	1.011116
P	-0.420001	1.929716	0.261835
C	-1.288035	2.256855	1.865198
H	-1.295352	3.335109	2.050470
H	-2.340635	1.997042	1.693045
Si	-0.873261	1.418014	3.505662
C	-1.438943	2.617438	4.847606
H	-0.868072	3.554377	4.822394
H	-2.500104	2.870985	4.730559
H	-1.312779	2.181536	5.846554
C	-1.906009	-0.148313	3.587715
H	-2.898726	0.085206	3.180524
H	-2.066333	-0.423647	4.638957
C	0.954487	1.042819	3.758824
H	1.544209	1.941648	3.533123
H	1.097549	0.858283	4.833745
H	0.115763	-2.234930	-0.406256
H	0.603675	-1.945881	-0.950001
C	0.684762	-4.716601	0.831483
O	-0.167454	-4.504909	-0.051896

O	1.201382	-3.889186	1.634913
H	1.049788	-5.768052	0.935621
H	0.710516	-2.152057	1.640210
C	1.076510	3.077497	0.385157
C	1.529046	3.595771	-0.992325
C	1.000384	4.227097	1.406126
H	1.864816	2.406297	0.741407
C	2.825924	4.410064	-0.912299
H	0.755718	4.243882	-1.416503
H	1.646643	2.758991	-1.689935
C	2.317690	5.006554	1.470105
H	0.190121	4.918458	1.147658
H	0.775664	3.835100	2.403086
C	2.713490	5.550886	0.098595
H	3.071567	4.800763	-1.906783
H	3.660378	3.760245	-0.615705
H	2.227603	5.820742	2.198969
H	3.112943	4.340466	1.836794
H	3.662311	6.096158	0.162024
H	1.953855	6.269500	-0.240791
C	-1.675822	2.837813	-0.833313
C	-1.898439	4.326939	-0.500824
C	-1.516355	2.632225	-2.347714
H	-2.604096	2.321074	-0.556959
C	-3.060293	4.925073	-1.301108
H	-0.995401	4.904086	-0.729443
H	-2.095457	4.461668	0.566741
C	-2.657968	3.277438	-3.143439
H	-0.561193	3.039241	-2.698758
H	-1.500488	1.565590	-2.568884
C	-2.841631	4.754972	-2.803440
H	-3.173627	5.985251	-1.044224
H	-3.997512	4.427267	-1.014059
H	-2.467376	3.146699	-4.215081
H	-3.595525	2.747326	-2.925093
H	-3.685625	5.174367	-3.363590
H	-1.946359	5.317276	-3.106229
C	-3.701731	-0.180645	0.070823
C	-4.262672	0.316688	-1.270713
C	-4.841838	-0.719904	0.950357
H	-3.297297	0.693133	0.596928
C	-5.335075	1.389765	-1.066389
H	-4.716019	-0.527008	-1.804306
H	-3.458264	0.692975	-1.911330

C	-5.921796	0.350212	1.152632
H	-5.288918	-1.608705	0.488067
H	-4.461605	-1.029768	1.928568
C	-6.467485	0.870923	-0.178484
H	-5.727372	1.715331	-2.037395
H	-4.882997	2.274986	-0.595981
H	-6.734515	-0.056441	1.765943
H	-5.489981	1.190095	1.717565
H	-7.209360	1.659053	-0.004345
H	-6.987356	0.053928	-0.699044
C	-2.576075	-2.547552	-1.469147
C	-3.882842	-3.332531	-1.267455
C	-2.453984	-2.084136	-2.928449
H	-1.750455	-3.251671	-1.287575
C	-3.945160	-4.533641	-2.218766
H	-4.745452	-2.680607	-1.462461
H	-3.970167	-3.682579	-0.233623
C	-2.513990	-3.285469	-3.879445
H	-3.263694	-1.388783	-3.182320
H	-1.516523	-1.549280	-3.084467
C	-3.794334	-4.098862	-3.678358
H	-4.891708	-5.069855	-2.076957
H	-3.138591	-5.232605	-1.959393
H	-2.439538	-2.939359	-4.917583
H	-1.642688	-3.928900	-3.693743
H	-3.797976	-4.974261	-4.338855
H	-4.660744	-3.483323	-3.962677
C	3.680610	0.737005	-1.105404
C	5.177342	0.500338	-0.847649
C	3.407445	0.784966	-2.617322
H	3.442726	1.732290	-0.708808
C	6.026568	1.588411	-1.514180
H	5.466136	-0.472793	-1.263571
H	5.390012	0.465291	0.226615
C	4.267937	1.852742	-3.302799
H	3.622444	-0.190164	-3.069367
H	2.353556	0.987739	-2.811875
C	5.758053	1.654980	-3.019191
H	7.089630	1.397795	-1.324322
H	5.792992	2.561280	-1.057911
H	4.079778	1.835024	-4.382849
H	3.961710	2.845357	-2.945325
H	6.342865	2.462373	-3.475852
H	6.094163	0.717336	-3.484482

C	3.109384	-2.113725	-0.263716
C	3.183370	-2.567917	-1.731633
C	4.365774	-2.560265	0.500953
H	2.289737	-2.669149	0.204445
C	3.320581	-4.090802	-1.820314
H	4.054297	-2.104961	-2.215356
H	2.298069	-2.238676	-2.290696
C	4.505392	-4.086221	0.413739
H	5.267825	-2.082661	0.100368
H	4.292174	-2.281592	1.557234
C	4.543255	-4.574983	-1.036425
H	3.397887	-4.395177	-2.871261
H	2.410090	-4.554017	-1.418093
H	5.410814	-4.404875	0.944929
H	3.647890	-4.535731	0.929868
H	4.603090	-5.669585	-1.064560
H	5.454228	-4.194933	-1.522593

A8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.002212	-0.496383	-0.145499
N	0.076223	-1.086122	2.118443
C	2.850959	-0.247217	1.649747
H	3.730102	-0.788363	2.018382
H	3.168281	0.793331	1.532982
C	-2.614548	-1.862469	1.484354
C	-0.003819	-0.555696	-1.883331
O	-0.014996	-0.740993	-3.045633
P	-2.392573	-0.856693	-0.054124
P	2.274430	-0.860912	-0.009400
Si	-1.526127	-1.207269	2.864948
Si	1.448550	-0.318601	2.920896
C	-1.538875	-2.455378	4.275014
H	-1.023600	-2.074697	5.164905
H	-2.569864	-2.691073	4.570123
H	-1.048053	-3.388061	3.977134
C	2.038389	-1.366923	4.370502
H	2.957490	-0.957557	4.809395
H	1.288218	-1.422218	5.168174
H	2.250736	-2.393575	4.047537

H	-3.660499	-1.970806	1.789543
H	-2.244797	-2.872664	1.280544
P	0.100518	1.915064	0.051599
C	-1.147229	2.446521	1.310460
H	-1.305135	3.530229	1.303503
H	-2.093855	1.998252	1.004206
Si	-0.879781	1.905297	3.113134
C	-1.372934	3.364957	4.207812
H	-0.735039	4.244503	4.059455
H	-2.406908	3.669419	4.000591
H	-1.316737	3.094572	5.269671
C	-2.024935	0.474095	3.539622
H	-3.054828	0.722243	3.251766
H	-2.035927	0.392413	4.636524
C	0.877133	1.363678	3.559160
H	1.602559	2.146807	3.309506
H	0.887880	1.302264	4.658384
H	-0.456125	-3.348296	-0.020732
H	-0.209600	-2.114601	-0.240307
C	-0.176621	-4.783971	1.241343
O	-0.681891	-4.355870	0.112877
O	0.436463	-4.118286	2.058143
H	-0.372044	-5.856115	1.391442
H	0.334485	-2.052634	1.885290
C	1.557750	3.039589	0.574887
C	2.495232	3.514881	-0.548060
C	1.209840	4.279465	1.422198
H	2.152018	2.382403	1.218171
C	3.785114	4.116026	0.018964
H	1.984317	4.290674	-1.131882
H	2.741459	2.712478	-1.243106
C	2.471582	4.933221	2.000296
H	0.664293	5.005962	0.803978
H	0.553219	4.027834	2.254964
C	3.477908	5.314855	0.915340
H	4.448342	4.414690	-0.801583
H	4.322350	3.349122	0.595762
H	2.191648	5.815072	2.589442
H	2.943765	4.225987	2.698545
H	4.396510	5.708371	1.366369
H	3.055784	6.121286	0.299022
C	-0.556463	2.652810	-1.548438
C	-1.188299	4.049823	-1.494541
C	0.386952	2.557871	-2.763004

H	-1.357146	1.935769	-1.765517
C	-1.954974	4.339701	-2.792445
H	-0.404841	4.807731	-1.349797
H	-1.878406	4.140045	-0.648626
C	-0.397670	2.798497	-4.056271
H	1.166873	3.320918	-2.701435
H	0.884510	1.585713	-2.797113
C	-1.072408	4.173306	-4.032433
H	-2.381150	5.349865	-2.759154
H	-2.801451	3.640603	-2.859162
H	0.275173	2.720932	-4.918793
H	-1.156866	2.013415	-4.174666
H	-1.665645	4.325635	-4.942174
H	-0.295661	4.951952	-4.027690
C	-3.871968	0.302430	0.178994
C	-3.940118	1.510352	-0.769656
C	-5.270957	-0.335289	0.256684
H	-3.666545	0.706510	1.181940
C	-4.956283	2.543582	-0.271524
H	-4.222235	1.182632	-1.777080
H	-2.965125	1.984693	-0.864012
C	-6.300087	0.677521	0.774671
H	-5.575245	-0.669249	-0.743282
H	-5.278155	-1.221731	0.898435
C	-6.347423	1.928330	-0.106156
H	-4.995275	3.391715	-0.966042
H	-4.612557	2.941676	0.695166
H	-7.291010	0.210225	0.823375
H	-6.034823	0.963517	1.803175
H	-7.045142	2.664125	0.311614
H	-6.735196	1.652248	-1.097146
C	-2.872676	-2.008238	-1.455716
C	-3.861598	-3.143552	-1.151104
C	-3.308937	-1.248471	-2.718667
H	-1.910009	-2.478856	-1.689514
C	-3.961782	-4.097595	-2.348653
H	-4.856018	-2.736567	-0.932024
H	-3.543290	-3.706645	-0.268317
C	-3.390064	-2.199588	-3.916636
H	-4.299705	-0.802641	-2.559605
H	-2.614459	-0.430562	-2.936425
C	-4.349294	-3.358394	-3.632353
H	-4.689041	-4.890032	-2.132697
H	-2.989375	-4.588689	-2.493055

H	-3.710286	-1.650360	-4.810445
H	-2.386511	-2.593639	-4.126088
H	-4.368563	-4.055427	-4.478858
H	-5.369432	-2.960772	-3.524873
C	3.375299	0.020680	-1.242763
C	4.780420	0.448412	-0.789794
C	3.456205	-0.683142	-2.607877
H	2.792656	0.931843	-1.414994
C	5.451957	1.342202	-1.840973
H	5.403011	-0.438669	-0.619037
H	4.738014	0.987202	0.162611
C	4.089177	0.239123	-3.654315
H	4.076519	-1.584002	-2.521529
H	2.464030	-1.001417	-2.939495
C	5.488325	0.681518	-3.220681
H	6.466955	1.599105	-1.513659
H	4.897705	2.287951	-1.914661
H	4.133959	-0.272842	-4.622882
H	3.448778	1.122456	-3.792032
H	5.919320	1.370054	-3.957545
H	6.147069	-0.198316	-3.185221
C	2.843618	-2.644576	0.049403
C	2.341327	-3.499015	-1.129579
C	4.348833	-2.888489	0.245671
H	2.326462	-3.016317	0.947438
C	2.615351	-4.986395	-0.882051
H	2.858024	-3.205735	-2.049811
H	1.277303	-3.321904	-1.301645
C	4.634428	-4.373619	0.499843
H	4.887788	-2.576546	-0.658520
H	4.750134	-2.292473	1.072740
C	4.104459	-5.246238	-0.640587
H	2.256374	-5.576488	-1.733747
H	2.051453	-5.323841	-0.002147
H	5.712402	-4.529694	0.629902
H	4.153077	-4.674560	1.441384
H	4.278065	-6.306736	-0.421391
H	4.663797	-5.016453	-1.559227

TSA7-8

Coordinates (Angstroms)		
X	Y	Z

Mn	0.096555	-0.438874	-0.252883
N	0.341313	-1.148683	1.967038
C	2.870333	0.338583	1.691402
H	3.862523	0.007143	2.013901
H	2.906889	1.433822	1.697525
C	-2.069477	-2.531725	1.217916
C	0.110673	-0.348067	-1.998906
O	0.134305	-0.429430	-3.169139
P	-2.083389	-1.405970	-0.241396
P	2.466215	-0.203749	-0.033569
Si	-1.195511	-1.699646	2.667907
Si	1.534427	-0.229415	2.905499
C	-0.927545	-2.986343	4.014803
H	-0.538091	-2.536921	4.936270
H	-1.875172	-3.480102	4.267196
H	-0.215340	-3.751406	3.688718
C	2.331289	-1.342149	4.195254
H	3.224053	-0.872159	4.627003
H	1.646891	-1.571133	5.020444
H	2.627701	-2.295274	3.742266
H	-3.051158	-2.943134	1.473748
H	-1.429291	-3.382328	0.945957
P	-0.539650	1.907707	0.171496
C	-1.543462	2.220087	1.704475
H	-1.618766	3.297279	1.877571
H	-2.569286	1.906925	1.475354
Si	-1.168721	1.420858	3.371695
C	-1.916827	2.572813	4.666416
H	-1.407695	3.544886	4.678255
H	-2.980548	2.757183	4.469353
H	-1.835547	2.147458	5.674484
C	-2.075008	-0.228529	3.441138
H	-3.064210	-0.065798	2.996360
H	-2.259805	-0.482041	4.494496
C	0.668959	1.220931	3.734499
H	1.188960	2.158660	3.498526
H	0.770489	1.091453	4.821935
H	0.569111	-3.023350	-0.240101
H	0.482773	-2.079298	-0.471985
C	1.191485	-4.588118	1.074548
O	0.672676	-4.253775	-0.051286
O	1.551633	-3.832650	1.979630
H	1.310308	-5.680352	1.195074

H	0.823617	-2.030845	1.735669
C	3.511795	0.971056	-1.048922
C	5.032240	0.866801	-0.857143
C	3.159003	0.992027	-2.545353
H	3.210945	1.943031	-0.639605
C	5.760021	2.009256	-1.574282
H	5.389123	-0.082827	-1.273796
H	5.289961	0.867403	0.208557
C	3.907975	2.108520	-3.282439
H	3.409885	0.029869	-3.006282
H	2.082178	1.122051	-2.677570
C	5.420445	2.024873	-3.065783
H	6.842357	1.907615	-1.429533
H	5.468304	2.968847	-1.124049
H	3.673385	2.061917	-4.352717
H	3.548828	3.082404	-2.922452
H	5.922586	2.863509	-3.563109
H	5.803355	1.104446	-3.529764
C	3.270117	-1.892557	-0.140267
C	3.343811	-2.370571	-1.599593
C	4.591009	-2.163935	0.598704
H	2.529281	-2.517526	0.361939
C	3.729180	-3.850085	-1.687539
H	4.096329	-1.781724	-2.140805
H	2.380964	-2.203909	-2.096139
C	4.953489	-3.652547	0.509173
H	5.411769	-1.570217	0.182407
H	4.500740	-1.892897	1.656037
C	5.035245	-4.130338	-0.942116
H	3.821139	-4.143954	-2.740431
H	2.919914	-4.452859	-1.257451
H	5.906110	-3.830753	1.023360
H	4.188889	-4.233139	1.042724
H	5.270740	-5.201135	-0.976349
H	5.861424	-3.608178	-1.447575
C	-2.545878	-2.493475	-1.702859
C	-1.405110	-3.393614	-2.200940
C	-3.801414	-3.355856	-1.485130
H	-2.756352	-1.768909	-2.503245
C	-1.796350	-4.131460	-3.485218
H	-1.156152	-4.129682	-1.429335
H	-0.501227	-2.811087	-2.378630
C	-4.202749	-4.105672	-2.761279
H	-3.599522	-4.083432	-0.686476

H	-4.648344	-2.751523	-1.153688
C	-3.059613	-4.970551	-3.291596
H	-0.962587	-4.766782	-3.807455
H	-1.963871	-3.397137	-4.286631
H	-5.090904	-4.718814	-2.564118
H	-4.488909	-3.372119	-3.529096
H	-3.350613	-5.455252	-4.231466
H	-2.850988	-5.773217	-2.569673
C	-3.650790	-0.388611	0.011703
C	-4.237619	0.111957	-1.320389
C	-4.774369	-0.936383	0.910537
H	-3.264055	0.493386	0.531891
C	-5.306085	1.183237	-1.086195
H	-4.700490	-0.723604	-1.859475
H	-3.444789	0.496443	-1.972429
C	-5.844483	0.137342	1.144290
H	-5.245822	-1.815108	0.456643
H	-4.377793	-1.265619	1.875532
C	-6.418287	0.660927	-0.174404
H	-5.719878	1.517137	-2.045506
H	-4.844292	2.064030	-0.617797
H	-6.644906	-0.267256	1.775138
H	-5.397422	0.975168	1.700611
H	-7.156475	1.448510	0.017144
H	-6.949314	-0.155487	-0.684743
C	-1.752726	2.710434	-1.041319
C	-2.153191	4.170384	-0.752240
C	-1.417349	2.523598	-2.529014
H	-2.648696	2.106314	-0.855431
C	-3.283805	4.645952	-1.673051
H	-1.293404	4.834037	-0.896845
H	-2.469821	4.288875	0.288655
C	-2.556259	3.010911	-3.432475
H	-0.503078	3.068950	-2.790546
H	-1.222265	1.471923	-2.734979
C	-2.922399	4.466610	-3.147133
H	-3.510151	5.697588	-1.458376
H	-4.197494	4.075744	-1.454968
H	-2.269469	2.882925	-4.483017
H	-3.443647	2.382497	-3.269190
H	-3.754589	4.786043	-3.785910
H	-2.066649	5.112201	-3.393215
C	0.846396	3.186347	0.396854
C	1.348218	3.760415	-0.940546

C	0.615709	4.327224	1.404309
H	1.664904	2.584927	0.805716
C	2.598862	4.628651	-0.762099
H	0.568441	4.384260	-1.389180
H	1.542553	2.952946	-1.652851
C	1.875403	5.183435	1.576800
H	-0.210456	4.969445	1.074683
H	0.333616	3.928435	2.383105
C	2.360620	5.753245	0.244718
H	2.902697	5.040188	-1.732073
H	3.434961	4.008970	-0.409278
H	1.674955	5.990887	2.291187
H	2.672467	4.564917	2.015628
H	3.278587	6.334854	0.389611
H	1.603416	6.445116	-0.151394

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.046206	-0.277286	-0.048123
N	0.146586	-0.822970	1.952368
C	3.034757	-0.580274	1.442635
H	3.823286	-1.290611	1.710424
H	3.512227	0.403101	1.345535
C	-2.793306	-0.550152	1.997610
C	-0.204121	-0.276874	-1.793265
O	-0.317127	-0.313505	-2.963942
P	-2.349153	-0.715596	0.231190
P	2.219349	-0.935019	-0.160149
Si	-1.218417	-0.865093	3.006467
Si	1.648081	-0.479320	2.731923
C	-1.455898	-2.514731	3.903700
H	-0.625386	-2.745619	4.580716
H	-2.378230	-2.513149	4.499668
H	-1.527600	-3.340262	3.183023
C	2.077661	-1.666768	4.145354
H	3.105198	-1.497210	4.493696
H	1.418185	-1.526376	5.011037
H	1.996043	-2.716259	3.836482
H	-3.121984	0.479764	2.176013
H	-3.623185	-1.202285	2.292168

P	-0.070356	2.003739	0.193493
C	-0.820555	2.497556	1.814328
H	-0.903145	3.589512	1.855500
H	-1.854612	2.132154	1.781607
Si	-0.109117	1.953604	3.510668
C	-0.196507	3.501044	4.596176
H	0.474923	4.289772	4.232326
H	-1.211414	3.917603	4.628899
H	0.096959	3.270172	5.627957
C	-1.141644	0.564766	4.255624
H	-2.155245	0.890321	4.525573
H	-0.649424	0.259892	5.190993
C	1.642104	1.271991	3.489929
H	2.346623	1.949825	2.993952
H	1.969576	1.211378	4.538802
C	-2.597411	-2.558693	-0.006020
C	-4.040382	-3.074135	0.110438
C	-1.934268	-3.121298	-1.272539
H	-2.033666	-2.963134	0.850047
C	-4.090933	-4.604685	0.109068
H	-4.622673	-2.711043	-0.746253
H	-4.523710	-2.686569	1.013588
C	-2.011071	-4.652026	-1.302924
H	-2.421117	-2.710766	-2.166691
H	-0.887071	-2.804114	-1.317926
C	-3.443722	-5.167019	-1.156953
H	-5.131288	-4.941542	0.191442
H	-3.561995	-4.988175	0.993513
H	-1.561782	-5.027429	-2.229775
H	-1.409090	-5.051562	-0.473675
H	-3.452378	-6.263371	-1.138943
H	-4.033519	-4.857619	-2.031872
C	-3.724732	0.202273	-0.646155
C	-3.742832	-0.044732	-2.162379
C	-5.142603	0.097183	-0.058278
H	-3.420691	1.248433	-0.492254
C	-4.715843	0.905385	-2.869089
H	-4.050534	-1.081691	-2.355826
H	-2.740073	0.069774	-2.584965
C	-6.090453	1.075804	-0.761657
H	-5.536672	-0.916313	-0.182141
H	-5.129062	0.302720	1.017235
C	-6.121936	0.827558	-2.271470
H	-4.741160	0.680627	-3.942121

H	-4.340689	1.934142	-2.771619
H	-7.097698	0.984182	-0.337765
H	-5.758557	2.106857	-0.569605
H	-6.784810	1.549305	-2.763417
H	-6.542314	-0.170474	-2.461885
C	-1.162672	2.911460	-1.041224
C	-1.877336	4.193585	-0.588813
C	-0.509556	3.146664	-2.412419
H	-1.938110	2.155116	-1.212334
C	-2.918629	4.630969	-1.628219
H	-1.141659	4.996618	-0.439055
H	-2.383117	4.045146	0.370288
C	-1.564036	3.527516	-3.454831
H	0.205136	3.974561	-2.336192
H	0.045710	2.263406	-2.740679
C	-2.318756	4.788604	-3.027367
H	-3.392009	5.567370	-1.309085
H	-3.714362	3.872866	-1.662850
H	-1.085753	3.683307	-4.429240
H	-2.269119	2.693683	-3.578194
H	-3.106389	5.029873	-3.751334
H	-1.619452	5.637136	-3.025254
C	1.584052	2.880337	0.285555
C	2.402730	2.877301	-1.013643
C	1.625820	4.287367	0.900805
H	2.113480	2.211072	0.976883
C	3.862045	3.243033	-0.726283
H	2.006268	3.623317	-1.708625
H	2.320017	1.911706	-1.517430
C	3.075345	4.717600	1.167927
H	1.147411	5.001655	0.215641
H	1.070854	4.328913	1.842738
C	3.949173	4.631679	-0.086209
H	4.448544	3.212752	-1.652887
H	4.304752	2.501369	-0.044700
H	3.092964	5.735943	1.574608
H	3.495962	4.062243	1.944631
H	4.989403	4.876659	0.158940
H	3.609627	5.380826	-0.815389
C	2.032052	-2.803443	-0.210946
C	1.958252	-3.330707	-1.653330
C	3.035679	-3.618518	0.619694
H	1.044059	-2.957938	0.249617
C	1.640645	-4.827507	-1.689636

H	2.923120	-3.174084	-2.150095
H	1.213451	-2.768330	-2.228403
C	2.714959	-5.116239	0.564995
H	4.055176	-3.452707	0.248289
H	3.017961	-3.289097	1.663365
C	2.655902	-5.629830	-0.874537
H	1.616490	-5.176588	-2.728963
H	0.640161	-4.995171	-1.274246
H	3.461033	-5.675248	1.142584
H	1.743244	-5.289648	1.050108
H	2.400513	-6.696206	-0.889037
H	3.649867	-5.533842	-1.335688
C	3.563968	-0.455735	-1.365146
C	4.887597	-1.228538	-1.249759
C	3.133722	-0.327255	-2.834676
H	3.783588	0.562860	-1.018332
C	5.983579	-0.537718	-2.069976
H	4.758140	-2.253884	-1.618922
H	5.199453	-1.303720	-0.201847
C	4.230167	0.361079	-3.654773
H	2.936516	-1.317054	-3.262194
H	2.197601	0.232310	-2.914590
C	5.567767	-0.374083	-3.534323
H	6.918753	-1.106476	-2.000525
H	6.182138	0.452900	-1.636114
H	3.924755	0.425644	-4.705937
H	4.350337	1.393743	-3.295645
H	6.347247	0.158387	-4.092559
H	5.472126	-1.368649	-3.993598

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.011833	-0.352170	-0.183751
N	0.428202	-0.891147	2.110234
C	3.092927	0.098205	1.322131
H	4.090759	-0.293507	1.549436
H	3.211721	1.176088	1.156539
C	-2.537605	-1.151725	1.970738
C	-0.208719	-0.252718	-1.903239
O	-0.375328	-0.230675	-3.070368

P	-2.130341	-1.160958	0.161784
P	2.363158	-0.578631	-0.238536
Si	-1.025473	-1.161507	3.087600
Si	1.898815	-0.137490	2.758735
C	-0.891650	-2.833348	3.940478
H	0.012459	-2.907097	4.556382
H	-1.756389	-3.027084	4.587157
H	-0.852257	-3.639643	3.195990
C	2.670147	-1.265820	4.056670
H	3.644443	-0.885802	4.389633
H	2.033585	-1.354203	4.946156
H	2.825634	-2.277448	3.660274
H	-3.068649	-0.212583	2.165252
H	-3.232583	-1.953958	2.244941
P	-0.422013	1.895289	0.221009
C	-1.229032	2.246161	1.864154
H	-1.509409	3.304114	1.918007
H	-2.180149	1.698828	1.849947
Si	-0.420834	1.850793	3.541036
C	-0.777215	3.327103	4.659054
H	-0.293581	4.237242	4.281497
H	-1.853665	3.527907	4.727681
H	-0.406058	3.154456	5.676736
C	-1.164144	0.280654	4.280326
H	-2.220535	0.428173	4.541203
H	-0.635666	0.068018	5.220420
C	1.431698	1.512123	3.535548
H	1.995603	2.333517	3.078529
H	1.734526	1.489952	4.593045
H	0.196988	-1.934599	-0.284816
H	0.644427	-1.762338	1.619248
C	-2.250025	-3.001070	-0.217692
C	-3.578333	-3.722467	0.055854
C	-1.747864	-3.389693	-1.618878
H	-1.506621	-3.393562	0.495390
C	-3.394200	-5.243509	-0.027012
H	-4.318714	-3.421325	-0.696538
H	-3.993677	-3.455472	1.034034
C	-1.556318	-4.905810	-1.724737
H	-2.471185	-3.068384	-2.378897
H	-0.807067	-2.878122	-1.828457
C	-2.842904	-5.664916	-1.391900
H	-4.349055	-5.746787	0.169052
H	-2.697818	-5.564037	0.761510

H	-1.208558	-5.167720	-2.731461
H	-0.763687	-5.212598	-1.026743
H	-2.668783	-6.747625	-1.414672
H	-3.596697	-5.449115	-2.162980
C	-3.692888	-0.378308	-0.538162
C	-3.793398	-0.573873	-2.060015
C	-5.050282	-0.679537	0.120819
H	-3.511050	0.689736	-0.352772
C	-4.903226	0.283215	-2.674968
H	-4.015481	-1.629373	-2.265033
H	-2.836424	-0.355452	-2.544491
C	-6.139751	0.221307	-0.474945
H	-5.331665	-1.725832	-0.037691
H	-5.002921	-0.525788	1.203982
C	-6.250203	0.039827	-1.991041
H	-4.978028	0.078679	-3.749828
H	-4.634391	1.343015	-2.576076
H	-7.103224	0.009497	0.004835
H	-5.900205	1.272000	-0.252512
H	-7.012626	0.713543	-2.400461
H	-6.584412	-0.985671	-2.204829
C	-1.691679	2.634104	-0.974553
C	-2.671825	3.679015	-0.417352
C	-1.093796	3.143425	-2.295010
H	-2.274782	1.749232	-1.249091
C	-3.759707	4.036311	-1.438659
H	-2.122324	4.586966	-0.131095
H	-3.162858	3.309946	0.488689
C	-2.197280	3.412233	-3.321939
H	-0.561396	4.086112	-2.117217
H	-0.373368	2.423620	-2.694777
C	-3.184461	4.455028	-2.793021
H	-4.398419	4.831411	-1.034388
H	-4.406765	3.160145	-1.579574
H	-1.753612	3.754076	-4.264706
H	-2.724250	2.473306	-3.541051
H	-3.995349	4.618714	-3.513149
H	-2.661248	5.416016	-2.681582
C	0.992055	3.133677	0.303495
C	1.842538	3.196846	-0.972609
C	0.728645	4.564196	0.796468
H	1.624536	2.653310	1.062526
C	3.195375	3.853136	-0.687919
H	1.336630	3.800500	-1.730753

H	1.951328	2.199511	-1.401924
C	2.058529	5.282413	1.071194
H	0.160848	5.117691	0.035570
H	0.126024	4.573020	1.710966
C	2.989647	5.271417	-0.145187
H	3.803283	3.882564	-1.600827
H	3.755420	3.254124	0.046276
H	1.868978	6.314704	1.389750
H	2.558900	4.780948	1.913004
H	3.952080	5.729452	0.112635
H	2.547988	5.890792	-0.938835
C	2.789645	-2.409432	-0.116242
C	2.597845	-3.099278	-1.475358
C	4.096169	-2.867241	0.551309
H	1.974638	-2.782537	0.519168
C	2.615824	-4.622543	-1.323397
H	3.403827	-2.800238	-2.158987
H	1.651999	-2.772420	-1.921401
C	4.102855	-4.394236	0.706497
H	4.967483	-2.569986	-0.041421
H	4.212128	-2.407056	1.539251
C	3.899353	-5.098257	-0.637538
H	2.506042	-5.100679	-2.304343
H	1.746974	-4.927672	-0.722515
H	5.044669	-4.717291	1.166550
H	3.297387	-4.690095	1.394851
H	3.877850	-6.185689	-0.496438
H	4.757510	-4.879287	-1.289448
C	3.555210	0.155407	-1.489243
C	5.011948	-0.328150	-1.449164
C	3.027082	0.152121	-2.930755
H	3.585057	1.203898	-1.167272
C	5.897075	0.546794	-2.345126
H	5.071210	-1.364822	-1.802837
H	5.397035	-0.314101	-0.422943
C	3.914370	1.010485	-3.838607
H	2.993334	-0.874949	-3.317002
H	2.000856	0.525255	-2.960108
C	5.379503	0.571568	-3.785385
H	6.931091	0.181476	-2.317852
H	5.911814	1.571019	-1.944945
H	3.540929	0.969404	-4.868703
H	3.838846	2.060097	-3.517467
H	5.999828	1.234030	-4.401279

H	5.469527	-0.436168	-4.216379

$R^1=R^2=R^3=CH_2F$

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.646901	0.977343	0.409397
N	0.014907	-0.017095	-1.375255
C	2.424101	-1.656863	-0.942555
H	3.231433	-1.695910	-1.682397
H	2.514069	-2.564120	-0.335007
C	-2.378588	1.689456	-1.049165
C	1.209045	1.843086	1.842243
O	1.569473	2.429258	2.786529
P	-1.176699	2.307214	0.170298
P	2.593640	-0.167409	0.101635
Si	-1.485678	0.373188	-2.112393
Si	0.712107	-1.532405	-1.783910
C	-1.353408	1.099928	-3.848379
H	-0.794506	0.442509	-4.524223
H	-2.343154	1.272069	-4.291615
H	-0.826087	2.061315	-3.816133
C	0.991869	-1.795687	-3.633297
H	1.518645	-2.741596	-3.816513
H	0.047411	-1.842631	-4.190271
H	1.593628	-0.984611	-4.060461
H	-3.202946	1.220302	-0.500563
H	-2.805627	2.503668	-1.646426
C	3.848340	0.815185	-0.854675
C	3.677156	-0.650922	1.518916
C	-0.749238	3.994422	-0.491761
C	-2.247454	2.895993	1.574274
P	-0.466693	-0.623092	1.611818
C	-2.036957	-1.316227	0.975368
H	-2.438188	-1.974178	1.753981
H	-2.733532	-0.472655	0.903174
Si	-2.072963	-2.280675	-0.680329
C	0.454898	-2.177583	2.077507
C	-0.936125	-0.101892	3.325378
C	-3.322030	-3.667856	-0.404464
H	-2.972571	-4.371179	0.361475

H	-4.292972	-3.274409	-0.077195
H	-3.490275	-4.236347	-1.327460
C	-2.614703	-1.154288	-2.094087
H	-3.671458	-0.866293	-2.014725
H	-2.517500	-1.725850	-3.029293
C	-0.392187	-2.964396	-1.174298
H	0.052768	-3.537942	-0.352418
H	-0.547961	-3.681901	-1.993380
H	1.236178	1.870861	-1.018773
H	1.519253	2.292868	-0.416016
F	-0.123168	3.852020	-1.722190
F	-3.055175	1.839643	1.992388
F	3.347732	1.063381	-2.125392
F	4.819638	-1.314208	1.086908
F	-0.388563	-3.251178	2.317742
F	-1.477296	-1.152928	4.057764
H	-0.065655	4.510413	0.191740
H	-1.641659	3.225320	2.424915
H	-0.045194	0.257691	3.853236
H	1.033704	-1.986345	2.989295
H	4.038417	1.773668	-0.358919
H	3.983129	0.244105	2.074144
H	1.141669	-2.473042	1.282842
H	-1.676510	0.699708	3.277091
H	-1.645999	4.606445	-0.641513
H	4.788036	0.263901	-0.956994
H	3.132153	-1.311084	2.201238
H	-2.910459	3.710383	1.262359

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.474953	0.985399	0.401111
N	-0.319012	-0.002199	-1.586083
C	1.834766	1.853479	-1.909623
H	1.242526	2.481937	-2.588302
H	2.895118	2.058352	-2.086650
C	-2.643085	-1.504082	-0.604009
C	-0.873633	2.051123	1.741593
O	-1.169548	2.778600	2.606213
P	-2.518349	-0.003191	0.431358

P	1.310309	2.259509	-0.202499
Si	-1.289149	-1.387904	-1.943635
Si	1.284328	0.063011	-2.223198
C	-2.156042	-1.307266	-3.612953
H	-1.442785	-1.159802	-4.432453
H	-2.712702	-2.231074	-3.817906
H	-2.866528	-0.472538	-3.633660
C	1.387673	-0.239768	-4.083841
H	2.407301	-0.060458	-4.449782
H	1.129837	-1.273169	-4.347393
H	0.713467	0.425764	-4.635869
H	-2.455905	-2.368250	0.042631
H	-3.648512	-1.625897	-1.024853
C	0.954545	4.088916	-0.264453
C	2.960767	2.467238	0.654752
C	-3.821561	1.091330	-0.327716
C	-3.494593	-0.464938	1.950720
P	0.548844	-0.591894	1.674796
C	0.556355	-2.314785	1.063276
H	1.089774	-2.933337	1.792427
H	-0.486619	-2.653786	1.069189
Si	1.271474	-2.649973	-0.678081
C	2.328979	-0.407226	2.184850
C	-0.165772	-0.752675	3.374944
C	2.309924	-4.214415	-0.511919
H	3.161309	-4.046031	0.159364
H	1.722414	-5.044837	-0.100927
H	2.708437	-4.538071	-1.481423
C	-0.181510	-2.924517	-1.853687
H	-0.757478	-3.810670	-1.552723
H	0.215884	-3.144635	-2.855832
C	2.345587	-1.252650	-1.370544
H	2.988404	-0.826019	-0.592847
H	3.030916	-1.694638	-2.108726
H	-1.217636	2.028567	-0.722787
H	-0.942380	1.279599	-1.251275
F	-3.501853	1.336114	-1.654630
F	-3.036068	-1.688635	2.433529
F	0.522513	-1.674390	4.155915
F	2.890436	-1.605065	2.607335
F	-0.221733	4.339954	-0.944598
F	3.847352	1.480386	0.235252
H	-3.863348	2.047367	0.204784
H	-4.559367	-0.585569	1.723140

H	0.860772	4.485127	0.754051
H	2.852176	2.400999	1.741857
H	2.385298	0.311584	3.012189
H	-0.111668	0.222936	3.873377
H	2.935198	-0.037524	1.360069
H	-1.208948	-1.067438	3.315149
H	1.762980	4.617724	-0.784187
H	-4.808369	0.613812	-0.306916
H	3.414427	3.432869	0.403368
H	-3.376115	0.286612	2.738418

A6

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.694731	0.609001	-0.640312
N	0.601916	-0.912983	1.039862
C	0.394853	1.603610	2.627836
H	1.190133	1.752478	3.367173
H	-0.465531	2.194062	2.964284
C	0.317592	-2.765056	-1.307039
C	0.921679	1.776054	-1.944300
O	1.120133	2.527325	-2.812805
P	0.804163	-1.165010	-2.063188
P	0.984575	2.167675	0.973836
Si	0.248477	-2.605942	0.584848
Si	-0.067461	-0.243150	2.545635
C	1.542212	-3.735340	1.332984
H	1.560811	-3.658247	2.426428
H	1.349562	-4.783669	1.072693
H	2.537334	-3.460090	0.968004
C	0.708463	-1.100294	4.026574
H	0.415078	-0.610991	4.963985
H	0.402705	-2.151402	4.096821
H	1.802550	-1.073366	3.959458
H	-0.678558	-3.023347	-1.684735
H	1.001045	-3.565442	-1.611888
C	2.719537	2.716485	1.385999
C	0.340307	3.898270	0.705153
C	2.517082	-1.542456	-2.705656
C	-0.053188	-1.254804	-3.714245
P	-1.604979	0.806603	-0.718562

C	-2.641830	-0.693292	-0.515565
H	-3.676486	-0.429542	-0.757501
H	-2.313684	-1.404933	-1.280476
Si	-2.631913	-1.544071	1.187033
C	-2.566454	1.985238	0.393068
C	-2.222929	1.482898	-2.326780
C	-4.402857	-2.049146	1.567958
H	-5.053247	-1.169124	1.637345
H	-4.806716	-2.700858	0.783225
H	-4.469075	-2.592668	2.518320
C	-1.492999	-3.042415	1.138914
H	-1.893044	-3.825501	0.481060
H	-1.460780	-3.472785	2.150485
C	-1.937539	-0.476081	2.576133
H	-2.473787	0.476117	2.640845
H	-2.172751	-1.009925	3.509153
C	3.618690	-0.208242	0.129835
O	2.817898	0.451017	-0.602186
O	3.349892	-0.971599	1.071254
H	4.688271	-0.058150	-0.122835
H	1.647282	-0.902068	1.136107
F	-0.666178	3.923622	-0.251620
F	3.340420	1.781278	2.192738
F	-3.802099	1.466998	0.769549
F	-3.607509	1.629441	-2.319410
F	-1.433028	-1.310486	-3.525979
F	3.213413	-2.281724	-1.762589
H	3.053820	-0.608821	-2.886846
H	0.178112	-0.373729	-4.322876
H	-1.777150	2.468283	-2.498238
H	-2.749234	2.923312	-0.131776
H	3.291620	2.826018	0.460355
H	1.156525	4.523875	0.326196
H	-2.015237	2.203720	1.309577
H	-1.952934	0.810128	-3.142750
H	0.235117	-2.159029	-4.261291
H	-0.047042	4.346562	1.626760
H	2.707528	3.668072	1.932708
H	2.477958	-2.136478	-3.627044

A7

Coordinates (Angstroms)

	X	Y	Z
Mn	-0.423000	0.929831	0.377670
N	-0.942020	-0.912369	-0.806086
C	-0.139389	0.877122	-3.027528
H	-0.891997	1.029966	-3.810177
H	0.834914	1.096968	-3.478268
C	-1.611997	-1.908795	1.821708
C	-0.269213	2.451024	1.280967
O	-0.213121	3.467733	1.837941
P	-0.810607	-0.334408	2.275504
P	-0.477575	2.003529	-1.614502
Si	-1.010570	-2.449439	0.119461
Si	-0.193088	-0.927997	-2.417060
C	-2.278436	-3.621773	-0.612621
H	-1.926359	-4.090649	-1.538554
H	-2.499218	-4.428043	0.099067
H	-3.206075	-3.082244	-0.829031
C	-1.254429	-1.905206	-3.616399
H	-0.979117	-1.692499	-4.657056
H	-1.155798	-2.986303	-3.465913
H	-2.311285	-1.645616	-3.482144
H	-1.520638	-2.675171	2.598732
H	-2.673220	-1.652464	1.687269
C	-2.098435	2.745738	-2.143374
C	0.510249	3.563373	-1.869322
C	-2.024702	0.467332	3.427013
C	0.380471	-0.870131	3.610180
P	1.871390	0.659139	0.345246
C	2.587142	-0.991729	0.618043
H	3.676308	-0.900327	0.643609
H	2.260529	-1.333269	1.604083
Si	2.089874	-2.336322	-0.621167
C	2.963238	1.218688	-1.087743
C	2.684792	1.650536	1.678699
C	3.590388	-3.443404	-0.863281
H	4.420490	-2.885394	-1.313199
H	3.942080	-3.849519	0.093218
H	3.361833	-4.291503	-1.520409
C	0.667508	-3.297919	0.139881
H	0.932769	-3.552027	1.173838
H	0.557619	-4.249576	-0.398895
C	1.538994	-1.661715	-2.298566
H	2.297669	-0.964289	-2.673554

H	1.565191	-2.516193	-2.991379
H	-2.218650	0.786845	0.638783
H	-2.062038	1.393601	0.142507
C	-4.422027	-0.369780	-0.047062
O	-4.054422	-0.058007	1.109342
O	-3.715204	-0.748296	-1.014482
H	-5.518872	-0.307712	-0.250482
H	-1.969334	-0.710391	-0.928947
F	-1.334656	1.446287	4.142465
F	1.091198	-1.997311	3.205710
F	4.054865	1.427343	1.706056
F	4.004414	0.329360	-1.323555
F	1.571778	3.642917	-0.977603
F	-2.999651	1.727829	-2.371600
H	-2.435881	-0.256175	4.140557
H	1.094055	-0.083416	3.867125
H	2.514596	2.717808	1.504250
H	3.402741	2.191232	-0.862433
H	-2.487719	3.400020	-1.354997
H	-0.134885	4.429140	-1.680847
H	2.396598	1.298618	-2.017043
H	2.266825	1.382722	2.654432
H	-0.179371	-1.144770	4.510798
H	0.907656	3.633810	-2.887437
H	-1.982179	3.321836	-3.070229
H	-2.839714	0.925075	2.863374

A8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.315024	0.193916	-0.961225
N	0.639893	-0.137721	1.304673
C	0.269069	2.786537	1.263869
H	0.965703	3.466979	1.766188
H	-0.672117	3.333915	1.144487
C	1.075933	-2.809124	0.345684
C	0.459192	0.500304	-2.678361
O	0.626857	0.705185	-3.819123
P	0.481770	-2.020196	-1.196611
P	0.893220	2.280990	-0.394425
Si	0.400264	-1.834287	1.803484

Si	-0.009910	1.204041	2.275428
C	1.366028	-2.235484	3.362612
H	0.899477	-1.801602	4.255058
H	1.407461	-3.322006	3.513900
H	2.393051	-1.863862	3.292403
C	0.929110	1.360349	3.893696
H	0.635578	2.272529	4.428536
H	0.745990	0.512041	4.562596
H	2.008716	1.412518	3.709955
H	0.856777	-3.881427	0.370332
H	2.164828	-2.678753	0.361746
C	2.702599	2.621655	-0.137317
C	0.518628	3.714550	-1.501247
C	1.694235	-2.648817	-2.460435
C	-0.911576	-3.152086	-1.680242
P	-1.931457	0.404648	-0.978231
C	-3.073587	-0.554576	0.095962
H	-4.076872	-0.128086	-0.000950
H	-3.138695	-1.573668	-0.305084
Si	-2.609028	-0.702045	1.921177
C	-2.704688	2.093602	-0.775646
C	-2.632267	0.011127	-2.651007
C	-4.203962	-1.057290	2.857576
H	-4.912546	-0.224483	2.769304
H	-4.699123	-1.955193	2.466964
H	-4.016157	-1.222602	3.925729
C	-1.425028	-2.153035	2.125256
H	-1.780217	-2.982588	1.498261
H	-1.508173	-2.512458	3.160897
C	-1.837633	0.881926	2.604587
H	-2.442836	1.738408	2.276944
H	-1.963432	0.842732	3.697046
H	3.319631	-0.239357	-0.837629
H	1.882685	-0.079297	-0.980574
C	4.506607	-0.533874	0.607767
O	4.298497	-0.170636	-0.638370
O	3.668749	-0.934292	1.389328
H	5.569940	-0.440190	0.869913
H	1.658608	-0.034538	1.224086
F	2.984704	-2.289143	-2.104115
F	-0.566480	-4.498884	-1.583053
F	-4.018534	0.077829	-2.684125
F	-4.079432	2.070143	-0.585758
F	3.109871	1.934344	1.007840

F	0.918196	4.926122	-0.946942
H	1.470815	-2.214589	-3.440771
H	-1.204653	-2.959328	-2.719271
H	-2.236490	0.719483	-3.387827
H	-2.498298	2.681386	-1.678214
H	3.289110	2.259409	-0.985556
H	-0.557317	3.764676	-1.693854
H	-2.266397	2.606245	0.084216
H	-2.332025	-0.998971	-2.949288
H	1.652177	-3.740672	-2.524463
H	2.895676	3.685948	0.027050
H	1.035916	3.582782	-2.458967
H	-1.776890	-2.979144	-1.033326

TSA7-8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.328374	0.002887	-0.995236
N	-0.693530	0.614110	1.145679
C	-1.662479	-2.195837	1.200302
H	-2.593056	-2.574857	1.635054
H	-0.962742	-3.035306	1.160543
C	0.435994	3.045378	0.101038
C	-0.337268	-0.395722	-2.716369
O	-0.388189	-0.652033	-3.851247
P	0.907998	1.920759	-1.255581
P	-1.930126	-1.547118	-0.492057
Si	0.287542	2.014109	1.672967
Si	-0.926422	-0.775081	2.238413
C	-0.573266	2.994871	3.016706
H	-0.549467	2.471286	3.980121
H	-0.078939	3.964429	3.159556
H	-1.618087	3.171716	2.742403
C	-2.117349	-0.317209	3.611274
H	-2.427139	-1.204473	4.177620
H	-1.667710	0.388525	4.319207
H	-3.014765	0.154300	3.197480
H	1.103429	3.909394	0.182013
H	-0.576653	3.404392	-0.126120
C	-3.742602	-1.136126	-0.369023
C	-2.121440	-2.990479	-1.633454

C	0.570075	2.888248	-2.807924
C	2.756027	2.100676	-1.291249
P	1.495071	-1.353402	-0.653833
C	2.803787	-0.998045	0.585045
H	3.407752	-1.907380	0.684454
H	3.488516	-0.250135	0.170850
Si	2.286417	-0.414909	2.312426
C	1.356720	-3.182661	-0.332579
C	2.484411	-1.447476	-2.231969
C	3.746950	-0.807770	3.434033
H	3.921789	-1.888654	3.500735
H	4.668853	-0.346230	3.058503
H	3.582138	-0.434371	4.452083
C	1.964106	1.437448	2.312248
H	2.777919	1.963809	1.795848
H	2.027395	1.765618	3.360154
C	0.743505	-1.287367	2.953909
H	0.870175	-2.375951	2.881535
H	0.707669	-1.073333	4.032884
H	-2.125887	1.209043	-1.219232
H	-1.317837	1.290339	-1.399464
C	-3.736172	2.286756	0.009571
O	-3.613442	1.714357	-1.107399
O	-2.907310	2.330940	0.942556
H	-4.699703	2.819978	0.165375
H	-1.622018	1.074860	0.996081
F	-0.784245	3.123386	-2.937147
F	3.122804	3.440410	-1.360168
F	3.810590	-1.778425	-2.022799
F	2.584564	-3.812807	-0.476899
F	-2.845682	-4.022843	-1.053451
F	-3.989499	-0.506993	0.843354
H	0.914844	2.317245	-3.678168
H	3.185155	1.588737	-2.159704
H	2.035661	-2.194716	-2.896889
H	0.658032	-3.653211	-1.029833
H	-4.050658	-0.464549	-1.171354
H	-2.655075	-2.650742	-2.530338
H	1.011586	-3.360307	0.690615
H	2.449924	-0.477533	-2.737403
H	1.088261	3.851256	-2.776925
H	-4.322112	-2.065502	-0.390389
H	-1.149830	-3.379106	-1.949471
H	3.195691	1.680436	-0.384561

A2

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.070284	-0.938186	0.175022
N	0.011922	0.494770	-1.237230
C	-2.949550	0.400141	-1.144445
H	-3.488207	0.109004	-2.051684
H	-3.654920	0.925142	-0.492108
C	2.917850	0.350094	-0.690820
C	-0.157135	-2.486564	1.014116
O	-0.212621	-3.517616	1.567529
P	2.136143	-1.211796	-0.221461
P	-2.291804	-1.064521	-0.290005
Si	1.520617	1.294319	-1.588629
Si	-1.412118	1.478178	-1.452376
C	1.985364	1.290538	-3.415763
H	1.195857	1.700465	-4.055204
H	2.894319	1.882073	-3.585168
H	2.195224	0.268469	-3.755980
C	-1.559449	2.239537	-3.174022
H	-2.528487	2.743984	-3.283304
H	-0.782398	2.987962	-3.372698
H	-1.495460	1.472947	-3.955857
H	3.204690	0.874803	0.227720
H	3.815041	0.209069	-1.301126
C	-2.336857	-2.358207	-1.613735
H	-2.156914	-3.344622	-1.170498
H	-1.535348	-2.137984	-2.328754
C	-3.572944	-1.666103	0.890547
H	-3.240359	-2.616820	1.324637
H	-3.689852	-0.927710	1.688416
C	2.197355	-2.192545	-1.791997
H	1.988221	-3.247199	-1.575881
H	1.423684	-1.811174	-2.467338
C	3.289187	-2.151727	0.866112
H	2.883728	-3.157721	1.029920
H	3.370850	-1.643205	1.829782
P	0.028701	0.255978	2.027156
C	0.720125	1.960522	1.933906
H	0.530914	2.455488	2.896934

H	1.809192	1.830695	1.882574
Si	0.264195	3.187404	0.534795
C	-1.527671	0.508045	3.018776
H	-1.855252	-0.453134	3.433023
H	-1.383174	1.222580	3.836670
C	1.028164	-0.385949	3.470232
H	0.810460	0.147441	4.403079
H	0.852971	-1.456623	3.613756
C	0.380032	4.887501	1.345210
H	-0.382955	5.014968	2.123650
H	1.361321	5.045303	1.810818
H	0.233614	5.685289	0.606491
C	1.492595	3.052814	-0.887791
H	2.503589	3.360775	-0.589104
H	1.167952	3.765620	-1.660776
C	-1.441048	2.887603	-0.181160
H	-2.143656	2.651393	0.625303
H	-1.796560	3.811711	-0.658370
F	3.420201	-2.102737	-2.441526
F	4.554335	-2.266133	0.309912
F	2.380439	-0.196991	3.189689
F	-2.552335	0.998726	2.212470
F	-3.535755	-2.394534	-2.308640
F	-4.804986	-1.858833	0.286147

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.012743	-1.113590	0.050944
N	0.189216	0.659513	-1.436071
C	-2.550231	-0.058855	-1.891281
H	-2.354422	-0.495680	-2.879453
H	-3.616372	0.186359	-1.856473
C	2.904621	0.626084	-0.265242
C	-0.032968	-2.607085	0.957449
O	-0.061597	-3.620662	1.545857
P	2.230969	-1.078336	-0.226507
P	-2.115056	-1.305989	-0.607672
Si	1.667988	1.655904	-1.264863
Si	-1.411776	1.417765	-1.648514
C	2.400865	1.967335	-2.965302

H	1.654706	2.350025	-3.671898
H	3.211459	2.704545	-2.906787
H	2.831548	1.048706	-3.382451
C	-1.428815	2.508273	-3.182310
H	-2.434678	2.907407	-3.364012
H	-0.752494	3.365954	-3.079430
H	-1.129367	1.951256	-4.078440
H	2.955978	0.974326	0.772356
H	3.912684	0.665806	-0.690688
C	-2.423250	-2.929186	-1.442393
H	-2.184428	-3.740601	-0.744223
H	-1.752521	-3.005771	-2.303805
C	-3.602235	-1.237399	0.501773
H	-3.619400	-2.140514	1.125643
H	-3.535613	-0.360606	1.149204
C	2.712616	-1.701558	-1.909104
H	2.671807	-2.797147	-1.902822
H	1.991879	-1.345738	-2.651746
C	3.381244	-2.067658	0.823457
H	3.075547	-3.120040	0.777442
H	3.319540	-1.719419	1.856567
P	-0.077165	0.056083	1.958242
C	0.253894	1.865115	2.173493
H	-0.172851	2.199600	3.128389
H	1.341458	1.969899	2.275839
Si	-0.282317	3.056983	0.802799
C	-1.612711	-0.052859	3.027527
H	-2.064249	-1.047282	2.954587
H	-1.401575	0.170452	4.079522
C	1.076192	-0.545596	3.308293
H	0.826386	-0.122976	4.287731
H	1.078217	-1.638409	3.370140
C	-0.646635	4.713530	1.616983
H	-1.480775	4.631166	2.324746
H	0.224391	5.084807	2.171069
H	-0.914851	5.474111	0.873678
C	1.160171	3.241064	-0.402966
H	2.027708	3.660709	0.124688
H	0.880971	3.980415	-1.168066
C	-1.800077	2.453039	-0.139376
H	-2.441464	1.901903	0.556691
H	-2.375695	3.329607	-0.468466
H	0.107511	-1.982166	-1.305033
H	0.312545	-0.000070	-2.205356

F	3.979050	-1.297291	-2.315134
F	4.701371	-1.972957	0.401703
F	2.375089	-0.124266	3.009323
F	-2.554350	0.887741	2.600254
F	-3.732023	-3.088246	-1.875381
F	-4.804215	-1.160881	-0.191427

R^1=R^3=Ph, R^2=NH_2

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.063655	-0.282286	0.291889
N	-0.037385	1.002514	-1.434544
C	-2.915050	1.256008	-0.892880
H	-3.760177	1.033173	-1.553793
H	-3.256091	1.989181	-0.155238
C	2.879141	0.786637	-1.053476
C	-0.145704	-1.399904	1.639189
O	-0.211185	-2.147698	2.542225
P	2.236377	-0.525020	0.034171
P	-2.360910	-0.213202	0.047221
Si	1.457584	1.451457	-2.136570
Si	-1.397994	1.986480	-1.783225
C	1.701859	0.825611	-3.903918
H	0.993481	1.308762	-4.588249
H	2.712648	1.024948	-4.283877
H	1.519534	-0.254705	-3.964113
C	-1.794301	2.118523	-3.632430
H	-2.746613	2.639600	-3.798447
H	-1.020443	2.687495	-4.164209
H	-1.859790	1.134595	-4.113226
H	3.172377	1.608840	-0.391703
H	3.777410	0.503159	-1.612508
P	0.108958	1.588393	1.580506
C	1.031861	3.076651	1.022597
H	0.931034	3.823481	1.826584
H	2.095106	2.807976	1.025570
Si	0.630105	3.978681	-0.620833
C	1.030200	5.797460	-0.284882
H	0.366904	6.222333	0.479679

H	2.063837	5.931583	0.059211
H	0.906084	6.395338	-1.196381
C	1.673748	3.336637	-2.055310
H	2.733410	3.610365	-1.966518
H	1.297625	3.826191	-2.966035
C	-1.155189	3.768473	-1.153556
H	-1.832559	3.977543	-0.318000
H	-1.375544	4.496578	-1.947784
H	-0.134759	-1.292857	-1.209950
H	-0.158745	-1.836061	-0.650909
C	2.596546	-2.103840	-0.848591
C	3.116234	-2.160581	-2.142523
C	2.269299	-3.304212	-0.204330
C	3.309941	-3.387371	-2.777627
H	3.369148	-1.250852	-2.676436
C	2.470618	-4.527149	-0.832181
H	1.843753	-3.285118	0.795604
C	2.991463	-4.572682	-2.124939
H	3.713402	-3.410421	-3.786032
H	2.215219	-5.446787	-0.313556
H	3.143297	-5.527617	-2.619626
C	3.461254	-0.631417	1.409031
C	3.122054	-1.260278	2.611308
C	4.758801	-0.131549	1.260277
C	4.056529	-1.391003	3.634615
H	2.123505	-1.656536	2.756309
C	5.691760	-0.252131	2.286658
H	5.053656	0.354261	0.335366
C	5.343521	-0.883996	3.476980
H	3.774945	-1.886863	4.559314
H	6.693544	0.146104	2.152236
H	6.072325	-0.980827	4.276673
C	-3.563409	-0.306502	1.441489
C	-4.938604	-0.228265	1.182581
C	-3.137724	-0.439996	2.765308
C	-5.860669	-0.278402	2.220463
H	-5.289417	-0.132807	0.158298
C	-4.062240	-0.490145	3.809336
H	-2.078704	-0.515133	2.987551
C	-5.423341	-0.408414	3.539055
H	-6.923120	-0.216210	2.003160
H	-3.713034	-0.598657	4.832203
H	-6.145462	-0.448161	4.349444
C	-2.911123	-1.644341	-0.966272

C	-3.099393	-2.886476	-0.349321
C	-3.022570	-1.557267	-2.355821
C	-3.408663	-4.012482	-1.104906
H	-3.004701	-2.976520	0.730084
C	-3.331007	-2.685937	-3.112893
H	-2.862195	-0.609327	-2.860411
C	-3.526637	-3.914901	-2.490444
H	-3.557004	-4.968281	-0.610509
H	-3.418158	-2.600118	-4.192320
H	-3.767335	-4.794439	-3.080670
N	-1.381190	2.372411	1.911808
H	-2.095538	1.760756	2.292183
H	-1.318998	3.220964	2.467894
N	0.941652	1.303057	3.044901
H	0.947584	2.045999	3.737060
H	0.740532	0.406178	3.470686

TSA5-1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.029687	0.307774	0.180154
N	-0.126730	-0.947930	-1.658961
C	2.574595	-0.047578	-1.956354
H	2.272161	0.663359	-2.736589
H	3.643241	-0.238295	-2.098127
C	-2.786499	-1.497913	-0.522440
C	0.010199	1.533512	1.432507
O	0.064832	2.342671	2.278788
P	-2.333821	0.133352	0.157691
P	2.171879	0.764724	-0.356762
Si	-1.522539	-1.941832	-1.879738
Si	1.427182	-1.542116	-2.127759
C	-2.331577	-1.705031	-3.564476
H	-1.660539	-2.032975	-4.368323
H	-3.266758	-2.271935	-3.659297
H	-2.556986	-0.645649	-3.738068
C	1.497357	-2.124984	-3.923744
H	2.526737	-2.372401	-4.214936
H	0.890376	-3.023428	-4.091650
H	1.136480	-1.346354	-4.606575
H	-2.640555	-2.211699	0.295157

H	-3.830104	-1.591769	-0.841109
P	0.192904	-1.387862	1.692623
C	-0.157010	-3.152857	1.287148
H	0.295406	-3.760351	2.085204
H	-1.237459	-3.309174	1.379269
Si	0.403247	-3.883942	-0.377797
C	0.788886	-5.705400	-0.059232
H	1.636060	-5.819072	0.629078
H	-0.070507	-6.227711	0.380077
H	1.048329	-6.223400	-0.991082
C	-1.020625	-3.748072	-1.613994
H	-1.879336	-4.340484	-1.267701
H	-0.702469	-4.196821	-2.566359
C	1.931319	-2.993333	-1.028872
H	2.501245	-2.653884	-0.153941
H	2.570919	-3.690752	-1.587286
H	-0.263714	1.357658	-1.169005
H	-0.256788	0.473134	-1.561812
C	-3.380329	0.374785	1.653026
C	-3.259385	1.575637	2.361623
C	-4.266183	-0.595412	2.125753
C	-3.998924	1.798257	3.518505
H	-2.575835	2.344773	2.016422
C	-5.007343	-0.373950	3.284638
H	-4.380913	-1.537227	1.598425
C	-4.874651	0.820975	3.985816
H	-3.887377	2.736585	4.054290
H	-5.691118	-1.140137	3.639446
H	-5.449605	0.990949	4.891647
C	-3.122105	1.353056	-0.982427
C	-4.157136	1.027305	-1.862062
C	-2.672696	2.678829	-0.943263
C	-4.718476	1.996739	-2.691848
H	-4.534136	0.011571	-1.920939
C	-3.242973	3.651587	-1.756580
H	-1.856957	2.946060	-0.277695
C	-4.265241	3.310684	-2.640072
H	-5.512572	1.719478	-3.379288
H	-2.879785	4.674338	-1.709019
H	-4.702396	4.065399	-3.287466
C	2.589032	2.532547	-0.704146
C	3.918517	2.900221	-0.952979
C	1.598683	3.513396	-0.778279
C	4.246685	4.214191	-1.265516

H	4.706133	2.153501	-0.894149
C	1.926195	4.832354	-1.090152
H	0.564769	3.244124	-0.595791
C	3.248765	5.185577	-1.334949
H	5.282815	4.480704	-1.454301
H	1.142830	5.583425	-1.139064
H	3.503867	6.213882	-1.575208
C	3.559349	0.366959	0.778031
C	4.476171	-0.663308	0.565484
C	3.643949	1.111656	1.963576
C	5.451878	-0.950269	1.519349
H	4.428906	-1.264183	-0.337205
C	4.616062	0.824750	2.915453
H	2.939274	1.919915	2.144063
C	5.522984	-0.211870	2.696075
H	6.156682	-1.757186	1.340021
H	4.665917	1.410754	3.828689
H	6.282202	-0.438897	3.438736
N	1.753247	-1.642461	2.337815
H	2.256606	-0.791629	2.561634
H	1.818874	-2.309918	3.100929
N	-0.930250	-1.216079	2.972704
H	-0.811310	-1.827766	3.774908
H	-1.084675	-0.257948	3.266147

A6

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.041499	-0.161883	0.411815
N	0.014137	0.752379	-1.693981
C	-2.874721	1.132016	-1.081061
H	-3.714679	0.800954	-1.700752
H	-3.225086	1.990821	-0.498799
C	2.939153	0.677365	-1.083023
C	-0.123613	-0.987914	1.951813
O	-0.182218	-1.563371	2.971479
P	2.272902	-0.446211	0.206583
P	-2.356601	-0.135906	0.150302
Si	1.614091	1.210667	-2.324585
Si	-1.403185	1.746598	-2.100558
C	1.879492	0.391731	-3.991499

H	1.211709	0.826707	-4.745193
H	2.909657	0.517138	-4.347872
H	1.647212	-0.677572	-3.938324
C	-1.774862	1.558166	-3.935841
H	-2.739116	2.010674	-4.199346
H	-1.007633	2.044158	-4.551608
H	-1.802524	0.499834	-4.221813
H	3.249893	1.585406	-0.553825
H	3.836791	0.285976	-1.574765
P	0.106181	1.909501	1.367758
C	1.055591	3.295819	0.616168
H	0.949910	4.158541	1.292812
H	2.116193	3.022589	0.671038
Si	0.663309	3.925791	-1.138259
C	0.988015	5.783396	-1.113827
H	0.297513	6.301379	-0.436377
H	2.009401	6.003228	-0.778241
H	0.865072	6.223383	-2.111127
C	1.743047	3.082600	-2.428398
H	2.798127	3.372233	-2.335545
H	1.406105	3.436947	-3.413322
C	-1.092944	3.559596	-1.686123
H	-1.802976	3.885990	-0.919106
H	-1.284887	4.157729	-2.588743
C	2.719688	-2.130757	-0.380837
C	3.102943	-2.403611	-1.693594
C	2.581301	-3.195920	0.516397
C	3.347576	-3.714445	-2.103333
H	3.197155	-1.604858	-2.421739
C	2.834055	-4.499961	0.112999
H	2.254986	-3.007914	1.535555
C	3.216831	-4.764233	-1.202099
H	3.634531	-3.909179	-3.132757
H	2.721900	-5.313528	0.824030
H	3.406377	-5.785416	-1.520329
C	3.493453	-0.256686	1.578647
C	3.122328	-0.553593	2.892893
C	4.815076	0.130946	1.330988
C	4.044244	-0.462639	3.932455
H	2.107258	-0.862673	3.110780
C	5.736094	0.231630	2.369305
H	5.139571	0.350347	0.318320
C	5.352387	-0.064134	3.674994
H	3.735772	-0.700001	4.946792

H	6.757464	0.534228	2.156030
H	6.072127	0.010950	4.485188
C	-3.554395	0.161111	1.527308
C	-4.910907	0.366403	1.241665
C	-3.145384	0.164047	2.863277
C	-5.830086	0.576999	2.261889
H	-5.253013	0.351859	0.210188
C	-4.067269	0.374066	3.889843
H	-2.103772	-0.007062	3.110554
C	-5.408802	0.582829	3.591804
H	-6.877849	0.733536	2.022024
H	-3.731146	0.368593	4.922854
H	-6.127935	0.744166	4.389674
C	-3.039386	-1.717573	-0.487235
C	-3.133204	-2.791925	0.405384
C	-3.387380	-1.918018	-1.822378
C	-3.582076	-4.033032	-0.025611
H	-2.842707	-2.659008	1.444135
C	-3.834989	-3.165373	-2.257093
H	-3.289952	-1.116490	-2.547233
C	-3.935485	-4.223500	-1.361529
H	-3.648813	-4.855460	0.680812
H	-4.093626	-3.307344	-3.302422
H	-4.282536	-5.195217	-1.701346
C	-0.219249	-2.478744	-1.657654
O	-0.147686	-2.067507	-0.468109
O	-0.266738	-1.796430	-2.703566
H	-0.246455	-3.581618	-1.763111
H	-0.159179	-0.198822	-2.106926
N	-1.379593	2.762964	1.532656
H	-2.109244	2.219244	1.982497
H	-1.306454	3.669628	1.988164
N	0.892872	1.884706	2.885821
H	0.869418	2.742362	3.429252
H	0.658758	1.085241	3.462445

A7

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.166111	0.281396	-0.344460
N	-0.035268	-0.573416	1.744204

C	-2.716115	-1.569009	1.033386
H	-3.575242	-1.347504	1.676259
H	-2.956931	-2.475396	0.468148
C	2.436631	0.869449	1.704356
C	-0.292619	1.142481	-1.872671
O	-0.347336	1.702221	-2.896180
P	2.059911	0.987800	-0.076456
P	-2.427767	-0.226227	-0.195805
Si	1.602450	-0.637579	2.456122
Si	-1.153318	-1.919239	2.053805
C	1.535011	-0.383867	4.316180
H	1.231724	-1.290083	4.852977
H	2.519995	-0.087534	4.699165
H	0.817390	0.408529	4.553655
C	-1.633030	-1.952017	3.871319
H	-2.533495	-2.558798	4.031063
H	-0.838719	-2.375389	4.497036
H	-1.829582	-0.932814	4.224173
H	3.493253	1.019758	1.948761
H	1.864776	1.706793	2.140763
P	0.312200	-1.680903	-1.448306
C	1.582599	-2.837373	-0.835070
H	1.599208	-3.712097	-1.503408
H	2.559631	-2.354061	-0.946419
Si	1.431492	-3.451068	0.955953
C	2.210418	-5.168363	0.985080
H	1.636167	-5.877947	0.376040
H	3.234909	-5.145805	0.592609
H	2.255509	-5.570044	2.004807
C	2.399820	-2.304472	2.086957
H	3.411426	-2.181390	1.683091
H	2.519542	-2.819180	3.051374
C	-0.343210	-3.553141	1.576541
H	-0.956741	-4.064422	0.826404
H	-0.333104	-4.191184	2.472862
H	-0.211064	1.737324	0.737826
H	-0.921116	1.661140	0.393549
C	2.448276	2.743947	-0.486422
C	3.775814	3.161399	-0.646660
C	1.429540	3.695428	-0.583683
C	4.075410	4.494720	-0.902885
H	4.584732	2.439846	-0.577679
C	1.729726	5.031059	-0.840114
H	0.394584	3.407569	-0.445541

C	3.051101	5.433678	-1.003504
H	5.110881	4.799196	-1.026816
H	0.924781	5.756825	-0.908436
H	3.283096	6.475654	-1.204877
C	3.445638	0.144306	-0.936280
C	3.464353	0.167117	-2.335731
C	4.485157	-0.502916	-0.263298
C	4.483486	-0.460788	-3.041745
H	2.674608	0.677624	-2.876290
C	5.502590	-1.142967	-0.969714
H	4.517380	-0.506964	0.820605
C	5.501016	-1.126832	-2.360983
H	4.481046	-0.432330	-4.127564
H	6.300598	-1.644004	-0.429265
H	6.294601	-1.622239	-2.913026
C	-3.454459	-0.744469	-1.639459
C	-4.727832	-1.292502	-1.436568
C	-3.000138	-0.571183	-2.949245
C	-5.517223	-1.669682	-2.516686
H	-5.108217	-1.419216	-0.426560
C	-3.792424	-0.945308	-4.034340
H	-2.021650	-0.140533	-3.127371
C	-5.049965	-1.498012	-3.819598
H	-6.500755	-2.096328	-2.343268
H	-3.422706	-0.800814	-5.045313
H	-5.668419	-1.791895	-4.662639
C	-3.431295	1.202414	0.380511
C	-3.846048	2.152253	-0.561947
C	-3.686403	1.431463	1.732801
C	-4.522723	3.297581	-0.158970
H	-3.645334	1.996229	-1.618992
C	-4.361329	2.582642	2.134505
H	-3.324236	0.747155	2.490646
C	-4.784181	3.514555	1.193119
H	-4.844405	4.022328	-0.901236
H	-4.541538	2.751894	3.191951
H	-5.307972	4.411841	1.509784
C	-0.748858	2.545251	3.245940
O	0.156888	2.968698	2.502791
O	-1.155183	1.357252	3.383830
H	-1.275663	3.301905	3.878014
H	-0.467152	0.237980	2.264412
N	0.887848	-1.417098	-3.029991
H	1.039308	-2.238799	-3.606168

H	0.415862	-0.685990	-3.547968
N	-0.969898	-2.824927	-1.520266
H	-1.812460	-2.465735	-1.956806
H	-0.715736	-3.703954	-1.964526

A8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.099769	0.149392	0.487686
N	0.080619	-0.639784	-1.703411
C	2.555643	-1.870358	-0.726730
H	3.539697	-1.907147	-1.206798
H	2.501935	-2.715743	-0.033679
C	-2.199415	1.063324	-1.751961
C	0.240865	0.950301	2.025122
O	0.323973	1.489230	3.066241
P	-1.938976	1.069368	0.071208
P	2.307802	-0.369959	0.321262
Si	-1.515985	-0.533262	-2.477674
Si	1.113103	-2.065608	-1.935393
C	-1.357146	-0.327561	-4.340644
H	-1.048211	-1.258251	-4.830941
H	-2.319093	-0.031172	-4.778774
H	-0.618736	0.443725	-4.583895
C	1.776466	-2.089317	-3.698352
H	2.601807	-2.804973	-3.804177
H	1.000961	-2.375892	-4.418330
H	2.143776	-1.099439	-3.995235
H	-3.215485	1.332178	-2.059139
H	-1.538151	1.851828	-2.135941
P	-0.535358	-1.781598	1.488810
C	-1.852706	-2.844907	0.792206
H	-1.960102	-3.745655	1.415690
H	-2.795778	-2.292184	0.884717
Si	-1.675710	-3.373665	-1.017807
C	-2.594745	-5.013032	-1.187764
H	-2.111817	-5.803185	-0.598900
H	-3.630844	-4.925167	-0.837184
H	-2.624697	-5.351212	-2.231027
C	-2.503953	-2.092989	-2.123696
H	-3.484199	-1.857931	-1.693702

H	-2.702991	-2.571388	-3.093549
C	0.102920	-3.617277	-1.598316
H	0.630222	-4.244845	-0.870480
H	0.047877	-4.193400	-2.534122
H	0.866854	2.474950	-1.120978
H	0.477318	1.521463	-0.261403
C	-2.199589	2.857687	0.473742
C	-3.472567	3.431333	0.357048
C	-1.129158	3.676292	0.841513
C	-3.668389	4.786806	0.597016
H	-4.322632	2.812940	0.081213
C	-1.324745	5.033947	1.087063
H	-0.137359	3.249332	0.930429
C	-2.592257	5.593073	0.964821
H	-4.662238	5.214748	0.499640
H	-0.479604	5.652911	1.374811
H	-2.744452	6.651625	1.156001
C	-3.516122	0.385509	0.743204
C	-3.629408	0.299665	2.136205
C	-4.586785	-0.059794	-0.037515
C	-4.768773	-0.232278	2.728609
H	-2.809360	0.636951	2.761421
C	-5.727222	-0.603409	0.552878
H	-4.547354	0.016449	-1.118998
C	-5.819766	-0.693807	1.938000
H	-4.833168	-0.293818	3.811208
H	-6.544568	-0.948423	-0.074409
H	-6.706958	-1.117520	2.399992
C	3.389917	-0.758714	1.770111
C	4.755905	-1.014281	1.589960
C	2.859221	-0.839782	3.059436
C	5.563155	-1.354902	2.668761
H	5.193498	-0.936148	0.597943
C	3.666975	-1.182653	4.144204
H	1.808422	-0.627913	3.223594
C	5.018626	-1.442574	3.950314
H	6.620332	-1.548955	2.511876
H	3.235350	-1.238517	5.139407
H	5.650417	-1.707722	4.793239
C	3.342403	0.920177	-0.486430
C	3.548306	2.116686	0.214604
C	3.879923	0.793965	-1.766970
C	4.283795	3.151036	-0.346920
H	3.115581	2.239743	1.204843

C	4.608900	1.838155	-2.338369
H	3.726228	-0.111742	-2.344642
C	4.814536	3.016136	-1.630684
H	4.433515	4.071543	0.209892
H	5.013488	1.723661	-3.340229
H	5.382625	3.828752	-2.074524
C	1.359623	2.756866	-2.947570
O	1.152468	3.229011	-1.746048
O	1.163849	1.613758	-3.320676
H	1.734973	3.536712	-3.625424
H	0.589894	0.179458	-2.062885
N	0.647849	-3.035245	1.650348
H	1.505379	-2.703247	2.081932
H	0.319083	-3.848980	2.166208
N	-1.186721	-1.521292	3.051621
H	-1.342537	-2.348477	3.619517
H	-0.716019	-0.798096	3.583269

TSA7-8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.128724	0.217013	0.458704
N	0.122350	-0.651624	-1.659680
C	2.636121	-1.817833	-0.673148
H	3.611913	-1.842832	-1.169578
H	2.613851	-2.648717	0.038388
C	-2.228644	0.963699	-1.792812
C	0.230210	1.057566	1.990225
O	0.282842	1.612437	3.019985
P	-2.007078	1.041822	0.026117
P	2.376814	-0.298706	0.333013
Si	-1.470210	-0.626171	-2.460148
Si	1.183396	-2.066810	-1.863628
C	-1.295707	-0.454856	-4.323460
H	-0.983922	-1.393117	-4.796891
H	-2.253428	-0.162332	-4.773075
H	-0.550525	0.309834	-4.566346
C	1.839494	-2.111695	-3.625439
H	2.700701	-2.786633	-3.711594
H	1.081651	-2.456529	-4.338706
H	2.150348	-1.107723	-3.937908

H	-3.245723	1.191560	-2.129265
H	-1.578918	1.762510	-2.180525
P	-0.478466	-1.702445	1.538304
C	-1.759607	-2.820615	0.869451
H	-1.842648	-3.697781	1.529319
H	-2.719018	-2.294041	0.938973
Si	-1.562681	-3.424468	-0.917529
C	-2.445266	-5.088656	-1.009178
H	-1.944461	-5.841388	-0.387265
H	-3.482559	-5.007342	-0.660545
H	-2.470081	-5.473484	-2.036172
C	-2.409343	-2.213115	-2.081749
H	-3.412794	-2.007620	-1.692653
H	-2.555945	-2.729615	-3.041389
C	0.226168	-3.640517	-1.468288
H	0.766953	-4.215062	-0.707114
H	0.203509	-4.258773	-2.378072
H	0.566489	2.056238	-0.990490
H	0.648309	1.655695	-0.218354
C	-2.339697	2.819581	0.399516
C	-3.642262	3.329950	0.321304
C	-1.295011	3.692668	0.711753
C	-3.892480	4.677684	0.552698
H	-4.471522	2.669071	0.083667
C	-1.545878	5.042719	0.946958
H	-0.278193	3.323005	0.763328
C	-2.842910	5.538320	0.869789
H	-4.908533	5.056742	0.487802
H	-0.720686	5.705598	1.190457
H	-3.037609	6.590963	1.054358
C	-3.531210	0.287148	0.723772
C	-3.655775	0.253410	2.117738
C	-4.567299	-0.240238	-0.051618
C	-4.773454	-0.314304	2.718220
H	-2.865752	0.663060	2.737631
C	-5.684804	-0.819138	0.548285
H	-4.518386	-0.198327	-1.134310
C	-5.788172	-0.861429	1.935032
H	-4.850090	-0.333786	3.801510
H	-6.476853	-1.227676	-0.072955
H	-6.658723	-1.310985	2.403996
C	3.447663	-0.618269	1.801796
C	4.813810	-0.881983	1.635869
C	2.914708	-0.630891	3.092675

C	5.619276	-1.165313	2.732249
H	5.251875	-0.855129	0.641459
C	3.721160	-0.915946	4.194878
H	1.863664	-0.411801	3.245605
C	5.072975	-1.185541	4.015891
H	6.676754	-1.366305	2.587247
H	3.288774	-0.918569	5.191224
H	5.703439	-1.406289	4.872368
C	3.355879	1.009839	-0.504450
C	3.432229	2.256415	0.131336
C	3.969464	0.848130	-1.745139
C	4.115297	3.310948	-0.457812
H	2.938398	2.403844	1.089132
C	4.651661	1.908906	-2.340723
H	3.901416	-0.093422	-2.279211
C	4.725193	3.139721	-1.701322
H	4.162243	4.272345	0.045233
H	5.111661	1.770185	-3.314780
H	5.248861	3.968333	-2.169405
C	1.165163	2.466888	-3.089269
O	0.613668	2.963268	-2.058466
O	1.355276	1.265930	-3.343653
H	1.497049	3.214829	-3.837934
H	0.631461	0.125733	-2.133548
N	0.748057	-2.898795	1.736082
H	1.590206	-2.533056	2.170381
H	0.444046	-3.720980	2.253041
N	-1.148259	-1.397039	3.080346
H	-1.334885	-2.207283	3.662736
H	-0.689565	-0.664488	3.609073

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.082146	-0.045048	0.350097
N	0.011730	0.880186	-1.470649
C	-2.931188	0.810213	-1.374165
H	-3.484604	0.283771	-2.159430
H	-3.609327	1.531053	-0.904744
C	2.885190	1.046829	-0.779213
C	-0.138837	-1.175323	1.691841

O	-0.160689	-1.933485	2.588056
P	2.178855	-0.305102	0.209037
P	-2.305059	-0.333866	-0.085956
Si	1.523772	1.496966	-2.037658
Si	-1.393914	1.733313	-2.008880
C	2.055392	0.801900	-3.708755
H	1.306634	0.988173	-4.487959
H	3.003802	1.240670	-4.044882
H	2.195570	-0.284468	-3.636618
C	-1.528114	1.863366	-3.892557
H	-2.487092	2.312862	-4.182180
H	-0.736416	2.491250	-4.320830
H	-1.464048	0.877529	-4.369799
H	3.017503	1.911849	-0.121442
H	3.856492	0.818962	-1.231324
P	-0.075644	1.770083	1.626002
C	0.668164	3.334388	1.002420
H	0.403859	4.125497	1.721874
H	1.755499	3.221510	1.088105
Si	0.265100	4.012993	-0.739301
C	0.407508	5.891577	-0.576896
H	-0.351240	6.297801	0.104310
H	1.392008	6.185731	-0.190287
H	0.275941	6.383011	-1.548969
C	1.483836	3.393874	-2.042441
H	2.493003	3.801158	-1.892028
H	1.134538	3.782296	-3.011148
C	-1.445425	3.498359	-1.310040
H	-2.135812	3.544056	-0.458962
H	-1.810181	4.199561	-2.074070
C	3.268281	-0.557298	1.664525
C	3.191532	-1.772406	2.355925
C	4.120279	0.438664	2.146871
C	3.946278	-1.984549	3.504250
H	2.539277	-2.561903	1.993898
C	4.878243	0.225650	3.296540
H	4.201388	1.389876	1.629811
C	4.792383	-0.984269	3.978861
H	3.873884	-2.934254	4.026435
H	5.539615	1.008672	3.656918
H	5.382277	-1.149179	4.876030
C	2.556588	-1.806214	-0.787119
C	3.826741	-2.027086	-1.333151
C	1.554818	-2.755866	-1.001755

C	4.082960	-3.165033	-2.089451
H	4.624828	-1.309887	-1.159618
C	1.810861	-3.899860	-1.755637
H	0.566833	-2.607075	-0.573863
C	3.073136	-4.103557	-2.303126
H	5.071309	-3.322695	-2.511737
H	1.018075	-4.625226	-1.913114
H	3.275148	-4.993791	-2.892175
C	-3.662890	-0.469810	1.141979
C	-5.004043	-0.429560	0.740399
C	-3.370826	-0.632049	2.499692
C	-6.026671	-0.543221	1.675961
H	-5.249330	-0.310954	-0.311517
C	-4.395436	-0.746662	3.438089
H	-2.337705	-0.679785	2.828088
C	-5.724031	-0.700716	3.027938
H	-7.062436	-0.508688	1.350471
H	-4.151911	-0.874696	4.488813
H	-6.522852	-0.787613	3.758776
C	-2.343413	-1.975410	-0.918828
C	-2.874580	-3.112047	-0.301632
C	-1.724934	-2.110188	-2.168892
C	-2.805956	-4.353343	-0.929822
H	-3.349615	-3.032882	0.671840
C	-1.665075	-3.349764	-2.798126
H	-1.254754	-1.248367	-2.635498
C	-2.207288	-4.475494	-2.181261
H	-3.227343	-5.226593	-0.439981
H	-1.180242	-3.436731	-3.766216
H	-2.158267	-5.443848	-2.671111
N	0.827668	1.615186	3.068066
H	0.749788	2.356418	3.757414
H	0.767762	0.699656	3.498613
N	-1.638368	2.386779	1.975337
H	-2.289822	1.680812	2.301540
H	-1.672671	3.202384	2.581380

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.133340	0.420227	-0.211754

N	-0.191435	-1.150974	1.539039
C	-2.682504	-1.777441	0.097627
H	-3.687325	-1.983703	0.482212
H	-2.556710	-2.279886	-0.865740
C	2.213223	0.287574	2.135575
C	-0.234335	1.737250	-1.346330
O	-0.284819	2.619521	-2.120081
P	1.935927	0.993310	0.452845
P	-2.364940	0.022549	-0.163676
Si	1.408050	-1.407019	2.268196
Si	-1.323339	-2.482414	1.202135
C	1.228481	-1.831214	4.095187
H	0.829884	-2.841682	4.244963
H	2.199090	-1.781314	4.604987
H	0.553970	-1.129427	4.601380
C	-2.094694	-3.078253	2.812120
H	-2.859756	-3.841834	2.622846
H	-1.356337	-3.512158	3.496660
H	-2.584455	-2.245123	3.333227
H	3.253793	0.339695	2.473602
H	1.635625	0.937878	2.806246
P	0.380403	-1.003587	-1.869172
C	1.610572	-2.343103	-1.627290
H	1.672251	-2.952698	-2.542063
H	2.586432	-1.852782	-1.520724
Si	1.401637	-3.504452	-0.148646
C	2.240706	-5.124892	-0.626194
H	1.749434	-5.590939	-1.489657
H	3.292101	-4.958735	-0.892870
H	2.219013	-5.850514	0.196331
C	2.275392	-2.809617	1.372129
H	3.295149	-2.525340	1.089271
H	2.379510	-3.638504	2.087590
C	-0.384395	-3.863005	0.338525
H	-0.946074	-4.170881	-0.552380
H	-0.353760	-4.733732	1.010370
H	-0.344770	1.416080	1.023696
H	-0.666058	-0.435665	2.092804
C	3.476645	0.539144	-0.463539
C	3.616109	1.049465	-1.760416
C	4.486993	-0.288760	0.033248
C	4.723518	0.733006	-2.538079
H	2.844263	1.696341	-2.165141
C	5.592510	-0.622090	-0.749761

H	4.430201	-0.680374	1.043344
C	5.712540	-0.112969	-2.038630
H	4.811921	1.143818	-3.539846
H	6.362201	-1.273493	-0.344813
H	6.574517	-0.367706	-2.648954
C	2.309894	2.785082	0.749362
C	3.625500	3.206152	0.983610
C	1.286688	3.735422	0.798157
C	3.910744	4.539884	1.256061
H	4.439223	2.487252	0.945347
C	1.571840	5.073184	1.065665
H	0.262959	3.420488	0.630179
C	2.882481	5.479459	1.295703
H	4.938143	4.845533	1.433984
H	0.764096	5.799473	1.090176
H	3.103501	6.523286	1.500908
C	-3.413392	0.470816	-1.610777
C	-4.107984	-0.460619	-2.387626
C	-3.494808	1.826389	-1.955733
C	-4.855066	-0.050761	-3.492247
H	-4.081161	-1.515888	-2.131961
C	-4.244795	2.236178	-3.051834
H	-2.966379	2.565122	-1.359792
C	-4.924234	1.297304	-3.827236
H	-5.389456	-0.788719	-4.084245
H	-4.297407	3.291686	-3.302699
H	-5.507414	1.617492	-4.685862
C	-3.425260	0.708200	1.201974
C	-2.870180	1.420840	2.264982
C	-4.806470	0.465932	1.207917
C	-3.668205	1.866501	3.319584
H	-1.805472	1.638301	2.248168
C	-5.605025	0.914452	2.253002
H	-5.266087	-0.070055	0.380835
C	-5.034998	1.613486	3.317391
H	-3.216234	2.418312	4.139290
H	-6.674140	0.721516	2.237460
H	-5.658480	1.963251	4.135507
N	1.116031	-0.217486	-3.203588
H	1.261697	-0.791032	-4.029274
H	0.666423	0.657044	-3.452122
N	-0.874181	-1.998621	-2.542206
H	-1.665731	-1.427732	-2.830610
H	-0.567704	-2.542603	-3.347129

$R^1=R^2=R^3=NMe_2$

A5

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.187641	-0.934914	-0.379497
N	-0.141440	1.080102	-1.205625
C	-2.808425	1.264381	-0.066648
H	-3.782715	1.669785	-0.352862
H	-2.717299	1.323701	1.022899
C	2.331978	0.150039	-2.317736
C	-0.401046	-2.636721	-0.018451
O	-0.594175	-3.786411	0.117773
P	2.161726	-1.079293	-0.991202
P	-2.551471	-0.493066	-0.433782
Si	1.281517	1.677699	-1.926174
Si	-1.354148	2.217497	-0.821821
C	1.094272	2.528478	-3.611215
H	0.651140	3.528048	-3.541260
H	2.078607	2.643785	-4.086270
H	0.466252	1.933251	-4.285979
C	-2.038384	3.207576	-2.288528
H	-2.972605	3.716641	-2.014790
H	-1.341009	3.983097	-2.625511
H	-2.243643	2.556761	-3.146999
H	3.357901	0.374271	-2.619852
H	1.833235	-0.301860	-3.185495
P	0.233462	-0.037149	1.816392
C	1.382591	1.386872	1.781178
H	1.659130	1.665315	2.803357
H	2.283472	0.943229	1.334805
Si	1.115103	3.018346	0.833090
C	1.865426	4.345169	1.960391
H	1.322422	4.432667	2.910860
H	2.914381	4.123538	2.196634
H	1.838070	5.329877	1.477314
C	2.120730	2.923582	-0.758852
H	3.154627	2.651540	-0.507429
H	2.167590	3.914847	-1.232179
C	-0.673101	3.466756	0.442910

H	-1.281625	3.496571	1.355280
H	-0.682059	4.486701	0.030774
H	-0.569346	-0.916687	-2.166390
H	-0.204035	-1.601443	-2.085241
N	-3.073018	-0.650144	-2.071106
N	-3.726857	-1.260341	0.553782
N	2.659200	-2.526441	-1.780908
N	3.403083	-0.609881	0.113414
N	1.033309	-1.043161	2.973562
N	-1.130870	0.612339	2.660142
C	3.836399	-2.538442	-2.635532
H	4.771621	-2.663277	-2.064270
H	3.765039	-3.377413	-3.339872
H	3.909696	-1.621855	-3.222907
C	2.516649	-3.797470	-1.087353
H	3.442320	-4.086905	-0.563070
H	1.712554	-3.758648	-0.355763
H	2.278325	-4.591997	-1.806948
C	4.636672	0.041199	-0.295552
H	5.351561	-0.645472	-0.778512
H	4.443133	0.874075	-0.971900
H	5.124242	0.455525	0.596149
C	3.651655	-1.578370	1.171544
H	3.975356	-1.068140	2.087648
H	2.738298	-2.125235	1.405938
H	4.432155	-2.302741	0.885715
C	0.775376	-2.469376	3.011845
H	-0.109031	-2.730211	3.618039
H	0.629096	-2.866680	2.011339
H	1.639871	-2.984658	3.454121
C	1.335038	-0.553575	4.308034
H	0.510201	-0.737385	5.016597
H	2.224623	-1.067914	4.697049
H	1.549913	0.515374	4.312440
C	-2.039064	-0.408133	3.158308
H	-3.069493	-0.030694	3.183187
H	-2.023675	-1.278454	2.502115
H	-1.769232	-0.734932	4.177194
C	-1.058553	1.730127	3.583464
H	-2.050277	2.196054	3.663220
H	-0.754547	1.429002	4.600151
H	-0.366708	2.496392	3.234954
C	-3.589364	-2.650818	0.941291
H	-4.016514	-3.349389	0.202620

H	-2.543438	-2.912806	1.086477
H	-4.111105	-2.815721	1.894392
C	-5.120443	-0.862549	0.468740
H	-5.674215	-1.430224	-0.297319
H	-5.614555	-1.038559	1.434152
H	-5.214805	0.201122	0.241371
C	-4.143911	0.138279	-2.654401
H	-4.047256	0.113622	-3.747611
H	-5.149161	-0.238456	-2.400552
H	-4.077017	1.183231	-2.349911
C	-3.094606	-2.019376	-2.561361
H	-2.302596	-2.610425	-2.093761
H	-4.056099	-2.521476	-2.359621
H	-2.929914	-2.034251	-3.647001

TSA5-1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.158362	-0.909877	-0.026028
N	-0.284037	0.743374	-1.512432
C	-2.898931	1.082665	-0.195454
H	-3.914499	1.340842	-0.509324
H	-2.755764	1.477741	0.815074
C	2.615161	0.178369	-1.776376
C	-0.165221	-2.436103	0.823481
O	-0.168247	-3.491601	1.337716
P	2.065643	-1.209069	-0.713257
P	-2.526609	-0.688309	-0.054157
Si	1.142269	1.216435	-2.368876
Si	-1.570792	1.880908	-1.281237
C	0.975906	0.992387	-4.231850
H	0.135933	1.570443	-4.635174
H	1.883991	1.299759	-4.766283
H	0.789833	-0.064405	-4.464023
C	-2.348843	2.431353	-2.912297
H	-3.249509	3.036537	-2.744851
H	-1.656598	3.040463	-3.507749
H	-2.629935	1.563043	-3.520832
H	3.255638	0.851923	-1.199483
H	3.202161	-0.166863	-2.633264
P	0.451054	0.578054	1.692274

C	1.526020	1.948394	1.090962
H	1.917608	2.502507	1.950895
H	2.398092	1.447220	0.656002
Si	0.927188	3.292023	-0.143386
C	1.633049	4.913265	0.527990
H	1.200387	5.180603	1.500696
H	2.721881	4.856559	0.653827
H	1.423746	5.740792	-0.161220
C	1.578468	2.988926	-1.887065
H	2.659411	3.158294	-1.975099
H	1.089010	3.722907	-2.543615
C	-0.932129	3.407760	-0.351886
H	-1.438907	3.500679	0.615279
H	-1.145715	4.324648	-0.920106
H	-0.446068	-1.599645	-1.565489
H	-0.490425	-0.630714	-1.731958
N	-3.583891	-1.200880	1.197298
N	-3.121886	-1.308235	-1.543975
N	2.258781	-2.529743	-1.807055
N	3.330117	-1.272676	0.452764
N	1.462414	-0.101979	2.914995
N	-0.782584	1.495584	2.500244
C	3.586307	-2.850727	-2.307510
H	4.148511	-3.503853	-1.619733
H	3.498817	-3.375179	-3.267861
H	4.181029	-1.950752	-2.477663
C	1.472725	-3.740556	-1.625869
H	1.874422	-4.403430	-0.841959
H	0.442094	-3.490652	-1.381215
H	1.467284	-4.303028	-2.568540
C	4.732134	-1.036872	0.152689
H	5.224834	-0.618462	1.041305
H	5.269888	-1.959520	-0.118540
H	4.856495	-0.322064	-0.662341
C	3.187044	-2.270861	1.498737
H	3.682470	-1.924573	2.415078
H	2.136911	-2.437869	1.727159
H	3.642005	-3.234742	1.213030
C	0.865955	-1.119810	3.758915
H	0.465763	-0.707995	4.700029
H	0.049651	-1.622175	3.235896
H	1.612018	-1.883308	4.021053
C	2.552125	0.589516	3.574269
H	2.225759	1.352881	4.300996

H	3.149072	-0.147633	4.126485
H	3.220883	1.059252	2.850067
C	-1.791420	0.714469	3.201100
H	-2.752690	1.246492	3.200271
H	-1.946941	-0.241718	2.703538
H	-1.517121	0.524230	4.251608
C	-0.462848	2.691356	3.263608
H	-1.396267	3.207955	3.521129
H	0.065243	2.471758	4.207102
H	0.140342	3.392263	2.685237
C	-3.305104	-2.419499	1.933737
H	-3.689560	-3.322906	1.431786
H	-2.234328	-2.544849	2.083485
H	-3.779337	-2.360949	2.923029
C	-5.009443	-0.944755	1.097398
H	-5.546928	-1.758159	0.582463
H	-5.439790	-0.846317	2.103515
H	-5.205263	-0.013172	0.562349
C	-2.939069	-2.737722	-1.738391
H	-2.059742	-3.086390	-1.192650
H	-3.813108	-3.317708	-1.396298
H	-2.783544	-2.957319	-2.803222
C	-4.321692	-0.833420	-2.207850
H	-4.256559	-1.078745	-3.276171
H	-5.245027	-1.293804	-1.817853
H	-4.418723	0.250665	-2.133714

A6

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.188171	-0.658892	-0.650357
N	-0.155053	-0.367815	1.690394
C	2.359275	-1.747527	1.386960
H	1.881275	-2.722932	1.542396
H	3.406886	-1.866074	1.679532
C	-2.690120	0.985235	1.041857
C	-0.390850	-1.180206	-2.310175
O	-0.577742	-1.630206	-3.375135
P	-2.540130	-0.282263	-0.263015
P	2.084800	-1.425757	-0.396611
Si	-1.322721	0.798526	2.325110

Si	1.407043	-0.587164	2.511191
C	-2.044211	0.173553	3.948999
H	-1.326570	0.277598	4.771191
H	-2.946401	0.730605	4.232657
H	-2.306932	-0.888576	3.877632
C	1.195802	-1.448200	4.169232
H	2.170122	-1.776425	4.555255
H	0.746947	-0.797523	4.928651
H	0.559585	-2.331443	4.050143
H	-2.492696	1.921437	0.507712
H	-3.677525	1.061633	1.506842
P	0.385066	1.672985	-1.102258
C	1.600895	2.335213	0.096719
H	2.441687	1.638905	-0.029495
H	1.967223	3.313430	-0.229351
Si	1.327620	2.494751	1.965401
C	2.112518	4.138293	2.461669
H	3.163026	4.185742	2.147952
H	1.593939	4.993711	2.009744
H	2.086760	4.277468	3.549507
C	-0.450696	2.446577	2.581580
H	-1.044381	3.254645	2.138279
H	-0.403158	2.657069	3.660446
C	2.240857	1.076965	2.785177
H	3.275290	1.055892	2.418551
H	2.296349	1.261004	3.866921
C	-0.666867	-3.443953	0.832183
O	-0.468684	-2.724705	-0.187084
O	-0.753908	-3.092915	2.022984
H	-0.766280	-4.529198	0.610098
H	-0.576107	-1.319750	1.776714
N	-3.247555	-1.665243	0.458650
N	-3.648611	0.298008	-1.440755
N	2.522457	-2.936966	-1.062402
N	3.354284	-0.321676	-0.793127
N	1.204053	2.062005	-2.576385
N	-0.897012	2.841127	-0.988304
C	3.877849	-3.427104	-0.906644
H	3.877742	-4.524909	-0.919865
H	4.555469	-3.083868	-1.706302
H	4.299202	-3.114369	0.052426
C	1.816922	-3.495340	-2.200063
H	0.746257	-3.359175	-2.064781
H	2.130170	-3.065605	-3.165631

H	2.011290	-4.575020	-2.238038
C	4.618875	-0.205283	-0.091841
H	5.353916	-0.975045	-0.379591
H	5.060994	0.773341	-0.322082
H	4.478748	-0.248566	0.989440
C	3.519793	-0.147180	-2.228092
H	2.565926	-0.300475	-2.735762
H	3.859916	0.870929	-2.453590
H	4.250899	-0.859809	-2.645601
C	0.854810	1.392744	-3.815876
H	0.566308	0.361754	-3.643093
H	0.030150	1.895258	-4.349396
H	1.725017	1.387657	-4.487279
C	1.626461	3.423036	-2.868278
H	2.497992	3.400021	-3.536804
H	0.837376	4.002729	-3.375900
H	1.919738	3.969621	-1.972011
C	-1.804321	2.797324	-2.126160
H	-1.870333	1.784006	-2.521470
H	-2.815963	3.100675	-1.828068
H	-1.470762	3.466390	-2.937568
C	-0.705693	4.212173	-0.549632
H	-0.339163	4.876614	-1.349884
H	-1.667412	4.616860	-0.205356
H	-0.009526	4.275908	0.286522
C	-3.547400	-0.153625	-2.816240
H	-3.958279	0.615098	-3.485796
H	-2.508931	-0.320261	-3.095342
H	-4.102033	-1.088354	-3.001001
C	-5.027711	0.559914	-1.068965
H	-5.460135	1.294162	-1.762274
H	-5.654847	-0.346259	-1.108286
H	-5.094291	0.978386	-0.062675
C	-3.435011	-2.774961	-0.462506
H	-4.411494	-2.722973	-0.974581
H	-2.639511	-2.786671	-1.210397
H	-3.391827	-3.726724	0.083096
C	-4.278448	-1.634979	1.477051
H	-5.292298	-1.487761	1.066202
H	-4.271038	-2.592835	2.012561
H	-4.088890	-0.855169	2.215801

A7

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.250241	-0.184198	-0.856923
N	0.414866	-0.909244	1.316409
C	2.498400	1.185447	1.263433
H	3.489801	1.287536	1.714230
H	2.064294	2.187034	1.171565
C	-1.748517	-2.565711	0.440628
C	0.227434	0.078812	-2.596173
O	0.208236	0.171948	-3.759405
P	-1.753329	-1.439078	-0.990842
P	2.481642	0.531323	-0.433492
Si	-1.000363	-1.787087	1.967900
Si	1.316716	0.200961	2.365837
C	-0.456190	-3.146547	3.143297
H	-0.158495	-2.750746	4.121724
H	-1.274570	-3.858517	3.311676
H	0.395909	-3.688608	2.721787
C	2.293382	-0.792411	3.626569
H	3.077013	-0.190291	4.103654
H	1.644244	-1.174390	4.423447
H	2.760057	-1.657490	3.140970
H	-2.679316	-3.117121	0.604118
H	-0.970077	-3.303120	0.160685
P	-0.838792	1.927883	-0.332163
C	-2.125707	1.734772	0.944888
H	-2.706633	2.656684	1.042891
H	-2.800051	0.972553	0.535107
Si	-1.688497	1.194666	2.714047
C	-2.772490	2.232029	3.859571
H	-2.563888	3.306044	3.775393
H	-3.836592	2.082643	3.637061
H	-2.612603	1.949738	4.907537
C	-2.141721	-0.613172	2.894990
H	-3.184000	-0.761481	2.585616
H	-2.096736	-0.876065	3.961412
C	0.116276	1.380502	3.213699
H	0.452988	2.414089	3.070796
H	0.153033	1.187774	4.296316
H	0.617844	-1.907284	-1.074356
H	1.318860	-1.556190	-0.990463
C	1.848358	-4.090460	0.313115

O	0.781236	-4.314679	-0.291471
O	2.143531	-3.116599	1.056254
H	2.659654	-4.853106	0.190080
H	1.081106	-1.700787	1.118382
N	3.544741	-0.790212	-0.376969
N	3.258546	1.779190	-1.328003
N	0.062104	3.253920	0.349443
N	-1.750848	2.568627	-1.642996
N	-1.913504	-2.453160	-2.372410
N	-3.277083	-0.661141	-0.940766
C	4.555575	-1.083653	0.616727
H	4.490038	-2.146271	0.878290
H	5.571110	-0.864138	0.248582
H	4.395649	-0.516519	1.533675
C	3.686169	-1.606075	-1.568852
H	2.945232	-1.330642	-2.325513
H	4.682033	-1.481023	-2.021745
H	3.548243	-2.668531	-1.325930
C	4.544240	2.264196	-0.852087
H	5.359169	1.541791	-1.026602
H	4.796983	3.191657	-1.380047
H	4.505677	2.492731	0.215420
C	3.244505	1.663401	-2.778108
H	4.039344	1.000600	-3.158729
H	2.286132	1.278442	-3.124388
H	3.392236	2.654096	-3.227778
C	0.990935	3.897845	-0.573786
H	1.786352	4.401862	-0.008541
H	1.475688	3.163907	-1.216932
H	0.491726	4.656616	-1.198316
C	-0.614176	4.281210	1.131073
H	0.142979	4.959276	1.543052
H	-1.312578	4.890362	0.533480
H	-1.158531	3.861744	1.977082
C	-1.052726	2.923939	-2.869315
H	-0.960794	4.015901	-2.975378
H	-0.046729	2.507846	-2.888515
H	-1.593142	2.544522	-3.747536
C	-2.971628	3.342288	-1.507493
H	-2.786211	4.408274	-1.295667
H	-3.525697	3.287617	-2.453680
H	-3.624504	2.941068	-0.731845
C	-3.648918	0.036023	-2.161831
H	-4.336474	0.856095	-1.921135

H	-2.764311	0.464860	-2.635648
H	-4.147054	-0.632297	-2.881703
C	-4.428774	-1.083409	-0.167203
H	-4.989179	-0.195229	0.157898
H	-5.125031	-1.717416	-0.740061
H	-4.130017	-1.627960	0.728583
C	-0.717731	-3.037853	-2.977541
H	-1.005350	-3.497878	-3.930371
H	0.021440	-2.270625	-3.202889
H	-0.249341	-3.801685	-2.340262
C	-2.990558	-3.433475	-2.325475
H	-3.894006	-2.998687	-1.893850
H	-3.231729	-3.753914	-3.346066
H	-2.722643	-4.329283	-1.741770

A8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.135542	0.266034	-0.819296
N	-0.187960	0.768875	1.507497
C	-2.658366	-0.767867	1.185207
H	-3.663346	-0.759381	1.615060
H	-2.400864	-1.796750	0.908537
C	2.254956	2.029414	0.753297
C	-0.431611	0.370635	-2.530623
O	-0.717220	0.559807	-3.654679
P	2.126757	1.013191	-0.769777
P	-2.455647	0.195422	-0.347322
Si	1.393840	1.186775	2.187902
Si	-1.355664	-0.201787	2.418829
C	1.231680	2.402275	3.616055
H	0.865836	1.912023	4.526575
H	2.204236	2.850909	3.856959
H	0.537717	3.209598	3.359309
C	-2.151323	0.840952	3.766955
H	-3.001033	0.323338	4.229806
H	-1.440401	1.084742	4.565110
H	-2.516228	1.788361	3.352101
H	3.269526	2.343736	1.009916
H	1.682591	2.942638	0.563278
P	0.292907	-2.042343	-0.639450

C	1.493261	-2.446352	0.690424
H	1.751580	-3.510668	0.680819
H	2.394455	-1.906859	0.369335
Si	1.297180	-1.954549	2.508546
C	2.077916	-3.351479	3.509883
H	1.533373	-4.295757	3.379999
H	3.118405	-3.525663	3.208343
H	2.079035	-3.118495	4.581964
C	2.262969	-0.364812	2.790137
H	3.238578	-0.463529	2.297159
H	2.456799	-0.255856	3.865995
C	-0.457888	-1.686093	3.136756
H	-1.063184	-2.587860	2.979811
H	-0.376170	-1.558855	4.226811
H	-0.152769	3.194111	-0.868821
H	-0.145076	1.886596	-0.846706
C	-0.454016	4.628199	0.360486
O	-0.125881	4.217098	-0.842128
O	-0.705429	3.926823	1.319613
H	-0.470815	5.728338	0.412633
H	-0.630015	1.660068	1.245077
N	-3.607761	-0.540281	-1.393057
N	-3.091244	1.730873	0.138380
N	-1.021926	-3.119711	-0.248754
N	1.083123	-2.811195	-1.970173
N	2.639561	2.105412	-1.990384
N	3.506592	-0.040921	-0.556214
C	-3.032620	2.784851	-0.865013
H	-2.970331	3.763313	-0.372761
H	-2.151962	2.649694	-1.498799
H	-3.927261	2.793521	-1.509643
C	-4.337000	1.828718	0.884437
H	-4.417874	2.835579	1.312952
H	-5.225123	1.664651	0.250436
H	-4.368046	1.121797	1.714256
C	-3.830522	0.081768	-2.687321
H	-4.702857	0.756344	-2.676633
H	-2.959668	0.655666	-3.001558
H	-4.013847	-0.688339	-3.450055
C	-4.791903	-1.227036	-0.912389
H	-5.617905	-0.545325	-0.649475
H	-5.156207	-1.896742	-1.702755
H	-4.565201	-1.845664	-0.041931
C	-1.946928	-3.307230	-1.355234

H	-2.934074	-3.601789	-0.973558
H	-2.072901	-2.373851	-1.907684
H	-1.609309	-4.095157	-2.049799
C	-0.891656	-4.336741	0.532502
H	-1.873285	-4.596238	0.954127
H	-0.549381	-5.203521	-0.055798
H	-0.205805	-4.203659	1.371381
C	0.853575	-2.370002	-3.333284
H	-0.087106	-2.753177	-3.763038
H	0.838837	-1.285898	-3.392953
H	1.676811	-2.726696	-3.966618
C	1.397785	-4.227502	-1.932730
H	0.592827	-4.846912	-2.361443
H	2.309581	-4.418462	-2.514984
H	1.583084	-4.577796	-0.916945
C	3.745874	-0.852084	-1.747415
H	2.809106	-1.282907	-2.101171
H	4.210939	-0.268701	-2.561031
H	4.417299	-1.683944	-1.499466
C	4.773265	0.517385	-0.098260
H	5.515731	-0.287852	-0.047101
H	5.170100	1.292263	-0.776089
H	4.687205	0.936535	0.906485
C	2.110870	1.976535	-3.335463
H	1.856685	0.938907	-3.553275
H	1.213272	2.592025	-3.501070
H	2.876418	2.286720	-4.059906
C	3.216539	3.410867	-1.738561
H	3.957071	3.643301	-2.516223
H	2.457022	4.209147	-1.743748
H	3.733622	3.439750	-0.779018

TSA7-8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.186650	-0.168017	-0.887116
N	0.400198	-0.881168	1.346877
C	2.519237	1.143068	1.255887
H	3.520928	1.230749	1.686961
H	2.110222	2.152781	1.137114
C	-1.735298	-2.581713	0.538946

C	0.334073	0.063093	-2.613786
O	0.517017	0.136140	-3.768905
P	-1.797091	-1.486154	-0.928957
P	2.453345	0.464352	-0.436590
Si	-1.005344	-1.733293	2.039546
Si	1.341974	0.205698	2.388283
C	-0.494652	-3.042492	3.288404
H	-0.214078	-2.600721	4.251999
H	-1.328884	-3.731321	3.476898
H	0.358149	-3.619149	2.917148
C	2.304651	-0.806333	3.648315
H	3.118111	-0.222959	4.098347
H	1.657042	-1.145276	4.465580
H	2.732316	-1.699915	3.179649
H	-2.657846	-3.133095	0.743166
H	-0.982539	-3.327986	0.247792
P	-0.866870	1.929618	-0.384725
C	-2.063821	1.835125	0.995479
H	-2.606894	2.779259	1.100538
H	-2.790571	1.102308	0.618736
Si	-1.631650	1.273914	2.750830
C	-2.669167	2.342598	3.910550
H	-2.391677	3.402752	3.847154
H	-3.737703	2.266035	3.673278
H	-2.539702	2.032278	4.954779
C	-2.153793	-0.520929	2.904667
H	-3.179464	-0.620230	2.527777
H	-2.184883	-0.793544	3.968770
C	0.176196	1.399902	3.256875
H	0.543672	2.426311	3.139169
H	0.206374	1.186536	4.335767
H	0.956768	-2.502517	-0.974820
H	0.864061	-1.676836	-1.239653
C	1.834887	-4.082324	0.306536
O	1.215590	-3.866517	-0.783571
O	1.997002	-3.301360	1.255737
H	2.264825	-5.103232	0.392144
H	1.055314	-1.655165	1.111532
N	3.386578	-0.962108	-0.324892
N	3.384264	1.619991	-1.306593
N	0.191323	3.200040	0.142829
N	-1.884537	2.663885	-1.575575
N	-1.968492	-2.621581	-2.186422
N	-3.328087	-0.705025	-0.763215

C	3.616242	-1.647094	-1.585442
H	4.551525	-1.314773	-2.067304
H	3.682367	-2.729217	-1.421103
H	2.791404	-1.468329	-2.279549
C	4.459047	-1.200349	0.619335
H	4.530163	-2.278911	0.803048
H	5.438527	-0.845345	0.255222
H	4.259072	-0.727290	1.580946
C	4.756907	1.864159	-0.897940
H	5.459411	1.121870	-1.312256
H	5.073546	2.854910	-1.250012
H	4.854678	1.855456	0.189518
C	3.234707	1.740397	-2.745750
H	3.869702	1.032270	-3.303557
H	2.202813	1.572794	-3.046297
H	3.514824	2.756345	-3.057092
C	1.002369	3.748469	-0.934589
H	1.964061	4.109568	-0.548879
H	1.214657	2.980440	-1.678279
H	0.497700	4.590173	-1.439096
C	-0.186406	4.247709	1.075125
H	0.722087	4.661020	1.534188
H	-0.719028	5.084467	0.593397
H	-0.813757	3.867753	1.881838
C	-1.598535	2.544651	-2.993178
H	-0.852920	3.277281	-3.345257
H	-1.242431	1.551679	-3.243927
H	-2.523839	2.716362	-3.559820
C	-2.519402	3.946444	-1.313584
H	-1.885074	4.794406	-1.620748
H	-3.458041	4.012685	-1.880174
H	-2.767324	4.079243	-0.260469
C	-3.733276	0.015882	-1.959866
H	-4.317834	0.905841	-1.694736
H	-2.854624	0.348673	-2.512764
H	-4.343530	-0.614710	-2.627983
C	-4.477039	-1.241397	-0.057257
H	-5.125453	-0.409348	0.249879
H	-5.087198	-1.920818	-0.675310
H	-4.180604	-1.773075	0.847579
C	-1.209770	-2.567168	-3.418965
H	-1.658873	-1.908035	-4.178973
H	-0.189934	-2.240314	-3.226758
H	-1.149865	-3.577348	-3.842628

C	-3.129154	-3.488055	-2.242628
H	-3.908058	-3.105618	-2.922546
H	-2.836361	-4.485829	-2.595789
H	-3.575672	-3.612807	-1.253323

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.172173	-0.703349	-0.439847
N	0.092820	0.159763	1.435519
C	2.940226	-0.254749	0.832763
H	3.810406	-0.632411	1.381128
H	3.269357	0.469610	0.081637
C	-2.770748	0.780998	1.124193
C	-0.297834	-1.630236	-1.924816
O	-0.353922	-2.232766	-2.931027
P	-2.483686	-0.565387	-0.049217
P	1.961982	-1.537355	0.009001
Si	-1.240190	0.867946	2.250953
Si	1.672879	0.609457	1.957487
C	-1.682464	0.011471	3.875419
H	-0.863067	0.070657	4.602026
H	-2.573620	0.444880	4.348308
H	-1.877467	-1.052443	3.690691
C	2.052905	0.137215	3.751992
H	3.111046	0.311341	3.988326
H	1.462956	0.734578	4.458950
H	1.830866	-0.918500	3.949585
H	-2.801382	1.698982	0.526425
H	-3.707028	0.736477	1.688149
P	0.298949	1.278906	-1.484867
C	-0.199695	2.798857	-0.554175
H	0.002533	3.671819	-1.188632
H	-1.296125	2.723177	-0.539594
Si	0.335291	3.269381	1.222920
C	0.481444	5.155901	1.189461
H	1.283929	5.489999	0.518668
H	-0.450085	5.625529	0.848056
H	0.703063	5.550980	2.188622
C	-0.941191	2.726760	2.500110
H	-1.882979	3.286307	2.425104

H	-0.521323	2.943234	3.493336
C	1.942719	2.484329	1.790672
H	2.776076	2.702736	1.113802
H	2.201237	2.928176	2.762960
C	-2.596077	-3.259285	0.246356
C	-3.996024	-2.044728	1.760494
H	-1.762512	-3.193808	-0.457316
H	-2.342659	-4.013221	1.002999
H	-3.480666	-3.620980	-0.302995
H	-4.130567	-1.120643	2.323944
H	-4.927165	-2.258676	1.209434
H	-3.849752	-2.851365	2.490214
C	-5.042595	0.152149	-0.863790
C	-3.807898	-1.342976	-2.279508
H	-4.972377	0.964912	-0.139014
H	-5.523274	0.553346	-1.765533
H	-5.706812	-0.625535	-0.451091
H	-2.831108	-1.788050	-2.478337
H	-4.505369	-2.159203	-2.029423
H	-4.161742	-0.872584	-3.206752
C	-0.109357	2.838106	-3.716375
C	-1.649113	1.025318	-3.410275
H	0.889870	3.211808	-3.487697
H	-0.170518	2.699335	-4.803561
H	-0.841348	3.616393	-3.438569
H	-1.785581	0.059868	-2.935300
H	-2.489259	1.674792	-3.108448
H	-1.702689	0.885367	-4.498392
C	2.673720	2.817496	-1.669849
C	2.580120	0.669937	-2.740103
H	2.152065	3.528489	-1.030200
H	3.671835	2.655293	-1.237077
H	2.822858	3.291905	-2.654512
H	2.104568	-0.311931	-2.722743
H	2.502709	1.078388	-3.761284
H	3.644529	0.531126	-2.508136
C	0.549073	-3.036295	1.837824
C	2.961710	-3.259141	1.897549
H	-0.290509	-2.666096	1.249065
H	0.412945	-4.116326	1.992304
H	0.489634	-2.534825	2.816055
H	3.872753	-3.130535	1.307224
H	3.095148	-2.729441	2.855749
H	2.858158	-4.330291	2.116926

C	2.575129	-3.451880	-1.771296
C	4.441858	-2.033270	-1.198815
H	1.489999	-3.555052	-1.718725
H	2.866402	-3.482433	-2.829493
H	3.019837	-4.324422	-1.264403
H	4.736151	-1.089877	-0.736465
H	4.981153	-2.850936	-0.689567
H	4.785696	-2.015526	-2.242300
N	-2.834491	-1.972280	0.888470
N	-3.727007	-0.353630	-1.215321
N	-0.357061	1.572148	-3.054036
N	1.971251	1.553472	-1.759142
N	1.805346	-2.793018	1.159894
N	3.004723	-2.203864	-1.168175

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.230229	-0.703042	-0.539223
N	0.068277	0.082174	1.675302
C	2.856243	-0.458721	0.745028
H	3.763375	-0.841555	1.224242
H	3.130249	0.240079	-0.050076
C	-2.667044	1.031429	0.952318
C	-0.310949	-1.403687	-2.132369
O	-0.338285	-1.892507	-3.200589
P	-2.453756	-0.463133	-0.080913
P	1.712637	-1.689469	0.032351
Si	-1.296591	1.071481	2.247896
Si	1.790032	0.474818	1.992835
C	-1.897075	0.333879	3.868559
H	-1.112136	0.384919	4.633329
H	-2.777070	0.858489	4.259888
H	-2.161775	-0.722043	3.735542
C	2.204743	-0.060265	3.747324
H	3.269291	0.092033	3.965851
H	1.632443	0.510848	4.489416
H	1.979802	-1.123647	3.889081
H	-2.522287	1.871506	0.265554
H	-3.645125	1.170297	1.424175
P	0.435636	1.296304	-1.438493

C	0.085918	2.914075	-0.578483
H	0.430804	3.742166	-1.210833
H	-1.009995	2.986960	-0.610807
Si	0.610797	3.302982	1.201119
C	0.964350	5.153695	1.289752
H	1.807345	5.438601	0.647381
H	0.092269	5.737789	0.969514
H	1.210459	5.459492	2.314133
C	-0.746460	2.852653	2.426862
H	-1.622633	3.503616	2.307170
H	-0.351205	3.031936	3.436956
C	2.095915	2.320086	1.792501
H	2.959838	2.462808	1.132928
H	2.377556	2.735345	2.771042
H	-0.638487	-2.085919	0.028722
H	-0.090444	-0.871885	2.005113
C	-3.064245	-3.032819	0.470834
C	-4.244168	-1.466880	1.807614
H	-2.197954	-3.194452	-0.173858
H	-3.038889	-3.774951	1.279720
H	-3.981164	-3.213464	-0.116124
H	-4.221798	-0.513154	2.336169
H	-5.163327	-1.507717	1.199133
H	-4.322779	-2.253436	2.569103
C	-4.979498	0.319801	-1.036575
C	-3.711297	-1.214926	-2.379775
H	-4.941141	1.061132	-0.236452
H	-5.316303	0.835309	-1.947501
H	-5.748222	-0.427420	-0.778780
H	-2.737034	-1.685431	-2.517554
H	-4.458197	-2.010190	-2.221621
H	-3.971703	-0.696173	-3.313857
C	0.285184	2.776931	-3.769114
C	-1.602846	1.411002	-3.253326
H	1.365048	2.889569	-3.673740
H	0.062266	2.632498	-4.834050
H	-0.192325	3.724855	-3.459464
H	-1.948521	0.562143	-2.671112
H	-2.218496	2.286787	-2.970838
H	-1.783264	1.208099	-4.317455
C	2.935720	2.678927	-1.670688
C	2.704514	0.498881	-2.645067
H	2.494352	3.433050	-1.019564
H	3.926893	2.433690	-1.259610

H	3.106499	3.146885	-2.655421
H	2.181607	-0.455256	-2.559345
H	2.656349	0.830130	-3.695901
H	3.761640	0.326488	-2.395977
C	0.469330	-3.573488	1.713215
C	2.841114	-3.410332	1.837446
H	-0.463326	-3.015233	1.636913
H	0.402617	-4.435512	1.027733
H	0.556029	-3.967209	2.734475
H	3.726273	-2.795013	1.669073
H	2.811051	-3.655947	2.907158
H	2.977781	-4.354271	1.283142
C	1.997131	-3.722786	-1.706324
C	4.077617	-2.618497	-1.161350
H	0.911424	-3.649666	-1.615964
H	2.242191	-3.804641	-2.773547
H	2.321986	-4.653238	-1.209998
H	4.521208	-1.710462	-0.747538
H	4.484466	-3.484871	-0.612333
H	4.411046	-2.702639	-2.205171
N	-3.030842	-1.685730	1.032183
N	-3.678879	-0.273169	-1.274148
N	-0.189857	1.628521	-3.024799
N	2.133536	1.476021	-1.735061
N	1.618920	-2.716753	1.453435
N	2.633300	-2.553238	-1.125950

R^1=R^2=R^3=OMe

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.258274	-1.082642	-0.559453
N	-0.004564	0.933560	-1.274172
C	-2.802950	1.174854	-0.412548
H	-3.625844	1.508419	-1.054480
H	-3.072247	1.381643	0.626276
C	2.643552	-0.112021	-1.869965
C	-0.564154	-2.768025	-0.082121
O	-0.779525	-3.869051	0.209899
P	1.943464	-1.380413	-0.772756
P	-2.432975	-0.595793	-0.612654

Si	1.576061	1.457289	-1.640914
Si	-1.176461	2.094523	-0.824285
C	1.771773	2.421611	-3.256469
H	1.288823	3.404769	-3.211127
H	2.832128	2.591009	-3.488009
H	1.324955	1.876073	-4.096869
C	-1.591191	3.363730	-2.165116
H	-2.455079	3.976928	-1.875021
H	-0.759487	4.052516	-2.357058
H	-1.832561	2.866366	-3.112721
H	3.719946	0.066150	-1.783801
H	2.445825	-0.455973	-2.894410
P	-0.071278	-0.447507	1.555430
C	1.136006	0.822292	2.073884
H	1.066046	0.988948	3.155547
H	2.128421	0.393923	1.898749
Si	1.110741	2.541622	1.246958
C	1.771352	3.712526	2.578436
H	1.086500	3.776380	3.434109
H	2.748233	3.385385	2.957653
H	1.895801	4.728185	2.182001
C	2.267792	2.548983	-0.239203
H	3.282681	2.257101	0.064458
H	2.350288	3.584480	-0.603116
C	-0.616622	3.065472	0.721994
H	-1.313787	2.912930	1.556306
H	-0.606873	4.145538	0.513941
H	-0.765178	-1.387224	-2.222640
H	0.012270	-1.561965	-2.236336
O	-3.086380	-0.952340	-2.087415
O	-3.408989	-1.424146	0.412219
O	-1.480575	0.181087	2.154510
O	0.226592	-1.705328	2.569887
O	2.892510	-1.342880	0.577259
O	2.316861	-2.828486	-1.451378
C	3.654795	-3.203579	-1.735367
H	4.191285	-3.461393	-0.815177
H	3.610735	-4.089464	-2.373221
H	4.195236	-2.412727	-2.271847
C	4.226871	-0.863969	0.626898
H	4.626701	-1.153375	1.602008
H	4.863277	-1.296817	-0.151745
H	4.259118	0.228674	0.543287
C	1.023994	-1.655583	3.737876

H	0.667524	-0.914179	4.463530
H	0.961756	-2.645189	4.196839
H	2.071502	-1.445142	3.495354
C	-1.687916	0.444631	3.528620
H	-1.721272	-0.487098	4.104243
H	-0.922022	1.109194	3.947403
H	-2.654594	0.947413	3.618922
C	-4.512544	-0.855361	1.090186
H	-5.120404	-1.685592	1.458966
H	-4.172092	-0.260161	1.945055
H	-5.133062	-0.226064	0.441417
C	-4.487081	-0.908933	-2.297981
H	-4.997494	-1.670171	-1.697246
H	-4.909556	0.078230	-2.069081
H	-4.657671	-1.119569	-3.356161

TSA5-1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.151956	-0.954110	-0.591275
N	0.183665	1.183862	-1.186771
C	-2.466265	0.499397	-2.027389
H	-2.129764	0.341216	-3.059968
H	-3.530161	0.758201	-2.044885
C	2.819520	0.905876	0.112091
C	0.239791	-2.720992	-0.535451
O	0.314298	-3.878742	-0.524090
P	2.364830	-0.721177	-0.573677
P	-2.034226	-0.974140	-1.034194
Si	1.519326	2.111343	-0.597890
Si	-1.399734	1.869972	-1.261135
C	2.368432	3.121025	-1.940603
H	1.663230	3.800989	-2.434289
H	3.192290	3.726331	-1.541042
H	2.778710	2.455451	-2.710542
C	-1.493047	3.423201	-2.327203
H	-2.529702	3.761026	-2.453861
H	-0.937095	4.253467	-1.872387
H	-1.071096	3.247536	-3.323940
H	2.719072	0.852636	1.202695
H	3.836524	1.245782	-0.114382

P	-0.024392	-0.812552	1.589223
C	-0.044587	0.813662	2.475554
H	-0.570880	0.721434	3.432608
H	1.006723	0.984145	2.748247
Si	-0.590174	2.457510	1.682577
C	-1.090595	3.549945	3.141130
H	-1.983586	3.158478	3.645410
H	-0.289106	3.614096	3.887922
H	-1.318787	4.571587	2.813008
C	0.888423	3.227266	0.793370
H	1.690625	3.458904	1.507826
H	0.568426	4.191495	0.369889
C	-2.024204	2.298309	0.473509
H	-2.722483	1.526970	0.823520
H	-2.576127	3.248548	0.451858
H	0.263022	-0.909466	-2.295898
H	0.306042	0.046178	-2.015874
O	2.976051	-0.628256	-2.103420
O	3.300975	-1.846015	0.146604
O	1.223864	-1.557884	2.377922
O	-1.290388	-1.637144	2.241839
O	-2.533178	-2.278672	-1.888589
O	-3.115301	-0.874260	0.207259
C	4.368798	-0.531562	-2.341010
H	4.868546	-1.482624	-2.124598
H	4.498437	-0.303778	-3.401773
H	4.842153	0.267445	-1.755919
C	4.527474	-1.612897	0.812796
H	5.359936	-1.989957	0.208288
H	4.695837	-0.552190	1.024584
H	4.501942	-2.158301	1.760208
C	1.157190	-1.789365	3.772779
H	0.316935	-2.445369	4.024781
H	2.088347	-2.284207	4.059985
H	1.069939	-0.853661	4.341474
C	-2.272900	-1.120955	3.108681
H	-3.075595	-1.861588	3.148338
H	-1.884357	-0.975077	4.126161
H	-2.693987	-0.178079	2.741897
C	-3.596938	-2.298353	-2.827443
H	-3.194995	-2.609571	-3.796703
H	-4.345735	-3.027956	-2.503399
H	-4.077521	-1.321902	-2.946640
C	-4.510600	-1.012731	0.021166

H	-4.898593	-0.354129	-0.766459
H	-4.771745	-2.050582	-0.213633
H	-4.988537	-0.736460	0.964672

A6

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.374063	-0.937633	-0.335398
N	0.124489	0.162814	1.603001
C	2.363431	-1.636409	1.425996
H	1.836070	-2.390746	2.022892
H	3.436279	-1.839421	1.513174
C	-2.438068	1.468431	0.900673
C	-0.975895	-1.865510	-1.726065
O	-1.432409	-2.477301	-2.598731
P	-2.436033	-0.160260	0.052529
P	1.718906	-1.796693	-0.266930
Si	-0.781593	1.671204	1.802765
Si	1.830262	0.045133	2.083926
C	-1.135717	1.990604	3.620983
H	-0.220334	2.185132	4.191443
H	-1.795116	2.858864	3.747663
H	-1.630229	1.123579	4.075532
C	2.002922	0.055010	3.954112
H	3.008024	-0.268123	4.254440
H	1.835916	1.048391	4.386979
H	1.278818	-0.636212	4.400796
H	-2.512039	2.258415	0.147716
H	-3.274492	1.583923	1.598867
P	0.115290	0.735980	-1.711835
C	1.588975	1.793989	-1.485749
H	2.439771	1.118823	-1.633548
H	1.658516	2.570948	-2.255834
Si	1.835893	2.617578	0.204743
C	2.836087	4.184499	-0.114552
H	3.779808	3.958422	-0.626483
H	2.280666	4.893400	-0.741803
H	3.083134	4.698252	0.822649
C	0.228103	3.086527	1.072987
H	-0.403220	3.691614	0.409686
H	0.513132	3.754424	1.900046

C	2.809547	1.463321	1.327330
H	3.670562	1.070839	0.769947
H	3.223478	2.062718	2.150925
C	-0.968946	-2.833813	2.058813
O	-0.732494	-2.671298	0.827260
O	-0.863518	-2.006435	2.984402
H	-1.294334	-3.860942	2.326548
H	-0.345359	-0.586294	2.167953
O	-3.313329	-1.104269	1.067133
O	-3.430571	0.003342	-1.240177
O	-1.088401	1.874987	-1.848489
O	0.311104	0.158606	-3.237346
O	2.020320	-3.391525	-0.501693
O	2.881732	-1.084324	-1.199170
C	-4.687956	-0.870349	1.311536
H	-5.015694	-1.624663	2.030167
H	-4.867793	0.122345	1.746069
H	-5.274419	-0.976498	0.391966
C	-4.319246	1.083671	-1.445189
H	-4.836369	1.389694	-0.528149
H	-3.781563	1.944708	-1.858215
H	-5.063732	0.750307	-2.172839
C	-0.960946	3.161974	-2.422947
H	-1.928366	3.658717	-2.305785
H	-0.203547	3.769448	-1.914201
H	-0.723150	3.120099	-3.490980
C	0.617335	0.919598	-4.389156
H	-0.293721	1.345383	-4.824879
H	1.337868	1.721372	-4.189377
H	1.059849	0.233872	-5.116495
C	1.204479	-4.132767	-1.404925
H	1.668080	-5.117718	-1.503105
H	0.196362	-4.239409	-0.996652
H	1.163031	-3.662476	-2.393103
C	4.247654	-1.461616	-1.098316
H	4.723451	-0.995232	-0.226767
H	4.359121	-2.548600	-1.035653
H	4.745368	-1.103696	-2.002871

A7

Coordinates (Angstroms)		
X	Y	Z

Mn	-0.229345	0.170956	-1.031673
N	-0.337866	0.904910	1.071505
C	-2.741608	-0.790379	1.047611
H	-3.711755	-0.428876	1.401538
H	-2.740856	-1.883129	1.121625
C	1.989288	2.324971	0.143456
C	-0.294043	-0.235747	-2.766397
O	-0.370806	-0.463240	-3.897038
P	1.800434	1.102870	-1.178298
P	-2.380257	-0.395499	-0.704279
Si	1.188715	1.591303	1.681775
Si	-1.332946	-0.119318	2.130272
C	0.846883	2.984634	2.888928
H	0.468896	2.623138	3.851977
H	1.760133	3.560397	3.085718
H	0.098536	3.662014	2.462840
C	-2.067235	0.911996	3.516030
H	-2.869231	0.370531	4.033940
H	-1.316288	1.181105	4.267849
H	-2.481071	1.841646	3.108573
H	3.001585	2.709637	0.304310
H	1.310502	3.160893	-0.099585
P	0.529609	-1.869441	-0.595646
C	1.839569	-2.178536	0.633597
H	2.054144	-3.251008	0.716383
H	2.747101	-1.697435	0.252539
Si	1.541858	-1.503174	2.381758
C	2.490463	-2.636445	3.551569
H	2.101263	-3.661912	3.515287
H	3.556761	-2.675278	3.295976
H	2.412436	-2.290425	4.589653
C	2.227397	0.244742	2.490698
H	3.239429	0.252901	2.063387
H	2.340673	0.498609	3.554394
C	-0.281839	-1.508496	2.850758
H	-0.713036	-2.482163	2.587407
H	-0.339179	-1.428596	3.946241
H	-0.451182	1.897316	-1.375716
H	-1.187203	1.589750	-1.394767
C	-1.641703	3.985748	0.071476
O	-0.521085	4.148998	-0.445779
O	-2.028583	3.049857	0.827746
H	-2.416502	4.760658	-0.150655

H	-0.942650	1.757506	0.898130
O	-3.387624	0.830469	-1.106785
O	-2.985985	-1.638574	-1.574214
O	-0.661600	-2.878487	-0.066968
O	1.090147	-2.600667	-1.952905
O	2.070942	1.885988	-2.590956
O	3.131934	0.141000	-1.049330
C	2.562663	3.219248	-2.667736
H	3.499432	3.347617	-2.113194
H	2.748300	3.417746	-3.725565
H	1.817972	3.929809	-2.294968
C	4.436515	0.669843	-1.237782
H	4.557999	1.057581	-2.254510
H	4.662745	1.460978	-0.512621
H	5.138752	-0.153015	-1.085774
C	2.134474	-3.558373	-1.999298
H	1.940268	-4.426065	-1.358356
H	2.195084	-3.897950	-3.035703
H	3.093310	-3.109203	-1.718909
C	-0.519545	-4.282729	0.029837
H	-0.400016	-4.734120	-0.960950
H	0.322334	-4.573614	0.671371
H	-1.440328	-4.665136	0.477362
C	-4.370546	-1.943909	-1.494225
H	-4.974157	-1.139293	-1.927929
H	-4.528208	-2.858028	-2.070362
H	-4.685730	-2.122092	-0.457747
C	-4.456409	1.349766	-0.327535
H	-4.988526	2.051830	-0.973873
H	-5.158287	0.567609	-0.013757
H	-4.062980	1.896739	0.533712

A8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.262363	0.424724	-0.849946
N	-0.474291	0.055664	1.391432
C	-1.805120	-2.322125	0.316318
H	-2.736192	-2.786138	0.657130
H	-1.211902	-3.079037	-0.207652
C	0.792016	2.628161	1.339073

C	-0.460590	0.831495	-2.549584
O	-0.645418	1.129108	-3.659952
P	1.032387	2.112737	-0.405762
P	-1.994232	-0.947615	-0.884500
Si	0.673203	1.035108	2.335198
Si	-0.759965	-1.662780	1.753494
C	-0.015454	1.393007	4.047063
H	-0.010030	0.499810	4.683491
H	0.582783	2.160474	4.554753
H	-1.048301	1.753749	3.982960
C	-1.738103	-1.798672	3.356148
H	-2.171600	-2.798623	3.483569
H	-1.110888	-1.598697	4.233046
H	-2.556068	-1.067996	3.369708
H	1.560176	3.317494	1.707226
H	-0.178471	3.135287	1.417896
P	1.261563	-1.081795	-1.315067
C	2.756313	-1.205128	-0.263666
H	3.448494	-1.959012	-0.660285
H	3.259720	-0.233363	-0.333588
Si	2.449597	-1.517622	1.576363
C	3.940709	-2.459299	2.242634
H	4.047612	-3.436163	1.754371
H	4.870457	-1.902134	2.073008
H	3.853256	-2.637330	3.321685
C	2.315382	0.135392	2.473840
H	3.119974	0.788742	2.110661
H	2.512669	-0.038885	3.541180
C	0.895359	-2.545293	1.894839
H	0.901020	-3.407811	1.216310
H	0.978011	-2.952050	2.913208
H	-2.504650	2.107811	-0.140679
H	-1.225498	1.659732	-0.508084
C	-3.547732	2.340698	1.436956
O	-3.292685	2.647669	0.191080
O	-2.921871	1.568725	2.140888
H	-4.428454	2.885293	1.807289
H	-1.374324	0.548901	1.477467
O	0.890322	3.516459	-1.262214
O	2.675947	2.010397	-0.507659
O	1.948298	-1.029796	-2.825659
O	0.785088	-2.660521	-1.402384
O	-3.407512	-0.236316	-0.406487
O	-2.383977	-1.658610	-2.306216

C	-0.381167	4.101752	-1.482128
H	-0.203646	5.049543	-1.997032
H	-1.014734	3.463945	-2.105282
H	-0.900369	4.308231	-0.537854
C	3.525646	3.142534	-0.403299
H	3.505830	3.727521	-1.327446
H	3.251697	3.795687	0.433336
H	4.537087	2.762172	-0.236749
C	2.710502	0.092518	-3.222574
H	2.917133	-0.028649	-4.289024
H	2.171745	1.033584	-3.072254
H	3.663288	0.142268	-2.679345
C	1.685005	-3.707956	-1.723654
H	2.355165	-3.426905	-2.541142
H	2.278823	-4.003084	-0.848211
H	1.080523	-4.563256	-2.037610
C	-3.492821	-2.530473	-2.437055
H	-4.435279	-1.971062	-2.422924
H	-3.394913	-3.027911	-3.404825
H	-3.506043	-3.296246	-1.650611
C	-4.441370	-0.845287	0.343986
H	-5.280102	-0.143950	0.345171
H	-4.783794	-1.791102	-0.091133
H	-4.133551	-1.019241	1.381513

TSA7-8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.359347	-0.239051	-0.951345
N	0.158462	-0.936765	1.175252
C	2.438163	0.902800	1.480628
H	3.351807	0.554637	1.975452
H	2.399514	1.992396	1.567547
C	-1.887956	-2.489835	-0.117279
C	0.722012	0.123851	-2.647096
O	0.998080	0.311397	-3.757742
P	-1.564354	-1.250505	-1.414737
P	2.376978	0.419654	-0.292540
Si	-1.429593	-1.672007	1.516010
Si	0.906592	0.183865	2.341452
C	-1.283539	-2.973639	2.860773

H	-1.143246	-2.525535	3.851398
H	-2.188511	-3.593004	2.904572
H	-0.426260	-3.627794	2.667008
C	1.455858	-0.765238	3.866823
H	2.111629	-0.151992	4.498276
H	0.604543	-1.074777	4.484566
H	2.003011	-1.668639	3.573883
H	-2.891776	-2.927935	-0.146851
H	-1.158799	-3.300017	-0.263009
P	-0.498768	1.780778	-0.705943
C	-2.023368	2.096378	0.247936
H	-2.266142	3.165237	0.279558
H	-2.837385	1.594812	-0.287572
Si	-2.034710	1.432017	2.023083
C	-3.233736	2.519184	2.989776
H	-2.861866	3.548544	3.069541
H	-4.217291	2.557530	2.505282
H	-3.380737	2.141623	4.009148
C	-2.658705	-0.343700	2.029188
H	-3.554382	-0.399543	1.395814
H	-2.991269	-0.576475	3.051016
C	-0.332455	1.518145	2.826152
H	0.097916	2.509252	2.635002
H	-0.481958	1.449651	3.913587
H	1.057906	-2.488726	-0.942918
H	1.116260	-1.675432	-1.325713
C	1.719976	-4.007861	0.500649
O	1.166387	-3.810625	-0.631748
O	1.850322	-3.198308	1.428500
H	2.112885	-5.035380	0.639973
H	0.820579	-1.741379	1.139716
O	-1.763605	-2.073130	-2.826261
O	-2.951378	-0.377640	-1.487917
O	-0.799466	2.500891	-2.153433
O	0.551611	2.842370	0.019133
O	3.492318	-0.779567	-0.392132
O	3.082311	1.640912	-1.128239
C	-0.745763	-2.963251	-3.268407
H	-0.563664	-3.762783	-2.541643
H	-1.104120	-3.403066	-4.201866
H	0.193375	-2.434520	-3.456695
C	-4.216988	-0.999309	-1.679240
H	-4.173873	-1.759536	-2.463795
H	-4.576537	-1.453048	-0.747927

H	-4.913553	-0.212919	-1.978905
C	-1.829273	3.439175	-2.407825
H	-1.777499	4.315955	-1.751745
H	-1.696193	3.770483	-3.440374
H	-2.818457	2.978046	-2.311697
C	0.358607	4.242821	0.039566
H	0.488923	4.671065	-0.960621
H	-0.626227	4.525265	0.432816
H	1.118198	4.664719	0.703816
C	4.870264	-0.538583	-0.171522
H	5.375649	-1.504329	-0.238303
H	5.279135	0.130859	-0.937095
H	5.062635	-0.113635	0.822668
C	3.856681	2.673512	-0.550474
H	4.547456	2.309740	0.219269
H	4.438966	3.123339	-1.358771
H	3.205269	3.440695	-0.116045

A2

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.138888	-1.036541	-0.128987
N	-0.125480	0.563317	-1.362465
C	-2.994929	0.704473	-0.629476
H	-3.810767	0.751122	-1.358722
H	-3.340507	1.147388	0.310356
C	2.811292	0.081340	-1.365528
C	-0.217004	-2.644209	0.615518
O	-0.263979	-3.704171	1.091854
P	2.033143	-1.301911	-0.465440
P	-2.351847	-0.965011	-0.307216
Si	1.374452	1.219483	-1.913716
Si	-1.454810	1.667182	-1.222410
C	1.499240	1.394126	-3.787769
H	0.728713	2.061448	-4.191371
H	2.475897	1.796034	-4.088166
H	1.372791	0.417169	-4.271594
C	-1.897064	2.536516	-2.841088
H	-2.825456	3.112713	-2.732726
H	-1.116162	3.239947	-3.155917
H	-2.042370	1.812207	-3.651883

H	3.465017	0.645657	-0.690260
H	3.414656	-0.223427	-2.227588
P	0.072472	0.016075	1.743103
C	1.166605	1.496327	1.716902
H	1.264188	1.922125	2.723649
H	2.168965	1.134589	1.451720
Si	0.734318	2.962804	0.556728
C	1.219634	4.508809	1.530278
H	0.632990	4.608601	2.452593
H	2.280355	4.488955	1.811942
H	1.053925	5.415704	0.935752
C	1.696384	2.885479	-1.061986
H	2.771554	3.056019	-0.918973
H	1.330840	3.714834	-1.686497
C	-1.078429	3.010267	0.073821
H	-1.713448	2.877178	0.956917
H	-1.297708	4.005336	-0.339315
O	0.591079	-0.833841	3.052340
O	-1.352933	0.656248	2.285791
O	-3.282915	-1.627461	0.861723
O	-2.716625	-1.788814	-1.684335
O	2.980563	-1.531913	0.859365
O	2.266969	-2.612016	-1.423201
C	4.385648	-1.711150	0.786576
H	4.787461	-1.524253	1.785566
H	4.632268	-2.738848	0.498929
H	4.856306	-1.012254	0.083202
C	3.472440	-2.973085	-2.080124
H	4.235409	-2.188617	-2.041317
H	3.873674	-3.881490	-1.619399
H	3.240732	-3.180528	-3.129042
C	1.502214	-0.373498	4.029961
H	1.148119	0.525777	4.549517
H	1.602885	-1.177627	4.763405
H	2.486698	-0.172426	3.593029
C	-1.467147	1.279391	3.550887
H	-1.318495	0.554418	4.359303
H	-0.758879	2.109892	3.670361
H	-2.481366	1.680950	3.622093
C	-4.680455	-1.426139	0.995104
H	-5.230446	-2.253891	0.534495
H	-4.906962	-1.403442	2.064493
H	-5.011311	-0.482379	0.546978
C	-4.037376	-1.987569	-2.157018

H	-4.481953	-2.873046	-1.688800
H	-4.686290	-1.121999	-1.975039
H	-3.976309	-2.154110	-3.235549

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.264221	-1.016769	-0.297654
N	0.021372	0.964207	-1.430140
C	-2.669282	1.315675	-0.301413
H	-3.544177	1.707297	-0.832398
H	-2.812848	1.482703	0.770078
C	2.436883	-0.446789	-2.073803
C	-0.680547	-2.643524	0.219179
O	-0.976710	-3.733425	0.504418
P	1.809726	-1.483962	-0.693856
P	-2.375802	-0.483295	-0.555932
Si	1.741902	1.273887	-1.767996
Si	-1.088114	2.216024	-0.814895
C	1.921780	2.337521	-3.309196
H	1.631214	3.378254	-3.122798
H	2.962522	2.347309	-3.657176
H	1.301842	1.959001	-4.131198
C	-1.499537	3.434588	-2.188269
H	-2.253767	4.159090	-1.855809
H	-0.620341	4.002361	-2.514860
H	-1.904330	2.914914	-3.065942
H	3.526638	-0.469426	-2.186501
H	1.996318	-0.825737	-3.004703
P	-0.109943	-0.300547	1.751452
C	1.253786	0.831464	2.217628
H	1.216807	1.068815	3.288577
H	2.178757	0.267336	2.044557
Si	1.409117	2.421097	1.208734
C	2.225335	3.705574	2.322793
H	1.597242	3.931923	3.193808
H	3.191457	3.345591	2.698316
H	2.404500	4.648560	1.791657
C	2.519706	2.126751	-0.289499
H	3.393314	1.551205	0.044843
H	2.901171	3.102285	-0.623504

C	-0.255885	3.096266	0.623597
H	-0.949029	3.121700	1.474619
H	-0.091312	4.143375	0.330069
H	-0.256215	-1.591913	-1.797478
H	-0.381975	0.522256	-2.258795
O	0.008304	-1.429387	2.964559
O	-1.426205	0.480113	2.391166
O	-3.508833	-1.254822	0.347045
O	-2.968979	-0.686924	-2.089451
O	2.981944	-1.266262	0.452807
O	2.265590	-3.015648	-1.109079
C	4.356778	-1.505309	0.194666
H	4.846403	-1.636419	1.163536
H	4.502255	-2.409019	-0.403761
H	4.818009	-0.649394	-0.314715
C	1.585590	-3.718017	-2.133995
H	0.529628	-3.866846	-1.892085
H	1.657966	-3.195094	-3.096597
H	2.078946	-4.689333	-2.226103
C	1.095326	-2.333597	2.982012
H	2.035508	-1.826449	3.234718
H	0.875580	-3.076444	3.753253
H	1.220220	-2.845698	2.022657
C	-1.445370	0.974422	3.719476
H	-1.048350	0.241699	4.428219
H	-0.878624	1.911024	3.805517
H	-2.489950	1.180634	3.968984
C	-4.544571	-0.606042	1.059406
H	-5.237638	-1.384798	1.387871
H	-4.143477	-0.095357	1.942027
H	-5.094632	0.113770	0.441025
C	-4.349934	-0.540735	-2.366424
H	-4.945763	-1.261067	-1.795136
H	-4.713140	0.474365	-2.155446
H	-4.486404	-0.738367	-3.432439

R^1=R^2=R^3=Me

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.345933	0.139633	-0.263318

N	-0.625989	-0.267472	-1.067276
C	0.072748	-3.057552	-0.418137
H	0.084855	-3.866513	-1.159376
H	-0.057438	-3.531741	0.561470
C	-0.819270	2.694197	-1.018633
C	2.981983	0.430464	0.318105
O	4.066894	0.620529	0.713894
P	0.942474	2.367797	-0.628573
P	1.656306	-2.127688	-0.448560
Si	-1.678642	1.036867	-1.423951
Si	-1.324738	-1.799308	-0.749785
C	-2.225741	1.132381	-3.233237
H	-2.732557	0.213544	-3.552536
H	-2.915775	1.969202	-3.404797
H	-1.361211	1.272998	-3.895683
C	-2.370417	-2.486876	-2.172360
H	-2.715858	-3.505939	-1.952440
H	-3.264149	-1.876551	-2.355028
H	-1.797621	-2.521447	-3.107832
H	-1.295164	3.126084	-0.129818
H	-0.916919	3.438870	-1.818766
C	2.322134	-2.583307	-2.105063
H	3.287954	-2.092720	-2.267057
H	2.453826	-3.666620	-2.205670
H	1.628955	-2.238509	-2.879676
C	2.803084	-3.076634	0.631980
H	2.838800	-4.134991	0.350390
H	3.810265	-2.653464	0.549524
H	2.492461	-3.004170	1.677770
C	1.813183	2.971241	-2.137203
H	1.611817	4.031926	-2.324563
H	2.893091	2.829427	-2.018405
H	1.488412	2.394643	-3.009427
C	1.390002	3.709686	0.550142
H	2.437965	3.612157	0.853397
H	1.242569	4.695685	0.094849
H	0.763230	3.653896	1.445371
P	0.501952	0.164497	1.867808
C	-1.194006	0.852872	2.110742
H	-1.380993	0.891609	3.193346
H	-1.158755	1.899508	1.778267
Si	-2.730970	0.054655	1.288202
C	0.403868	-1.396876	2.849949
H	-0.062967	-2.206256	2.287159

H	1.419853	-1.705204	3.116648
H	-0.160576	-1.247402	3.777867
C	1.460298	1.140216	3.107578
H	1.531889	2.190023	2.814519
H	1.002072	1.084186	4.101752
H	2.479189	0.743714	3.169400
C	-4.106571	0.201726	2.578363
H	-3.870705	-0.362646	3.489788
H	-4.274411	1.246945	2.868422
H	-5.054767	-0.186677	2.185744
C	-3.204230	0.969049	-0.289362
H	-3.595845	1.975358	-0.089519
H	-4.022257	0.404808	-0.762095
C	-2.475084	-1.735676	0.777500
H	-2.110908	-2.349442	1.610149
H	-3.460223	-2.144584	0.507588
H	1.421932	0.088425	-2.054549
H	2.176469	0.199546	-1.868293

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.281566	0.009054	-0.266827
N	-0.740890	0.247504	-1.223937
C	-0.231466	-2.474022	-1.966773
H	0.026109	-2.171004	-2.990611
H	-0.541022	-3.525180	-1.999513
C	-0.443186	2.900123	0.019989
C	2.991592	-0.061620	0.118177
O	4.133790	-0.095808	0.371817
P	1.249371	2.297440	-0.341979
P	1.247542	-2.213925	-0.898769
Si	-1.635897	1.671375	-0.821254
Si	-1.548883	-1.274072	-1.334367
C	-2.375400	2.540786	-2.324066
H	-3.013358	1.861496	-2.902905
H	-2.989448	3.401958	-2.029280
H	-1.591585	2.907733	-2.998888
C	-3.005204	-1.272507	-2.539012
H	-3.417628	-2.282550	-2.662652
H	-3.825778	-0.630371	-2.194346

H	-2.697446	-0.915282	-3.529341
H	-0.588962	2.870898	1.107065
H	-0.601023	3.936327	-0.306272
C	2.666540	-2.634719	-1.993513
H	3.594407	-2.645803	-1.410858
H	2.535180	-3.612408	-2.471198
H	2.764775	-1.865431	-2.764878
C	1.216300	-3.742503	0.135299
H	1.312497	-4.627031	-0.504999
H	2.039966	-3.741872	0.855111
H	0.274977	-3.825285	0.685473
C	1.513512	2.937994	-2.049281
H	1.343563	4.019252	-2.112523
H	2.539511	2.717700	-2.361806
H	0.839919	2.428742	-2.744997
C	2.390326	3.415641	0.570085
H	3.423619	3.174102	0.297626
H	2.196258	4.465302	0.322565
H	2.294713	3.290205	1.650758
P	0.691396	-0.157741	1.934372
C	-1.033292	0.215701	2.502755
H	-1.150891	-0.204195	3.511841
H	-1.100284	1.304711	2.632189
Si	-2.543108	-0.277950	1.453814
C	0.969524	-1.766575	2.792948
H	0.276637	-2.527108	2.424919
H	1.992330	-2.107554	2.604662
H	0.824093	-1.666615	3.874752
C	1.629434	0.920086	3.104215
H	1.364024	1.967632	2.936430
H	1.403024	0.677883	4.149035
H	2.705783	0.808047	2.937075
C	-3.931843	-0.655684	2.677399
H	-3.698426	-1.536874	3.288711
H	-4.106073	0.185763	3.360025
H	-4.876097	-0.856778	2.156103
C	-3.021935	1.197520	0.379154
H	-3.298626	2.052346	1.012378
H	-3.924976	0.938655	-0.193866
C	-2.215776	-1.785363	0.365459
H	-1.510332	-2.447512	0.884409
H	-3.146309	-2.357530	0.243924
H	1.508906	0.142864	-1.977169
H	0.545781	0.235662	-1.851342

A6

	Coordinates (Angstroms)		
	X	Y	Z
Mn	1.211182	-0.153592	-0.319580
N	-0.481695	0.212913	1.193935
C	0.116977	3.032572	0.442681
H	0.382176	3.748639	1.230521
H	-0.279661	3.624495	-0.391274
C	-0.754227	-2.759729	0.831210
C	2.587529	-0.404903	-1.383636
O	3.508062	-0.568713	-2.084232
P	0.861682	-2.413908	0.006432
P	1.622296	2.109234	-0.117674
Si	-1.497941	-1.195355	1.596754
Si	-1.216098	1.824009	1.037950
C	-1.576613	-1.387965	3.461973
H	-2.048787	-0.520175	3.937656
H	-2.146986	-2.280894	3.747536
H	-0.566590	-1.475002	3.878563
C	-1.863582	2.391635	2.711557
H	-2.222120	3.428094	2.665491
H	-2.701388	1.771655	3.054631
H	-1.078269	2.341216	3.475257
H	-1.453260	-3.140402	0.076115
H	-0.644554	-3.556515	1.577895
C	2.835998	2.597297	1.176091
H	3.789672	2.090925	1.003204
H	2.994040	3.681947	1.167614
H	2.463598	2.301578	2.160187
C	2.264591	3.120969	-1.516133
H	2.439458	4.158675	-1.210265
H	3.211837	2.690266	-1.858960
H	1.569269	3.120596	-2.357834
C	2.039807	-3.229685	1.161115
H	1.851837	-4.308611	1.205369
H	3.067649	-3.050697	0.834496
H	1.927864	-2.812276	2.164931
C	0.865021	-3.659108	-1.352712
H	1.810743	-3.606330	-1.902893
H	0.743995	-4.672563	-0.953368

H	0.044008	-3.469748	-2.050640
P	-0.193838	-0.030561	-2.139578
C	-1.909608	-0.717524	-1.999891
H	-2.374568	-0.667411	-2.994517
H	-1.816200	-1.787144	-1.768499
Si	-3.133647	0.045405	-0.754407
C	-0.562661	1.577593	-2.987359
H	-0.768025	2.384344	-2.281734
H	0.307864	1.864444	-3.585847
H	-1.416718	1.480802	-3.667969
C	0.394402	-0.909213	-3.655712
H	0.576246	-1.968285	-3.462589
H	-0.330965	-0.819938	-4.472882
H	1.342168	-0.466446	-3.978884
C	-4.821644	0.075862	-1.593276
H	-4.822531	0.730070	-2.474374
H	-5.121574	-0.926307	-1.924714
H	-5.594936	0.442775	-0.907179
C	-3.200984	-0.959789	0.833369
H	-3.661625	-1.943680	0.673277
H	-3.855936	-0.418709	1.531890
C	-2.655621	1.772663	-0.184584
H	-2.486941	2.444616	-1.032884
H	-3.534778	2.172685	0.342256
C	2.450265	-0.225147	2.558386
O	2.562422	-0.367991	1.312218
O	1.449810	0.143278	3.209437
H	3.372512	-0.458596	3.133589
H	0.219052	0.267244	1.969077

A7

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.934151	-0.845914	0.181940
N	0.042324	1.175536	-0.312106
C	0.214922	0.086395	-3.053375
H	0.698474	0.637306	-3.869633
H	-0.472033	-0.627455	-3.522393
C	0.306749	1.464151	2.556559
C	1.819535	-2.335479	0.508534
O	2.415564	-3.316983	0.711897

P	0.681895	-0.322909	2.429862
P	1.465404	-0.845623	-2.074833
Si	-0.708873	2.010379	1.076343
Si	-0.745026	1.253849	-1.904869
C	-0.539669	3.872626	0.887317
H	-1.271636	4.295294	0.189331
H	-0.679375	4.371859	1.854697
H	0.462001	4.117434	0.516582
C	-0.627660	2.999110	-2.590016
H	-0.880767	3.023301	-3.657542
H	-1.301416	3.693654	-2.075647
H	0.394470	3.377078	-2.468627
H	-0.120469	1.741730	3.527531
H	1.273773	1.974135	2.430564
C	3.005231	0.090177	-2.430273
H	3.854820	-0.413827	-1.955573
H	3.192002	0.155438	-3.508303
H	2.925218	1.099174	-2.008526
C	1.781123	-2.366014	-3.059210
H	2.121853	-2.107596	-4.068089
H	2.557848	-2.960269	-2.566132
H	0.882946	-2.981560	-3.145990
C	2.244884	-0.502399	3.376858
H	2.140299	-0.122641	4.399343
H	2.546249	-1.554862	3.413692
H	3.025407	0.070386	2.866954
C	-0.507921	-1.075156	3.616882
H	-0.296533	-2.140325	3.752277
H	-0.417279	-0.584666	4.592598
H	-1.539386	-0.963846	3.272425
P	-0.995619	-2.104180	0.013280
C	-2.636976	-1.439907	0.528690
H	-3.403338	-2.164984	0.222519
H	-2.661547	-1.432608	1.625397
Si	-3.169491	0.288999	-0.028233
C	-1.461915	-2.863199	-1.602141
H	-1.564210	-2.111126	-2.388014
H	-0.687048	-3.575084	-1.899623
H	-2.409235	-3.407671	-1.518431
C	-0.957172	-3.658576	1.004885
H	-0.743932	-3.439293	2.054079
H	-1.915844	-4.185738	0.943012
H	-0.169384	-4.321730	0.634574
C	-5.055467	0.290821	-0.016677

H	-5.463914	-0.414593	-0.751329
H	-5.447594	0.007479	0.968235
H	-5.453017	1.284757	-0.256149
C	-2.531778	1.550554	1.209719
H	-2.756626	1.200658	2.226478
H	-3.111668	2.475073	1.076670
C	-2.553535	0.730496	-1.752907
H	-2.781171	-0.090464	-2.445677
H	-3.163684	1.579645	-2.095264
H	2.245684	0.338811	0.626218
H	2.545264	-0.187130	0.114320
C	3.140029	2.834448	0.248980
O	3.133732	2.220841	1.332933
O	2.309614	2.757881	-0.701102
H	3.984245	3.547569	0.079798
H	0.949187	1.699087	-0.432915

A8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.788498	-0.935636	0.155580
N	0.094909	1.233508	-0.302858
C	0.172463	0.091646	-3.020563
H	0.634065	0.577425	-3.890101
H	-0.558091	-0.627003	-3.408541
C	0.489879	1.369878	2.546819
C	1.613876	-2.448103	0.429065
O	2.208875	-3.443368	0.603551
P	0.601628	-0.463513	2.358650
P	1.413509	-0.839870	-2.014207
Si	-0.560408	2.043950	1.137523
Si	-0.690428	1.348453	-1.892060
C	-0.335943	3.908563	1.017208
H	-1.030016	4.357808	0.296586
H	-0.517745	4.386030	1.988808
H	0.683202	4.157917	0.701432
C	-0.432339	3.067139	-2.615258
H	-0.810514	3.121052	-3.644240
H	-0.947247	3.840933	-2.033853
H	0.632952	3.327374	-2.636550
H	0.140456	1.671562	3.542419

H	1.501814	1.777041	2.418122
C	2.941401	0.125751	-2.368077
H	3.786417	-0.340817	-1.851863
H	3.156450	0.168305	-3.442689
H	2.837949	1.146526	-1.987732
C	1.781555	-2.337349	-3.018642
H	1.988857	-2.085581	-4.065033
H	2.662074	-2.834412	-2.596687
H	0.952060	-3.048409	-2.983554
C	2.065066	-0.906044	3.381955
H	1.998777	-0.480912	4.390064
H	2.142821	-1.995776	3.461261
H	2.971830	-0.540185	2.893189
C	-0.729016	-0.998913	3.527953
H	-0.780213	-2.091573	3.574280
H	-0.543186	-0.621807	4.540686
H	-1.702827	-0.625367	3.199468
P	-1.194175	-2.023718	-0.112063
C	-2.796835	-1.288710	0.458740
H	-3.624373	-1.914921	0.096597
H	-2.823642	-1.365255	1.553224
Si	-3.156497	0.514617	0.024835
C	-1.777783	-2.661010	-1.752821
H	-2.012283	-1.842337	-2.438201
H	-1.003619	-3.281948	-2.212428
H	-2.680179	-3.272629	-1.635460
C	-1.256871	-3.634908	0.790064
H	-1.015532	-3.484900	1.846302
H	-2.244926	-4.103918	0.714311
H	-0.509380	-4.318412	0.374295
C	-5.032033	0.718759	0.071306
H	-5.521828	0.087984	-0.681172
H	-5.436064	0.436687	1.051874
H	-5.328304	1.756962	-0.122913
C	-2.393336	1.658114	1.314288
H	-2.603017	1.256410	2.314360
H	-2.931467	2.615555	1.259672
C	-2.535092	1.016084	-1.686810
H	-2.873973	0.282844	-2.430419
H	-3.057433	1.950761	-1.940964
H	3.137533	0.654947	0.676676
H	2.204777	-0.201411	0.457558
C	3.641292	2.500900	0.425048
O	3.901614	1.315056	0.908004

O	2.657803	2.823300	-0.220386
H	4.438299	3.219373	0.667404
H	1.052888	1.598008	-0.386608

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.879015	-0.873660	0.164628
N	0.051994	1.214391	-0.294447
C	0.241500	0.146315	-3.035614
H	0.718267	0.695061	-3.857858
H	-0.438078	-0.579911	-3.495774
C	0.372671	1.404544	2.565777
C	1.770709	-2.354477	0.454044
O	2.393900	-3.326801	0.638380
P	0.623009	-0.411589	2.396637
P	1.492467	-0.773424	-2.035104
Si	-0.680820	2.002559	1.125547
Si	-0.726919	1.308660	-1.890939
C	-0.545333	3.873947	0.996333
H	-1.267448	4.295102	0.286785
H	-0.730499	4.343216	1.971214
H	0.458481	4.160585	0.663194
C	-0.594019	3.061083	-2.560943
H	-0.891916	3.104275	-3.616250
H	-1.231743	3.761112	-2.008893
H	0.437202	3.425637	-2.483698
H	-0.017178	1.687610	3.551406
H	1.360146	1.872135	2.452284
C	3.010212	0.218439	-2.333997
H	3.850978	-0.248484	-1.810808
H	3.243749	0.284824	-3.403244
H	2.882304	1.226693	-1.928175
C	1.891124	-2.251440	-3.054220
H	2.129684	-1.971574	-4.086593
H	2.759721	-2.757658	-2.619049
H	1.060931	-2.961571	-3.065894
C	2.123160	-0.736243	3.407451
H	2.025699	-0.324731	4.418546
H	2.296534	-1.815583	3.477044
H	2.989630	-0.282519	2.918383

C	-0.667981	-1.063661	3.542634
H	-0.608610	-2.154585	3.608994
H	-0.533409	-0.651668	4.549604
H	-1.668763	-0.793578	3.195081
P	-1.043068	-2.095332	-0.096198
C	-2.689203	-1.447941	0.444914
H	-3.467724	-2.134512	0.084332
H	-2.724963	-1.510484	1.539811
Si	-3.163915	0.321750	-0.021448
C	-1.533341	-2.775067	-1.745170
H	-1.692740	-1.979801	-2.477819
H	-0.744460	-3.433858	-2.119202
H	-2.456906	-3.360739	-1.669426
C	-1.021892	-3.697274	0.821174
H	-0.799550	-3.525801	1.878168
H	-1.983863	-4.216487	0.740822
H	-0.237922	-4.346029	0.418060
C	-5.048944	0.395490	-0.008266
H	-5.480234	-0.270035	-0.766634
H	-5.451753	0.091201	0.966066
H	-5.411779	1.410241	-0.213277
C	-2.493458	1.515983	1.271794
H	-2.697220	1.105800	2.269994
H	-3.080923	2.443054	1.205558
C	-2.543003	0.822041	-1.731331
H	-2.796482	0.034344	-2.453082
H	-3.135433	1.698191	-2.034914
H	2.739734	0.675585	0.681947
H	2.350346	-0.103707	0.378748
C	3.237623	2.753664	0.451285
O	3.461544	1.684804	1.112377
O	2.381257	2.931004	-0.426417
H	3.904743	3.595686	0.720356
H	0.966604	1.692865	-0.394550

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.207495	0.079646	-0.132353
N	-0.568005	-0.117034	-1.123691
C	-0.038569	-3.017434	-0.899913

H	0.010271	-3.631289	-1.807564
H	-0.249737	-3.692145	-0.061820
C	-0.678126	2.821340	-0.774569
C	2.910597	0.251644	0.254755
O	4.053795	0.367963	0.495713
P	1.054695	2.302320	-0.535211
P	1.532843	-2.124625	-0.595979
Si	-1.616052	1.249133	-1.305642
Si	-1.359260	-1.649488	-0.974941
C	-2.214738	1.538885	-3.074519
H	-2.742298	0.669346	-3.482673
H	-2.898992	2.396249	-3.124217
H	-1.368151	1.750835	-3.740593
C	-2.541566	-2.051348	-2.398280
H	-2.897270	-3.087536	-2.322364
H	-3.429697	-1.406572	-2.397516
H	-2.048697	-1.938926	-3.371933
H	-1.068571	3.154298	0.195451
H	-0.781064	3.658786	-1.475873
C	2.334423	-2.140256	-2.252295
H	3.326296	-1.680438	-2.183214
H	2.437865	-3.154472	-2.655778
H	1.728326	-1.541296	-2.940603
C	2.598490	-3.292919	0.338682
H	2.714028	-4.243490	-0.194157
H	3.586334	-2.845085	0.491110
H	2.161016	-3.493781	1.321390
C	1.808598	2.583781	-2.191430
H	1.628964	3.599942	-2.561542
H	2.888982	2.411896	-2.133978
H	1.392521	1.865202	-2.905872
C	1.831954	3.648090	0.446553
H	2.879220	3.403440	0.653592
H	1.787319	4.604742	-0.086220
H	1.311325	3.763812	1.402434
P	0.560360	0.059658	1.994833
C	-1.155832	0.673954	2.305693
H	-1.363574	0.557127	3.379136
H	-1.130745	1.757965	2.124182
Si	-2.659000	-0.012389	1.340024
C	0.557960	-1.551525	2.893961
H	0.042039	-2.320109	2.312263
H	1.595177	-1.872756	3.038631
H	0.077980	-1.472431	3.876585

C	1.506177	1.055047	3.225524
H	1.505599	2.110700	2.938623
H	1.085719	0.965718	4.234229
H	2.547487	0.716318	3.243427
C	-4.080133	-0.030021	2.587106
H	-3.883330	-0.729965	3.409448
H	-4.242004	0.962045	3.028142
H	-5.019195	-0.336812	2.109883
C	-3.097611	1.087575	-0.127359
H	-3.448646	2.078791	0.190679
H	-3.946001	0.609929	-0.641393
C	-2.385976	-1.731557	0.629686
H	-1.929172	-2.396255	1.373418
H	-3.373014	-2.162804	0.405243

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.333884	0.119575	-0.229108
N	-0.742676	-0.261147	-1.231688
C	0.049121	-3.034984	-0.568233
H	0.067376	-3.809327	-1.345798
H	-0.071524	-3.558027	0.388822
C	-0.734128	2.728299	-1.023395
C	2.992448	0.369721	0.244318
O	4.118985	0.541490	0.528905
P	1.030710	2.301063	-0.635198
P	1.646888	-2.084184	-0.522765
Si	-1.756012	1.189577	-1.415166
Si	-1.407187	-1.850219	-0.789886
C	-2.374888	1.278383	-3.189118
H	-2.963742	0.393580	-3.459072
H	-3.003963	2.162642	-3.349434
H	-1.533589	1.341750	-3.891730
C	-2.530917	-2.478657	-2.165789
H	-2.880367	-3.497524	-1.955035
H	-3.420022	-1.846758	-2.284502
H	-2.007168	-2.501743	-3.129636
H	-1.164646	3.201807	-0.131430
H	-0.790655	3.473720	-1.826949
C	2.384865	-2.568183	-2.139302

H	3.352692	-2.068580	-2.248653
H	2.520902	-3.652641	-2.233035
H	1.742318	-2.212440	-2.951208
C	2.699387	-3.104656	0.595199
H	2.729289	-4.154633	0.281835
H	3.718978	-2.703664	0.583537
H	2.329527	-3.052744	1.622552
C	1.912457	2.950772	-2.116196
H	1.746607	4.024654	-2.264876
H	2.984649	2.761204	-1.999648
H	1.578564	2.403235	-3.002416
C	1.457396	3.644467	0.560714
H	2.502996	3.542350	0.871595
H	1.316653	4.638132	0.119087
H	0.826347	3.575037	1.452389
P	0.552031	0.125112	1.888668
C	-1.128019	0.848739	2.215286
H	-1.305870	0.856633	3.300359
H	-1.076257	1.903880	1.910639
Si	-2.661136	0.094304	1.383996
C	0.442118	-1.427167	2.902805
H	0.005036	-2.255368	2.340100
H	1.458014	-1.718589	3.190855
H	-0.138181	-1.279508	3.821955
C	1.548708	1.084236	3.114872
H	1.598763	2.140388	2.840644
H	1.135651	1.002913	4.127723
H	2.572891	0.696491	3.118832
C	-4.062108	0.158325	2.643865
H	-3.840220	-0.467497	3.517595
H	-4.227876	1.181280	3.004420
H	-5.004960	-0.198379	2.211207
C	-3.150655	1.053381	-0.165656
H	-3.504497	2.061089	0.089824
H	-4.007795	0.528720	-0.613041
C	-2.417123	-1.676708	0.792201
H	-2.009104	-2.304382	1.592225
H	-3.420798	-2.075484	0.582561
H	1.780760	0.160401	-1.789830
H	-0.132727	-0.342841	-2.049401

R^1=NH_2, R^2=R^3=Ph

A5

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.096313	-0.372719	-1.124147
N	-0.008001	-2.018790	0.264952
C	1.711845	-0.272478	1.880431
H	2.630555	-0.415338	2.458753
H	1.161621	0.552439	2.346998
C	-2.038837	-3.032579	-1.644249
C	0.256097	0.864100	-2.364674
O	0.367402	1.625845	-3.248133
P	-1.429368	-1.486813	-2.391715
P	1.989978	0.218300	0.149873
Si	-1.062515	-3.338900	-0.028953
Si	0.579421	-1.806411	1.859199
C	-0.200439	-5.008365	-0.232344
H	0.335241	-5.306815	0.676637
H	-0.916881	-5.805549	-0.471585
H	0.535957	-4.962577	-1.045216
C	1.531069	-3.295872	2.542927
H	2.056539	-3.047698	3.474878
H	0.841153	-4.117138	2.777250
H	2.264209	-3.681632	1.825198
H	-3.106138	-2.930054	-1.421190
H	-1.920021	-3.870849	-2.340501
P	-1.603563	0.707376	0.093692
C	-2.869197	-0.407569	0.830115
H	-3.685172	0.207275	1.229972
H	-3.298795	-0.949362	-0.022320
Si	-2.467847	-1.731777	2.161894
C	-3.933612	-1.651781	3.355727
H	-3.986296	-0.688095	3.878962
H	-4.888526	-1.796246	2.834009
H	-3.856619	-2.434558	4.120713
C	-2.352247	-3.434746	1.366939
H	-3.322166	-3.791626	0.996034
H	-2.034355	-4.145188	2.144792
C	-0.848796	-1.477648	3.075098
H	-0.779521	-0.480350	3.523354
H	-0.818117	-2.201203	3.902755
H	1.129300	-1.727163	-1.647847
H	1.322089	-1.174641	-2.169516
C	-2.644815	1.894939	-0.887999

C	-4.022072	1.734898	-1.070447
C	-2.023154	2.991306	-1.498516
C	-4.753723	2.640201	-1.836237
H	-4.537774	0.886762	-0.635579
C	-2.751601	3.899689	-2.260107
H	-0.955180	3.144150	-1.387837
C	-4.122335	3.726600	-2.433761
H	-5.821852	2.490208	-1.966651
H	-2.243692	4.741383	-2.722001
H	-4.693067	4.431037	-3.032046
C	-1.186206	1.838329	1.497465
C	-0.162208	2.771489	1.309996
C	-1.858900	1.836440	2.723421
C	0.196719	3.664085	2.314658
H	0.378063	2.793075	0.370979
C	-1.496710	2.720040	3.737668
H	-2.671212	1.141839	2.907439
C	-0.467057	3.635532	3.538200
H	1.003051	4.370165	2.139580
H	-2.025254	2.691461	4.686267
H	-0.185135	4.322798	4.330573
C	2.800469	1.873907	0.237313
C	3.496186	2.282289	1.379267
C	2.747708	2.737863	-0.861473
C	4.122878	3.524275	1.424208
H	3.546567	1.631730	2.246977
C	3.374792	3.981036	-0.818351
H	2.201417	2.450070	-1.754068
C	4.064000	4.377693	0.324700
H	4.657363	3.825117	2.320853
H	3.320509	4.641305	-1.679229
H	4.551140	5.347813	0.359931
C	3.449941	-0.770259	-0.394134
C	3.923208	-0.576251	-1.698584
C	4.094124	-1.705399	0.415933
C	5.010432	-1.296350	-2.177268
H	3.430303	0.142572	-2.350256
C	5.179834	-2.437032	-0.065724
H	3.756196	-1.881799	1.431143
C	5.641602	-2.234839	-1.360870
H	5.363817	-1.129666	-3.190861
H	5.662626	-3.165653	0.579403
H	6.487499	-2.803699	-1.735668
N	-0.658072	-2.098246	-3.794955

H	-1.262241	-2.590932	-4.447712
H	-0.117400	-1.393213	-4.286630
N	-2.883926	-0.704260	-2.811561
H	-2.771985	0.268243	-3.077716
H	-3.491365	-1.193087	-3.462987

TSA5-1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.029687	0.307774	0.180154
N	-0.126730	-0.947930	-1.658961
C	2.574595	-0.047578	-1.956354
H	2.272161	0.663359	-2.736589
H	3.643241	-0.238295	-2.098127
C	-2.786499	-1.497913	-0.522440
C	0.010199	1.533512	1.432507
O	0.064832	2.342671	2.278788
P	-2.333821	0.133352	0.157691
P	2.171879	0.764724	-0.356762
Si	-1.522539	-1.941832	-1.879738
Si	1.427182	-1.542116	-2.127759
C	-2.331577	-1.705031	-3.564476
H	-1.660539	-2.032975	-4.368323
H	-3.266758	-2.271935	-3.659297
H	-2.556986	-0.645649	-3.738068
C	1.497357	-2.124984	-3.923744
H	2.526737	-2.372401	-4.214936
H	0.890376	-3.023428	-4.091650
H	1.136480	-1.346354	-4.606575
H	-2.640555	-2.211699	0.295157
H	-3.830104	-1.591769	-0.841109
P	0.192904	-1.387862	1.692623
C	-0.157010	-3.152857	1.287148
H	0.295406	-3.760351	2.085204
H	-1.237459	-3.309174	1.379269
Si	0.403247	-3.883942	-0.377797
C	0.788886	-5.705400	-0.059232
H	1.636060	-5.819072	0.629078
H	-0.070507	-6.227711	0.380077
H	1.048329	-6.223400	-0.991082
C	-1.020625	-3.748072	-1.613994

H	-1.879336	-4.340484	-1.267701
H	-0.702469	-4.196821	-2.566359
C	1.931319	-2.993333	-1.028872
H	2.501245	-2.653884	-0.153941
H	2.570919	-3.690752	-1.587286
H	-0.263714	1.357658	-1.169005
H	-0.256788	0.473134	-1.561812
C	-3.380329	0.374785	1.653026
C	-3.259385	1.575637	2.361623
C	-4.266183	-0.595412	2.125753
C	-3.998924	1.798257	3.518505
H	-2.575835	2.344773	2.016422
C	-5.007343	-0.373950	3.284638
H	-4.380913	-1.537227	1.598425
C	-4.874651	0.820975	3.985816
H	-3.887377	2.736585	4.054290
H	-5.691118	-1.140137	3.639446
H	-5.449605	0.990949	4.891647
C	-3.122105	1.353056	-0.982427
C	-4.157136	1.027305	-1.862062
C	-2.672696	2.678829	-0.943263
C	-4.718476	1.996739	-2.691848
H	-4.534136	0.011571	-1.920939
C	-3.242973	3.651587	-1.756580
H	-1.856957	2.946060	-0.277695
C	-4.265241	3.310684	-2.640072
H	-5.512572	1.719478	-3.379288
H	-2.879785	4.674338	-1.709019
H	-4.702396	4.065399	-3.287466
C	2.589032	2.532547	-0.704146
C	3.918517	2.900221	-0.952979
C	1.598683	3.513396	-0.778279
C	4.246685	4.214191	-1.265516
H	4.706133	2.153501	-0.894149
C	1.926195	4.832354	-1.090152
H	0.564769	3.244124	-0.595791
C	3.248765	5.185577	-1.334949
H	5.282815	4.480704	-1.454301
H	1.142830	5.583425	-1.139064
H	3.503867	6.213882	-1.575208
C	3.559349	0.366959	0.778031
C	4.476171	-0.663308	0.565484
C	3.643949	1.111656	1.963576
C	5.451878	-0.950269	1.519349

H	4.428906	-1.264183	-0.337205
C	4.616062	0.824750	2.915453
H	2.939274	1.919915	2.144063
C	5.522984	-0.211870	2.696075
H	6.156682	-1.757186	1.340021
H	4.665917	1.410754	3.828689
H	6.282202	-0.438897	3.438736
N	1.753247	-1.642461	2.337815
H	2.256606	-0.791629	2.561634
H	1.818874	-2.309918	3.100929
N	-0.930250	-1.216079	2.972704
H	-0.811310	-1.827766	3.774908
H	-1.084675	-0.257948	3.266147

A6

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.101659	-0.369065	-0.970642
N	0.586673	-1.992359	0.570491
C	1.440225	0.427633	2.032208
H	2.298051	0.651104	2.676089
H	0.617759	1.075013	2.360451
C	-0.547226	-3.606574	-1.563726
C	0.007554	0.740841	-2.329806
O	0.021334	1.379021	-3.308672
P	-1.040765	-1.952856	-2.157647
P	1.701397	0.830956	0.262275
Si	-0.236177	-3.549827	0.295513
Si	0.865986	-1.373316	2.205100
C	0.888840	-4.978190	0.767665
H	1.041309	-5.045933	1.851316
H	0.462006	-5.933059	0.434410
H	1.868715	-4.856592	0.293290
C	2.199474	-2.389996	3.059961
H	2.583190	-1.880553	3.953009
H	1.808989	-3.362352	3.383542
H	3.042790	-2.584247	2.387178
H	-1.270471	-4.372826	-1.867653
H	0.409753	-3.852905	-2.040082
P	-1.836816	0.443274	0.095814
C	-2.903124	-0.821407	0.892335

H	-3.811745	-0.348844	1.284329
H	-3.218890	-1.481533	0.074729
Si	-2.248740	-2.028579	2.200579
C	-3.676922	-2.315712	3.398920
H	-3.938060	-1.399920	3.944916
H	-4.577620	-2.656620	2.873470
H	-3.418306	-3.078788	4.143183
C	-1.817292	-3.626719	1.312974
H	-2.659379	-3.913854	0.669305
H	-1.704818	-4.427371	2.057635
C	-0.741440	-1.458976	3.176240
H	-0.937939	-0.496781	3.664473
H	-0.610444	-2.190184	3.987849
C	-3.043949	1.226965	-1.087303
C	-4.349245	0.753229	-1.265954
C	-2.639606	2.329536	-1.851373
C	-5.212639	1.348912	-2.184936
H	-4.714358	-0.091202	-0.692368
C	-3.502309	2.933322	-2.759467
H	-1.635555	2.724747	-1.749159
C	-4.793495	2.441377	-2.935500
H	-6.217733	0.954650	-2.305997
H	-3.159127	3.786749	-3.336906
H	-5.465735	2.906661	-3.650433
C	-1.812163	1.771756	1.392302
C	-1.164147	2.977661	1.105246
C	-2.405918	1.633439	2.652209
C	-1.097851	4.005636	2.040067
H	-0.684144	3.118492	0.144574
C	-2.331309	2.654502	3.597329
H	-2.941134	0.728789	2.917099
C	-1.675369	3.844113	3.296215
H	-0.579886	4.925011	1.784815
H	-2.796094	2.517802	4.569707
H	-1.618152	4.639072	4.034063
C	1.919278	2.661992	0.229829
C	2.335282	3.377178	1.356032
C	1.703786	3.355987	-0.965012
C	2.518459	4.755780	1.294090
H	2.509611	2.862894	2.296051
C	1.887675	4.734901	-1.029106
H	1.377750	2.823491	-1.852038
C	2.291343	5.439636	0.102030
H	2.836666	5.296501	2.180990

H	1.711975	5.257161	-1.965230
H	2.432984	6.515476	0.053566
C	3.446070	0.363940	-0.084350
C	3.925201	0.606631	-1.377465
C	4.307279	-0.201239	0.855509
C	5.234299	0.292568	-1.718827
H	3.258529	1.019758	-2.128885
C	5.619717	-0.523430	0.512355
H	3.968282	-0.403942	1.866213
C	6.086602	-0.276818	-0.773333
H	5.588261	0.484024	-2.727901
H	6.275321	-0.968973	1.255161
H	7.109118	-0.527659	-1.040554
C	2.588465	-2.123904	-1.956556
O	1.663408	-1.281473	-2.174548
O	2.820365	-2.753445	-0.911578
H	3.250812	-2.308759	-2.827826
H	1.516591	-2.160398	0.125817
N	-0.623456	-2.042286	-3.836427
H	-1.063254	-1.262704	-4.324960
H	0.383003	-1.871216	-3.889211
N	-2.739794	-2.100722	-2.190532
H	-3.207957	-1.215168	-2.362642
H	-3.072408	-2.797539	-2.853831

A7

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.211015	-0.321225	-0.962291
N	1.361872	-1.497484	0.597559
C	1.109763	1.104906	1.969619
H	1.780738	1.728886	2.568947
H	0.092527	1.303183	2.326790
C	0.973579	-3.548106	-1.384713
C	-0.283641	0.578285	-2.387983
O	-0.477763	1.120899	-3.405050
P	-0.230556	-2.334345	-1.984087
P	1.092750	1.524346	0.192535
Si	1.228099	-3.274195	0.459972
Si	1.466697	-0.742196	2.200627
C	2.832637	-4.081911	1.001705

H	2.931026	-4.108299	2.093861
H	2.893657	-5.116073	0.639687
H	3.680821	-3.520060	0.596285
C	3.190860	-0.972745	2.901054
H	3.381355	-0.294444	3.742403
H	3.343885	-1.996784	3.262295
H	3.931249	-0.789028	2.113683
H	0.724028	-4.582109	-1.654756
H	1.935034	-3.266883	-1.846139
P	-1.886484	-0.301478	0.116563
C	-2.280008	-1.722674	1.212196
H	-3.229793	-1.521214	1.721650
H	-2.458735	-2.547901	0.511287
Si	-1.114860	-2.561417	2.453413
C	-2.273666	-3.325325	3.730483
H	-2.807464	-2.554939	4.301443
H	-3.026500	-3.963769	3.251153
H	-1.721315	-3.944934	4.447412
C	-0.187339	-3.906062	1.528294
H	-0.899584	-4.471065	0.913245
H	0.229670	-4.612112	2.260154
C	0.152280	-1.480928	3.327281
H	-0.326343	-0.688961	3.917080
H	0.651163	-2.139126	4.054408
H	1.657247	-0.815122	-1.897250
H	1.843864	-0.132959	-1.539581
C	-3.350662	-0.346079	-1.037586
C	-4.422522	-1.232501	-0.867329
C	-3.407593	0.539564	-2.121036
C	-5.496026	-1.244915	-1.755782
H	-4.435358	-1.935271	-0.042708
C	-4.484598	0.539196	-3.002295
H	-2.605861	1.245511	-2.291442
C	-5.531563	-0.361059	-2.829001
H	-6.306612	-1.951534	-1.601856
H	-4.497112	1.242490	-3.829885
H	-6.367082	-0.371609	-3.522740
C	-2.395861	1.133557	1.170623
C	-2.675397	2.369597	0.578007
C	-2.497068	1.031896	2.562047
C	-3.049163	3.465911	1.346547
H	-2.597204	2.491689	-0.495970
C	-2.854323	2.133459	3.337498
H	-2.300726	0.088898	3.059996

C	-3.133589	3.353875	2.731722
H	-3.256267	4.413039	0.858698
H	-2.924471	2.028419	4.416434
H	-3.416581	4.212177	3.334096
C	0.402380	3.228787	0.121934
C	0.399585	4.066923	1.239893
C	-0.088417	3.722785	-1.090585
C	-0.094202	5.365129	1.151283
H	0.773613	3.709415	2.193830
C	-0.580926	5.021267	-1.181191
H	-0.095543	3.092246	-1.973027
C	-0.588221	5.845533	-0.058395
H	-0.095685	6.000735	2.032195
H	-0.961290	5.387783	-2.130423
H	-0.975752	6.857963	-0.127375
C	2.842899	1.876015	-0.252897
C	3.143308	2.043030	-1.610030
C	3.871246	1.984556	0.682217
C	4.444482	2.304729	-2.021173
H	2.359232	1.949738	-2.358170
C	5.176613	2.241838	0.270984
H	3.676573	1.845571	1.740311
C	5.466613	2.402455	-1.079118
H	4.661127	2.421602	-3.078814
H	5.968642	2.305304	1.011488
H	6.486626	2.594510	-1.398974
C	4.319144	-1.445311	-1.410677
O	3.667973	-2.010888	-2.307313
O	3.954911	-1.159918	-0.234824
H	5.369615	-1.149870	-1.658038
H	2.323588	-1.330573	0.180008
N	0.065665	-2.275573	-3.651652
H	0.000615	-3.140464	-4.177759
H	-0.351215	-1.496641	-4.146977
N	-1.696655	-3.177073	-1.685517
H	-2.518320	-2.648445	-1.967152
H	-1.731989	-4.100786	-2.110647

A8

Coordinates (Angstroms)		
X	Y	Z

Mn	0.109203	-0.261839	-0.927315
N	1.096968	-1.650296	0.659801
C	1.051166	0.935737	2.073412
H	1.762102	1.436687	2.739365
H	0.049687	1.293166	2.342103
C	0.645885	-3.534757	-1.477217
C	-0.203134	0.731540	-2.316309
O	-0.292506	1.318865	-3.332203
P	-0.321565	-2.110887	-2.109284
P	1.244400	1.330530	0.291349
Si	0.791650	-3.386343	0.394707
Si	1.075204	-0.945496	2.288553
C	2.239742	-4.421203	1.004422
H	2.269382	-4.472599	2.099619
H	2.159667	-5.450625	0.631207
H	3.192376	-4.004799	0.660787
C	2.625510	-1.467638	3.217834
H	2.749152	-0.898477	4.147915
H	2.587924	-2.530176	3.485964
H	3.520630	-1.318845	2.602979
H	0.236038	-4.500131	-1.801142
H	1.653800	-3.444436	-1.899725
P	-1.987695	-0.105042	0.030028
C	-2.665845	-1.605402	0.847093
H	-3.684148	-1.422652	1.210607
H	-2.740427	-2.344987	0.039956
Si	-1.694654	-2.536550	2.177536
C	-2.980925	-3.265377	3.349623
H	-3.534934	-2.477196	3.875743
H	-3.711662	-3.880340	2.809692
H	-2.510521	-3.900552	4.110415
C	-0.760142	-3.918958	1.311972
H	-1.447138	-4.416192	0.614579
H	-0.468501	-4.670241	2.058780
C	-0.467700	-1.525888	3.189590
H	-0.969648	-0.665691	3.649972
H	-0.153769	-2.174918	4.020793
H	2.636413	-1.101466	-2.193478
H	1.506940	-0.518925	-1.656357
C	-3.332355	0.236533	-1.216904
C	-4.423012	-0.618649	-1.414643
C	-3.250817	1.382000	-2.019896
C	-5.387536	-0.347497	-2.384930
H	-4.537848	-1.516411	-0.817777

C	-4.218293	1.662957	-2.978489
H	-2.415652	2.063842	-1.911309
C	-5.291061	0.795307	-3.170222
H	-6.218114	-1.035342	-2.517974
H	-4.126210	2.560844	-3.582793
H	-6.042647	1.009130	-3.924604
C	-2.418169	1.207025	1.274142
C	-2.130344	2.540783	0.963779
C	-2.990897	0.936821	2.522178
C	-2.402365	3.567921	1.861487
H	-1.663847	2.784599	0.016379
C	-3.249790	1.959830	3.432632
H	-3.245805	-0.078540	2.805193
C	-2.958013	3.280400	3.105342
H	-2.161589	4.591167	1.589651
H	-3.689357	1.720441	4.396988
H	-3.161888	4.078182	3.813736
C	0.973668	3.154980	0.194745
C	1.047165	3.983630	1.317642
C	0.714521	3.736526	-1.051378
C	0.856456	5.358233	1.201534
H	1.239627	3.560167	2.298257
C	0.525513	5.110822	-1.169280
H	0.646623	3.115004	-1.938076
C	0.592101	5.926267	-0.041935
H	0.910654	5.984940	2.087458
H	0.322808	5.543702	-2.144743
H	0.440101	6.997891	-0.133301
C	3.072313	1.335087	0.023731
C	3.525474	1.505462	-1.289398
C	4.016884	1.210703	1.044146
C	4.884612	1.548573	-1.574788
H	2.803431	1.575923	-2.098360
C	5.381305	1.232749	0.758453
H	3.704369	1.084172	2.075573
C	5.819256	1.402068	-0.550429
H	5.213788	1.677394	-2.601936
H	6.101400	1.117837	1.563838
H	6.882486	1.422934	-0.772842
C	4.278650	-1.764588	-1.491827
O	3.544224	-1.412242	-2.519723
O	3.906528	-1.868637	-0.338464
H	5.311989	-1.984379	-1.795862
H	2.033978	-1.495503	0.260760

N	0.212017	-2.011925	-3.731313
H	-0.131710	-2.731461	-4.359639
H	0.086755	-1.091221	-4.137635
N	-1.880722	-2.849098	-2.129594
H	-2.603029	-2.185961	-2.400831
H	-1.954392	-3.678206	-2.715382

TSA7-8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.106381	-0.284293	-0.967621
N	1.087366	-1.660321	0.573732
C	1.148819	0.925665	2.004850
H	1.888089	1.409395	2.651899
H	0.163883	1.299879	2.308622
C	0.494659	-3.573483	-1.510530
C	-0.298265	0.725574	-2.341041
O	-0.462589	1.322421	-3.334602
P	-0.501534	-2.170716	-2.113374
P	1.308463	1.333455	0.228287
Si	0.726481	-3.397612	0.352910
Si	1.157905	-0.960586	2.208869
C	2.176050	-4.459213	0.901997
H	2.254828	-4.508124	1.994902
H	2.059986	-5.487204	0.534705
H	3.116413	-4.052986	0.515672
C	2.748707	-1.500612	3.049236
H	2.958854	-0.900839	3.943743
H	2.696807	-2.550499	3.361725
H	3.591136	-1.408684	2.354577
H	0.090735	-4.548714	-1.811690
H	1.488662	-3.454187	-1.961702
P	-1.977981	-0.051968	0.086576
C	-2.642750	-1.525021	0.951462
H	-3.639092	-1.307995	1.354226
H	-2.771422	-2.272891	0.159260
Si	-1.646931	-2.479610	2.249719
C	-2.913409	-3.160922	3.469879
H	-3.424090	-2.354517	4.011913
H	-3.681473	-3.754903	2.959023
H	-2.435532	-3.807825	4.215845

C	-0.793474	-3.888049	1.347516
H	-1.524640	-4.376410	0.690183
H	-0.479971	-4.639458	2.085413
C	-0.347010	-1.503632	3.197393
H	-0.798939	-0.635331	3.692305
H	0.000218	-2.166879	4.003629
H	2.118763	-1.042500	-1.948532
H	1.537836	-0.418030	-1.845771
C	-3.363411	0.307712	-1.107072
C	-4.471419	-0.535516	-1.254503
C	-3.304731	1.452400	-1.912724
C	-5.472449	-0.256121	-2.184051
H	-4.571945	-1.428407	-0.647919
C	-4.307431	1.740006	-2.832513
H	-2.463715	2.131381	-1.838076
C	-5.395343	0.882665	-2.977413
H	-6.316332	-0.933836	-2.278430
H	-4.232075	2.635944	-3.441753
H	-6.174457	1.102148	-3.701431
C	-2.303015	1.287819	1.326641
C	-2.015936	2.612401	0.980221
C	-2.811437	1.041960	2.607404
C	-2.223403	3.655132	1.877355
H	-1.601598	2.840373	0.005459
C	-3.005506	2.080837	3.515291
H	-3.066430	0.035203	2.918563
C	-2.712636	3.392291	3.153605
H	-1.983491	4.670688	1.577838
H	-3.394978	1.860877	4.505280
H	-2.864591	4.202033	3.861323
C	1.052542	3.155722	0.128955
C	1.187645	3.987839	1.243376
C	0.755950	3.733724	-1.109827
C	1.020125	5.365087	1.125418
H	1.411587	3.564835	2.217591
C	0.588218	5.110644	-1.229237
H	0.643065	3.108454	-1.989301
C	0.717082	5.930567	-0.110609
H	1.123804	5.996186	2.003582
H	0.355700	5.542180	-2.198512
H	0.583349	7.004446	-0.203073
C	3.118262	1.295963	-0.112121
C	3.527913	1.404361	-1.445411
C	4.091323	1.204245	0.883903

C	4.877616	1.408536	-1.775117
H	2.784169	1.459542	-2.235398
C	5.444448	1.198228	0.554684
H	3.810608	1.116612	1.928361
C	5.840991	1.296594	-0.774466
H	5.175373	1.481753	-2.816999
H	6.188596	1.108306	1.340933
H	6.896490	1.285346	-1.031302
C	4.078442	-1.950066	-1.349106
O	3.276022	-1.820922	-2.322850
O	3.823730	-1.842780	-0.137083
H	5.122534	-2.198764	-1.634165
H	2.067517	-1.587644	0.217006
N	-0.088342	-2.083810	-3.757686
H	-0.327994	-2.872320	-4.348996
H	-0.293875	-1.199527	-4.207142
N	-2.074381	-2.853916	-1.975717
H	-2.797087	-2.195357	-2.256783
H	-2.196206	-3.720109	-2.496073

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.145342	-0.395004	-0.960431
N	0.542898	-1.865834	0.383707
C	1.718585	0.346823	1.945465
H	2.676246	0.432854	2.470990
H	1.000490	1.035467	2.406073
C	-1.065022	-3.556510	-1.448196
C	0.295386	0.635839	-2.367732
O	0.451385	1.237772	-3.366747
P	-0.804019	-1.960501	-2.272823
P	1.823039	0.745673	0.174053
Si	-0.106887	-3.458635	0.195339
Si	0.998359	-1.414507	1.992391
C	1.205921	-4.812906	0.152046
H	1.790234	-4.865152	1.077432
H	0.755691	-5.800530	-0.013928
H	1.908373	-4.618518	-0.668744
C	2.292923	-2.545316	2.777288
H	2.633111	-2.137533	3.738357

H	1.899194	-3.550039	2.974169
H	3.169532	-2.649610	2.126185
H	-2.133741	-3.673391	-1.241412
H	-0.747792	-4.401677	-2.070685
P	-1.787867	0.360297	-0.037735
C	-2.719614	-1.005405	0.791484
H	-3.676301	-0.616676	1.161152
H	-2.992601	-1.679505	-0.032110
Si	-2.002891	-2.100718	2.199117
C	-3.462302	-2.354587	3.375804
H	-3.782365	-1.413979	3.842928
H	-4.331213	-2.777498	2.855340
H	-3.193225	-3.046413	4.183681
C	-1.395752	-3.765795	1.555581
H	-2.212819	-4.400904	1.189594
H	-0.951976	-4.290701	2.414946
C	-0.531093	-1.382404	3.119345
H	-0.725793	-0.369730	3.488959
H	-0.363037	-2.014068	4.004030
C	-3.132797	1.154405	-1.042768
C	-4.386492	1.431156	-0.483676
C	-2.898066	1.545124	-2.362224
C	-5.383700	2.047665	-1.230967
H	-4.587262	1.186107	0.555615
C	-3.894091	2.165816	-3.115769
H	-1.924282	1.378535	-2.807203
C	-5.142420	2.411296	-2.554709
H	-6.349064	2.250356	-0.776062
H	-3.687304	2.459462	-4.141110
H	-5.920799	2.893788	-3.138908
C	-1.664999	1.667198	1.258053
C	-0.958611	2.828914	0.927744
C	-2.265482	1.584964	2.517085
C	-0.836426	3.873089	1.838870
H	-0.493798	2.913438	-0.051026
C	-2.135357	2.624236	3.436488
H	-2.840694	0.708066	2.796967
C	-1.417755	3.768883	3.100895
H	-0.277061	4.761959	1.563102
H	-2.600410	2.537429	4.414401
H	-1.316466	4.577908	3.818660
C	2.269652	2.525633	0.075986
C	2.539102	3.287736	1.215935
C	2.352907	3.138762	-1.180014

C	2.881989	4.633970	1.105462
H	2.473728	2.835819	2.200669
C	2.690800	4.483712	-1.290480
H	2.148332	2.565977	-2.079024
C	2.955616	5.235689	-0.147178
H	3.088171	5.211052	2.002623
H	2.747312	4.945439	-2.271937
H	3.217402	6.286317	-0.234512
C	3.417679	-0.035317	-0.323441
C	4.634307	0.392555	0.219467
C	3.419973	-1.093887	-1.236214
C	5.826176	-0.231681	-0.132710
H	4.652277	1.223151	0.921077
C	4.613547	-1.719443	-1.590417
H	2.486905	-1.451826	-1.663567
C	5.817102	-1.291795	-1.037849
H	6.762859	0.110424	0.298222
H	4.598178	-2.543119	-2.298512
H	6.747637	-1.781375	-1.311140
N	-2.308524	-1.696748	-3.024530
H	-2.448850	-0.758317	-3.380710
H	-2.618956	-2.396275	-3.692441
N	0.401902	-2.406460	-3.403931
H	0.182608	-3.176712	-4.029972
H	0.781408	-1.622272	-3.924329

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.006401	-0.270914	-1.073553
N	0.431777	-2.191279	0.215495
C	1.690339	-0.083703	1.826765
H	2.604373	-0.051465	2.429104
H	0.997888	0.650837	2.253027
C	-1.012887	-3.296848	-2.037031
C	0.063815	0.971173	-2.283193
O	0.157727	1.708466	-3.196279
P	-1.300496	-1.512688	-2.355318
P	1.892381	0.381577	0.058811
Si	-0.640409	-3.547579	-0.211852
Si	0.865241	-1.784503	1.890733

C	0.279862	-5.174428	0.014990
H	0.485087	-5.384450	1.071614
H	-0.305319	-6.014836	-0.379603
H	1.240500	-5.164330	-0.514764
C	2.082167	-3.052515	2.564869
H	2.505036	-2.726562	3.523730
H	1.601328	-4.023939	2.731750
H	2.914604	-3.211070	1.868404
H	-1.833224	-3.931043	-2.397410
H	-0.111129	-3.567424	-2.599627
P	-1.667196	0.629235	0.201311
C	-2.885014	-0.538849	0.935440
H	-3.685383	0.000708	1.456517
H	-3.343328	-1.029822	0.066947
Si	-2.321267	-1.993328	2.004357
C	-3.694526	-2.292243	3.263431
H	-3.782961	-1.454833	3.967431
H	-4.666906	-2.414956	2.770259
H	-3.505048	-3.198401	3.852081
C	-2.155407	-3.506321	0.894919
H	-3.058673	-3.581223	0.274557
H	-2.137937	-4.402260	1.531907
C	-0.697536	-1.749854	2.928903
H	-0.733533	-0.814837	3.502147
H	-0.637232	-2.560511	3.669948
H	0.988449	-1.057476	-2.058313
H	1.282773	-2.297262	-0.342017
C	-2.799836	1.739835	-0.775978
C	-4.167993	1.494067	-0.936426
C	-2.259017	2.866461	-1.409222
C	-4.965080	2.335782	-1.713066
H	-4.633315	0.638500	-0.458760
C	-3.052794	3.714358	-2.172503
H	-1.200289	3.081795	-1.319593
C	-4.411356	3.450279	-2.332650
H	-6.023805	2.118025	-1.825273
H	-2.604192	4.580698	-2.650196
H	-5.030861	4.107338	-2.936332
C	-1.336068	1.775409	1.627550
C	-0.410447	2.807672	1.435353
C	-1.929864	1.654835	2.888327
C	-0.088787	3.691225	2.460209
H	0.088147	2.908384	0.476980
C	-1.600327	2.528211	3.923940

H	-2.659114	0.875638	3.083416
C	-0.679858	3.550331	3.713651
H	0.638934	4.476762	2.279104
H	-2.070772	2.408364	4.896021
H	-0.423387	4.231601	4.519912
C	2.575901	2.094449	0.103880
C	3.088596	2.676028	1.266617
C	2.595729	2.835591	-1.083323
C	3.603882	3.969997	1.245509
H	3.077504	2.128748	2.203952
C	3.111216	4.128477	-1.105299
H	2.195393	2.407411	-1.996352
C	3.615682	4.700420	0.060088
H	3.996259	4.407705	2.159321
H	3.115146	4.688453	-2.036142
H	4.017139	5.709664	0.044493
C	3.442033	-0.518230	-0.429476
C	3.703068	-0.690448	-1.794478
C	4.383913	-0.989390	0.491031
C	4.867357	-1.318974	-2.224363
H	2.973890	-0.344783	-2.520494
C	5.542272	-1.636289	0.063196
H	4.228484	-0.858942	1.557063
C	5.787150	-1.802739	-1.296127
H	5.050082	-1.441506	-3.288197
H	6.254594	-2.004652	0.796260
H	6.690276	-2.304550	-1.631778
N	-0.966576	-1.378123	-4.033767
H	-1.743150	-1.604879	-4.647008
H	-0.582203	-0.471441	-4.277015
N	-3.025966	-1.518029	-2.228344
H	-3.405291	-0.577667	-2.311850
H	-3.502675	-2.127095	-2.890441

$R^1=R^2=R^3=Et$

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.098334	-1.170868	0.228327
N	-0.124888	0.203359	-1.448874
C	-2.995354	0.398155	-0.786216

H	-3.828371	0.243498	-1.479764
H	-3.379349	1.045328	0.010057
C	2.823079	-0.118505	-1.247719
C	-0.157887	-2.363468	1.520282
O	-0.221547	-3.161284	2.375522
P	2.208851	-1.366842	-0.046945
P	-2.393870	-1.173572	-0.055695
Si	1.355008	0.715304	-2.134791
Si	-1.491114	1.217623	-1.630038
C	1.541710	0.322194	-3.977113
H	0.752618	0.796138	-4.573456
H	2.507586	0.664521	-4.372003
H	1.473404	-0.759703	-4.153533
C	-1.974531	1.549894	-3.432963
H	-2.910017	2.121872	-3.496171
H	-1.206084	2.127872	-3.962297
H	-2.116437	0.611058	-3.983407
H	3.356003	0.650300	-0.673615
H	3.554306	-0.529501	-1.951452
P	0.052038	0.600159	1.741506
C	1.105074	2.018345	1.203941
H	1.234752	2.709068	2.046428
H	2.101263	1.606981	0.996967
Si	0.609282	3.079245	-0.318903
C	1.020486	4.861974	0.167059
H	0.454425	5.194867	1.046468
H	2.087471	4.978042	0.397300
H	0.786475	5.550814	-0.654456
C	1.595080	2.581845	-1.845406
H	2.659323	2.838652	-1.758333
H	1.200370	3.166275	-2.690265
C	-1.197602	2.921917	-0.817939
H	-1.882911	3.101451	0.018784
H	-1.401165	3.716579	-1.551370
H	-0.019349	-2.085822	-1.287950
H	-0.238891	-2.639933	-0.770848
C	3.423738	-1.224522	1.348699
C	4.896901	-1.454036	1.014430
H	3.100922	-1.927959	2.126698
H	3.297477	-0.218913	1.766420
H	5.522462	-1.229028	1.886028
H	5.092000	-2.493810	0.733615
H	5.230265	-0.810360	0.192800
C	2.670365	-3.047146	-0.731823

C	3.725622	-3.116878	-1.835337
H	1.752551	-3.518589	-1.092881
H	2.985583	-3.641831	0.135360
H	3.952505	-4.163867	-2.067952
H	3.365049	-2.648489	-2.757363
H	4.663425	-2.627535	-1.556011
C	0.792982	0.040142	3.354261
C	1.160519	1.056937	4.432402
H	1.670239	-0.557215	3.099274
H	0.066854	-0.678809	3.754331
H	1.687411	0.555136	5.252731
H	1.823557	1.841632	4.051506
H	0.276600	1.534960	4.864554
C	-1.479787	1.454560	2.388403
C	-1.370169	2.895502	2.892650
H	-1.852705	0.809560	3.194452
H	-2.238928	1.419128	1.604905
H	-2.330535	3.215434	3.313978
H	-0.611645	3.019314	3.669421
H	-1.126001	3.589659	2.083385
C	-3.442652	-1.509662	1.430760
C	-4.963672	-1.503828	1.293407
H	-3.131004	-0.759725	2.166290
H	-3.097661	-2.471566	1.830399
H	-5.434725	-1.526840	2.283018
H	-5.321791	-0.605969	0.777075
H	-5.322803	-2.379490	0.744683
C	-2.919627	-2.465397	-1.289907
C	-4.247490	-2.301649	-2.031803
H	-2.892623	-3.418543	-0.744963
H	-2.116346	-2.517090	-2.031987
H	-4.472672	-3.215023	-2.594823
H	-5.091768	-2.105874	-1.366319
H	-4.196623	-1.482988	-2.757078

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.054011	-1.021648	0.397796
N	0.073485	-0.087830	-1.649630
C	-2.723788	-0.678566	-1.650143

H	-2.530201	-1.504333	-2.345851
H	-3.762784	-0.364883	-1.797278
C	2.875625	0.188080	-0.779847
C	-0.093307	-2.092027	1.785307
O	-0.107627	-2.814523	2.707470
P	2.209166	-1.293773	0.075371
P	-2.371975	-1.241326	0.071008
Si	1.554720	0.700580	-2.057774
Si	-1.435481	0.644506	-2.051087
C	2.206450	0.233782	-3.767028
H	1.480546	0.492554	-4.547824
H	3.143257	0.757307	-3.998944
H	2.398783	-0.843887	-3.844531
C	-1.605260	1.086709	-3.882575
H	-2.619099	1.443483	-4.107323
H	-0.910186	1.879822	-4.185814
H	-1.411812	0.213915	-4.518179
H	2.988011	0.985950	-0.038017
H	3.860626	0.032065	-1.234629
P	0.148210	0.849953	1.737501
C	0.701194	2.459589	1.009327
H	0.548321	3.259585	1.743005
H	1.788894	2.388983	0.883911
Si	0.009451	3.031535	-0.667452
C	-0.173512	4.908388	-0.560150
H	-0.921124	5.193411	0.191229
H	0.773466	5.388747	-0.283431
H	-0.492727	5.334276	-1.519435
C	1.281629	2.574395	-1.983822
H	2.227505	3.098727	-1.786712
H	0.933999	2.930085	-2.964990
C	-1.663309	2.246796	-1.065214
H	-2.196886	2.066204	-0.122040
H	-2.276336	2.956601	-1.638187
H	-0.174786	-2.281806	-0.791141
H	-0.051032	-1.466900	-1.310580
C	3.396896	-1.757812	1.435783
C	4.743974	-1.037033	1.439932
H	3.548704	-2.841473	1.356985
H	2.886721	-1.598860	2.389677
H	5.373952	-1.408501	2.256338
H	5.289573	-1.182790	0.502157
H	4.620470	0.042236	1.583527
C	2.539939	-2.636944	-1.162798

C	3.985497	-2.863259	-1.599771
H	1.912399	-2.415450	-2.033901
H	2.124103	-3.552086	-0.723603
H	4.032936	-3.667935	-2.342626
H	4.418177	-1.969010	-2.061287
H	4.626614	-3.155120	-0.760649
C	1.413257	0.647553	3.086625
C	1.526721	1.714324	4.173507
H	2.375245	0.556605	2.568059
H	1.220819	-0.329649	3.545444
H	2.373051	1.489002	4.833225
H	1.693833	2.712025	3.752887
H	0.629062	1.751519	4.799270
C	-1.362905	1.338901	2.711627
C	-1.561852	2.794260	3.135631
H	-1.378782	0.672812	3.584798
H	-2.216131	1.044470	2.104780
H	-2.464887	2.880347	3.751578
H	-0.726363	3.193586	3.716679
H	-1.702538	3.443748	2.264273
C	-3.781744	-0.468793	1.007497
C	-5.197601	-0.943351	0.679377
H	-3.718918	0.611505	0.831113
H	-3.581391	-0.627787	2.073722
H	-5.927683	-0.360862	1.253272
H	-5.437729	-0.815887	-0.381454
H	-5.345333	-1.996809	0.936572
C	-2.829545	-3.048264	0.158077
C	-3.725158	-3.608930	-0.945944
H	-3.288896	-3.203525	1.143188
H	-1.886079	-3.601240	0.172256
H	-3.989239	-4.649258	-0.722369
H	-4.654624	-3.044633	-1.065213
H	-3.208472	-3.606960	-1.911393

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.143139	-0.745681	-0.775775
N	0.038198	-0.413607	1.478608
C	2.931240	0.151862	1.059175

H	3.647969	-0.436102	1.645256
H	3.440418	1.089849	0.812586
C	-2.896953	-0.598062	0.838949
C	0.318531	-1.174119	-2.470281
O	0.452362	-1.487461	-3.589092
P	-2.162054	-1.081892	-0.793133
P	2.435429	-0.770054	-0.473283
Si	-1.593459	-0.212794	2.156198
Si	1.400277	0.536061	2.108859
C	-1.808880	-1.379064	3.611441
H	-1.127278	-1.124535	4.431774
H	-2.833164	-1.348138	4.003479
H	-1.579858	-2.407855	3.311339
C	1.744915	0.035617	3.890836
H	2.657382	0.515881	4.266975
H	0.925068	0.321476	4.561546
H	1.878179	-1.049740	3.972966
H	-3.470663	0.322629	0.671891
H	-3.615841	-1.335440	1.210803
P	-0.052882	1.505633	-1.291296
C	-1.181045	2.529380	-0.238186
H	-1.286743	3.527783	-0.679531
H	-2.175992	2.070483	-0.300910
Si	-0.791223	2.763618	1.610615
C	-1.203315	4.555079	2.032672
H	-0.586471	5.258925	1.459899
H	-2.254223	4.783075	1.814840
H	-1.033969	4.757068	3.097395
C	-1.817500	1.587596	2.660054
H	-2.884525	1.844119	2.619155
H	-1.506164	1.724643	3.705927
C	0.993368	2.379904	2.063857
H	1.695726	2.933739	1.431159
H	1.142491	2.766380	3.083130
C	0.264993	-3.545389	0.721170
O	0.181403	-2.851542	-0.327874
O	0.466369	-3.154647	1.889821
H	0.150304	-4.639599	0.561522
H	0.276200	-1.416175	1.650398
C	3.164265	-2.437936	-0.133611
C	4.685886	-2.541714	-0.048858
H	2.777204	-3.106422	-0.910295
H	2.710333	-2.769377	0.805998
H	4.974621	-3.562301	0.228109

H	5.167997	-2.316194	-1.006079
H	5.106453	-1.867793	0.706415
C	3.509590	-0.174494	-1.876732
C	4.748205	0.653657	-1.544472
H	2.862820	0.382520	-2.559697
H	3.795855	-1.081062	-2.424676
H	5.333846	0.839198	-2.452332
H	4.477631	1.630602	-1.128159
H	5.399676	0.152678	-0.821702
C	1.486000	2.566388	-1.358403
C	1.351969	4.087580	-1.330774
H	2.001090	2.268236	-2.278266
H	2.137826	2.246027	-0.541672
H	2.342844	4.552772	-1.393281
H	0.762962	4.464003	-2.172225
H	0.884017	4.444354	-0.407220
C	-0.709123	1.790327	-3.020995
C	-1.577107	3.013639	-3.309483
H	-1.261533	0.889091	-3.296693
H	0.174830	1.796145	-3.671277
H	-1.855229	3.028259	-4.369852
H	-2.506657	2.998251	-2.729472
H	-1.067766	3.957208	-3.091819
C	-3.321447	-0.233602	-1.973199
C	-4.808600	-0.534527	-1.787638
H	-3.004832	-0.518095	-2.984715
H	-3.151049	0.845789	-1.889794
H	-5.406795	0.032334	-2.510253
H	-5.031592	-1.595855	-1.939349
H	-5.155163	-0.260955	-0.785138
C	-2.629807	-2.863008	-1.110817
C	-3.343985	-3.610385	0.011921
H	-1.685933	-3.361150	-1.336845
H	-3.239508	-2.887447	-2.021472
H	-3.482378	-4.661559	-0.266218
H	-2.765022	-3.592756	0.942775
H	-4.335252	-3.192564	0.221420

A7

Coordinates (Angstroms)		
X	Y	Z

Mn	0.126798	-0.243444	-1.018670
N	0.132372	-0.979589	1.116747
C	2.946935	-0.056952	0.897335
H	3.826212	-0.634101	1.204852
H	3.236716	0.996962	0.944783
C	-2.597698	-1.591867	0.404963
C	0.240291	0.099887	-2.743466
O	0.353855	0.296376	-3.888018
P	-2.188187	-0.556712	-1.048040
P	2.423583	-0.466057	-0.818553
Si	-1.493196	-1.106458	1.841368
Si	1.488201	-0.353349	2.076404
C	-1.521296	-2.478320	3.124257
H	-1.056017	-2.173442	4.069259
H	-2.552220	-2.780512	3.349030
H	-0.979335	-3.351493	2.744742
C	2.008112	-1.635944	3.345597
H	2.963156	-1.369611	3.815925
H	1.266635	-1.751297	4.144463
H	2.119721	-2.612792	2.859671
H	-3.665643	-1.618822	0.648023
H	-2.264756	-2.610357	0.150922
P	0.034892	2.050720	-0.608355
C	-0.910355	2.726179	0.822421
H	-0.693327	3.796724	0.922013
H	-1.977889	2.671750	0.582774
Si	-0.743919	1.922138	2.528966
C	-1.175184	3.271460	3.773763
H	-0.443622	4.088912	3.746404
H	-2.163341	3.702851	3.570272
H	-1.191592	2.878354	4.797776
C	-1.981872	0.516475	2.664469
H	-2.958227	0.853774	2.291421
H	-2.128874	0.304071	3.733377
C	0.970675	1.250727	2.926522
H	1.729755	2.030515	2.780651
H	0.964824	1.051023	4.009176
H	-0.221328	-2.013745	-1.175727
H	0.467936	-1.866943	-1.540410
C	0.015273	-4.419038	0.097489
O	-0.948632	-4.077161	-0.613455
O	0.727698	-3.700261	0.854849
H	0.299923	-5.500339	0.071004
H	0.366484	-1.987594	0.921749

C	2.970351	-2.224106	-1.005013
C	4.458651	-2.524886	-0.843454
H	2.636246	-2.530317	-2.005624
H	2.375043	-2.815537	-0.297602
H	4.632316	-3.600959	-0.955132
H	5.068317	-2.014094	-1.597111
H	4.831826	-2.239428	0.146099
C	3.570773	0.411391	-1.994855
C	4.847701	1.007189	-1.405430
H	2.994221	1.188042	-2.507738
H	3.821223	-0.324591	-2.769088
H	5.477134	1.418162	-2.202855
H	4.626890	1.823589	-0.708832
H	5.436657	0.259879	-0.864425
C	-2.722834	-1.511450	-2.552203
C	-3.729285	-2.641321	-2.337376
H	-1.810841	-1.926065	-2.992809
H	-3.101682	-0.774491	-3.273208
H	-4.016952	-3.072232	-3.303546
H	-3.283163	-3.439575	-1.737518
H	-4.642394	-2.302842	-1.838116
C	-3.440615	0.809581	-0.962239
C	-4.908961	0.426638	-1.144673
H	-3.162064	1.559956	-1.710724
H	-3.308377	1.282281	0.016694
H	-5.545294	1.309792	-1.016184
H	-5.101830	0.025538	-2.144575
H	-5.231464	-0.320142	-0.411818
C	1.638633	2.968647	-0.381398
C	1.639523	4.494523	-0.465213
H	2.331988	2.573692	-1.128985
H	2.028957	2.660652	0.594026
H	2.647238	4.875062	-0.262446
H	1.353741	4.846455	-1.461286
H	0.966858	4.955994	0.265270
C	-0.694098	2.948424	-2.075103
C	-1.513832	4.213846	-1.829058
H	-1.309573	2.221719	-2.612834
H	0.149368	3.163462	-2.743711
H	-1.825389	4.645308	-2.787234
H	-2.422634	3.998511	-1.257050
H	-0.956334	4.981496	-1.285378

A8

	Coordinates (Angstroms)		
	X	Y	Z
Mn	-0.125951	-0.340346	-0.938577
N	-0.465559	-0.601500	1.345181
C	2.126907	-1.957832	1.085088
H	2.226613	-2.961669	1.516051
H	3.141250	-1.546543	1.040615
C	-2.977644	0.556992	0.556316
C	-0.015096	-0.516511	-2.669692
O	0.038461	-0.704294	-3.827495
P	-2.076036	0.841288	-1.031074
P	1.371922	-2.013976	-0.613386
Si	-1.723436	0.486885	1.957100
Si	1.063088	-0.855698	2.198225
C	-2.570860	-0.247889	3.470210
H	-1.952829	-0.173560	4.372780
H	-3.516999	0.269023	3.677231
H	-2.793689	-1.308386	3.304995
C	0.763316	-1.758914	3.823041
H	1.710041	-2.069923	4.283261
H	0.235340	-1.131259	4.550678
H	0.157665	-2.659120	3.662617
H	-3.791566	1.269435	0.735552
H	-3.430182	-0.441516	0.513547
P	1.375846	1.404743	-0.947215
C	1.144392	2.812668	0.228175
H	1.970972	3.529811	0.157247
H	0.250156	3.353104	-0.104080
Si	0.889660	2.365181	2.047595
C	1.524853	3.824982	3.060869
H	2.597442	3.989449	2.897124
H	1.003996	4.752256	2.790129
H	1.375062	3.663787	4.135638
C	-0.947125	2.137629	2.418123
H	-1.503778	2.967094	1.961401
H	-1.077628	2.260325	3.503365
C	1.850130	0.818142	2.554895
H	2.854856	0.861999	2.116232
H	2.003869	0.876944	3.642490
H	-2.239213	-2.284075	-0.711157
H	-1.246567	-1.524219	-0.980625

C	-3.001368	-3.358177	0.701237
O	-3.055826	-2.898095	-0.521155
O	-2.144634	-3.111741	1.533742
H	-3.847959	-4.026367	0.919879
H	-0.922959	-1.515347	1.234017
C	-3.216236	0.252822	-2.382180
C	-4.695433	0.076812	-2.039508
H	-2.807423	-0.702614	-2.723128
H	-3.093498	0.953778	-3.218603
H	-5.258964	-0.199130	-2.938660
H	-4.834744	-0.727118	-1.309709
H	-5.146435	0.985124	-1.628752
C	-2.233091	2.692103	-1.187824
C	-3.620447	3.299547	-1.391866
H	-1.581261	2.995346	-2.015265
H	-1.784866	3.109378	-0.279195
H	-3.553887	4.393870	-1.416814
H	-4.067791	2.977680	-2.337624
H	-4.310683	3.032224	-0.584553
C	1.358691	2.272344	-2.593903
C	2.232427	3.505835	-2.805651
H	0.308240	2.515619	-2.786805
H	1.616778	1.503860	-3.331602
H	2.029458	3.947964	-3.788242
H	2.044302	4.280157	-2.053776
H	3.298338	3.257703	-2.779260
C	3.213654	1.058992	-0.772045
C	4.147702	2.132262	-0.210262
H	3.553309	0.770383	-1.775060
H	3.310142	0.158347	-0.160246
H	5.186520	1.784157	-0.259581
H	4.090164	3.075354	-0.760362
H	3.930621	2.352262	0.840455
C	0.594905	-3.697043	-0.621902
C	1.497961	-4.922354	-0.500179
H	0.018579	-3.739806	-1.553933
H	-0.144994	-3.685453	0.186930
H	0.893257	-5.836877	-0.479130
H	2.186512	-5.006842	-1.347801
H	2.095061	-4.907666	0.418933
C	2.776792	-2.239538	-1.818326
C	4.126544	-2.701058	-1.272665
H	2.894439	-1.289082	-2.346487
H	2.407935	-2.949274	-2.569860

H	4.825617	-2.892797	-2.095094
H	4.580783	-1.936752	-0.632053
H	4.042091	-3.619709	-0.683761

TSA7-8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.208838	0.212452	-0.994557
N	-0.509013	0.650718	1.234502
C	-2.673068	-1.297063	0.856610
H	-3.682271	-1.096362	1.231359
H	-2.592564	-2.387037	0.766808
C	1.577224	2.549388	0.616097
C	-0.255994	0.089731	-2.740862
O	-0.349044	0.039274	-3.907156
P	1.665152	1.584015	-0.951526
P	-2.374925	-0.553078	-0.813914
Si	0.893609	1.447533	1.978855
Si	-1.357400	-0.666380	2.066400
C	0.362514	2.547417	3.409803
H	0.067051	1.968022	4.292348
H	1.182784	3.211541	3.711964
H	-0.491644	3.170714	3.122484
C	-2.214625	-0.012487	3.608909
H	-2.937476	-0.741548	3.997568
H	-1.501471	0.200538	4.414099
H	-2.754129	0.916451	3.388944
H	2.522028	3.037553	0.881248
H	0.828181	3.339342	0.478978
P	0.902554	-1.815777	-0.863099
C	2.197209	-2.042542	0.431945
H	2.604561	-3.059465	0.394355
H	3.029716	-1.379626	0.173278
Si	1.705163	-1.655470	2.217488
C	2.759879	-2.761602	3.323935
H	2.556004	-3.824404	3.142141
H	3.829316	-2.594527	3.143955
H	2.568082	-2.564797	4.386027
C	2.094295	0.144646	2.615860
H	3.117069	0.369266	2.284547
H	2.112828	0.238412	3.711742

C	-0.119849	-1.999963	2.562236
H	-0.399851	-2.963499	2.118189
H	-0.217738	-2.139979	3.648844
H	-1.072685	2.556173	-0.851316
H	-0.919800	1.715424	-1.233149
C	-2.050918	3.814974	0.576511
O	-1.345889	3.768416	-0.491922
O	-2.366633	2.870283	1.308452
H	-2.395085	4.834421	0.837011
H	-1.212350	1.403281	1.118696
C	1.626058	2.825889	-2.338754
C	1.940020	4.281509	-1.995935
H	0.621491	2.765627	-2.767511
H	2.311485	2.449092	-3.109579
H	1.959778	4.884645	-2.911273
H	1.166327	4.700077	-1.345223
H	2.906836	4.400075	-1.497449
C	3.450960	1.060321	-0.943070
C	4.515397	2.145403	-1.103944
H	3.577054	0.307191	-1.729289
H	3.609145	0.542413	0.009241
H	5.515529	1.703052	-1.026447
H	4.449011	2.639010	-2.078357
H	4.437778	2.915242	-0.328675
C	1.856281	-2.108726	-2.434687
C	2.834989	-3.277080	-2.518942
H	2.377113	-1.168120	-2.643312
H	1.100447	-2.200088	-3.223562
H	3.376611	-3.241116	-3.471465
H	3.581061	-3.251074	-1.717288
H	2.322526	-4.242951	-2.476972
C	-0.039081	-3.431891	-0.735336
C	0.626950	-4.657802	-0.107960
H	-0.346396	-3.667298	-1.762292
H	-0.962394	-3.225569	-0.188873
H	-0.041822	-5.522823	-0.188986
H	1.570306	-4.924602	-0.591629
H	0.833213	-4.507964	0.957053
C	-3.004218	-1.820147	-2.009787
C	-4.448700	-2.291804	-1.857642
H	-2.323357	-2.674391	-1.950711
H	-2.850046	-1.383863	-3.004805
H	-4.661465	-3.097630	-2.569883
H	-4.645263	-2.679181	-0.851285

H	-5.161635	-1.485618	-2.056692
C	-3.656637	0.789632	-0.992216
C	-4.909136	0.739349	-0.119897
H	-3.924627	0.786290	-2.057170
H	-3.143264	1.734432	-0.813962
H	-5.611753	1.518294	-0.437959
H	-5.432126	-0.220682	-0.174100
H	-4.663767	0.937652	0.928191

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.049932	-0.804035	0.613885
N	-0.025058	-0.274419	-1.375992
C	-2.969873	-0.236243	-1.080261
H	-3.639413	-0.801044	-1.737251
H	-3.558283	0.581371	-0.645386
C	2.895337	-0.155666	-0.905561
C	-0.093866	-1.663941	2.141641
O	-0.123070	-2.248624	3.160737
P	2.167428	-1.231213	0.375603
P	-2.263272	-1.225383	0.289869
Si	1.462528	0.202009	-2.114118
Si	-1.452548	0.491689	-1.972949
C	1.850656	-0.723645	-3.716504
H	1.045548	-0.621492	-4.453804
H	2.774956	-0.354148	-4.179940
H	1.982214	-1.796697	-3.524829
C	-1.712194	0.285575	-3.837149
H	-2.686030	0.690291	-4.143103
H	-0.946334	0.812591	-4.420458
H	-1.682063	-0.771249	-4.130661
H	3.192352	0.785455	-0.427476
H	3.786058	-0.569642	-1.392574
P	-0.000192	1.224292	1.573811
C	0.832136	2.559205	0.602380
H	0.766404	3.499588	1.165056
H	1.899659	2.300021	0.588243
Si	0.323738	2.936683	-1.202111
C	0.470398	4.813895	-1.379027
H	-0.232434	5.338220	-0.718705

H	1.480884	5.163187	-1.130766
H	0.255383	5.130228	-2.407273
C	1.474623	2.075523	-2.421853
H	2.497975	2.471016	-2.366691
H	1.107186	2.302034	-3.434406
C	-1.416821	2.366755	-1.627748
H	-2.124709	2.641491	-0.835685
H	-1.741524	2.906857	-2.529609
C	2.205842	-2.917726	-0.398692
C	3.560163	-3.508725	-0.786122
H	1.551747	-2.852236	-1.276991
H	1.695241	-3.583333	0.309239
H	3.422864	-4.469422	-1.295931
H	4.115275	-2.852981	-1.465557
H	4.184213	-3.692353	0.094873
C	3.386230	-1.375875	1.769482
C	4.847231	-1.068215	1.441679
H	3.284409	-2.393954	2.167077
H	3.039021	-0.712442	2.568583
H	5.474379	-1.213175	2.328745
H	5.238383	-1.712242	0.648371
H	4.971966	-0.030540	1.114175
C	0.918642	1.319045	3.186099
C	0.866116	2.594864	4.023883
H	1.960527	1.096807	2.923592
H	0.572142	0.467257	3.782992
H	1.551824	2.512126	4.875514
H	1.163869	3.479776	3.450690
H	-0.135478	2.769373	4.430080
C	-1.660582	1.963776	1.984991
C	-1.811361	3.483460	2.068889
H	-1.964497	1.491054	2.928693
H	-2.353348	1.584656	1.226688
H	-2.833374	3.741749	2.370720
H	-1.127997	3.939724	2.789570
H	-1.631803	3.956132	1.097370
C	-3.556453	-1.266911	1.607750
C	-4.909992	-1.862350	1.225476
H	-3.680550	-0.230896	1.945411
H	-3.120261	-1.810648	2.454805
H	-5.627235	-1.749513	2.046610
H	-5.332980	-1.366781	0.344226
H	-4.828963	-2.932334	1.006934
C	-2.200928	-2.984248	-0.324581

C	-3.135045	-3.393825	-1.461999
H	-2.362081	-3.614813	0.559290
H	-1.164045	-3.160728	-0.635377
H	-3.038603	-4.468094	-1.657327
H	-4.186265	-3.188612	-1.236746
H	-2.881015	-2.869986	-2.389458

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.120743	-1.115109	0.354906
N	-0.075589	0.108802	-1.633360
C	-2.965839	0.306593	-0.915473
H	-3.786990	0.088397	-1.606881
H	-3.368921	1.014062	-0.179763
C	2.847119	-0.136409	-0.940291
C	-0.227659	-2.225696	1.688047
O	-0.313060	-3.002955	2.567519
P	2.066085	-1.521101	0.003792
P	-2.360623	-1.185268	0.008938
Si	1.564678	0.625507	-2.101330
Si	-1.512372	1.152063	-1.780178
C	1.896878	0.039862	-3.857417
H	1.146213	0.419853	-4.561072
H	2.881786	0.372893	-4.207810
H	1.882839	-1.056261	-3.916335
C	-1.909630	1.399915	-3.605955
H	-2.836766	1.972360	-3.736175
H	-1.109803	1.946906	-4.121306
H	-2.038266	0.439562	-4.121237
H	3.151208	0.636125	-0.226639
H	3.750802	-0.430471	-1.487666
P	0.110989	0.730723	1.700548
C	1.077627	2.223117	1.143523
H	1.070686	2.977191	1.940602
H	2.123315	1.899977	1.061694
Si	0.618439	3.111688	-0.467761
C	0.930179	4.952532	-0.203979
H	0.274344	5.364758	0.573240
H	1.966347	5.139342	0.105008
H	0.751841	5.521690	-1.124522

C	1.648635	2.488894	-1.919731
H	2.700583	2.786491	-1.813411
H	1.271749	2.981869	-2.827669
C	-1.167596	2.824507	-0.985151
H	-1.849775	2.987801	-0.142511
H	-1.414007	3.597946	-1.727272
C	2.382319	-2.945319	-1.149343
C	3.826356	-3.285444	-1.513169
H	1.798800	-2.736249	-2.054091
H	1.888870	-3.806428	-0.683213
H	3.852384	-4.142017	-2.197287
H	4.332726	-2.454655	-2.017611
H	4.419413	-3.555336	-0.632355
C	3.252115	-1.948555	1.386463
C	4.617352	-1.263355	1.378187
H	3.379439	-3.037958	1.357734
H	2.737473	-1.741341	2.328706
H	5.241270	-1.641420	2.196609
H	5.156804	-1.432945	0.440330
H	4.523794	-0.179801	1.513138
C	1.047763	0.336156	3.263668
C	1.094197	1.342125	4.411451
H	2.070488	0.125427	2.929849
H	0.645818	-0.617030	3.625394
H	1.755590	0.972441	5.204259
H	1.480882	2.316915	4.094066
H	0.106665	1.493595	4.859353
C	-1.434172	1.541342	2.389045
C	-1.415452	3.003189	2.839248
H	-1.749850	0.896322	3.220110
H	-2.204815	1.427741	1.621505
H	-2.390988	3.277918	3.258449
H	-0.661513	3.204640	3.604088
H	-1.222259	3.681884	2.001418
C	-3.508138	-1.319524	1.461198
C	-5.013825	-1.396438	1.218677
H	-3.275379	-0.463032	2.101894
H	-3.167185	-2.202351	2.016595
H	-5.555229	-1.333526	2.170241
H	-5.365941	-0.575102	0.583379
H	-5.299989	-2.339970	0.743788
C	-2.926532	-2.607250	-1.065147
C	-4.158965	-2.450291	-1.956583
H	-3.050531	-3.450895	-0.372891

H	-2.062022	-2.869199	-1.681300
H	-4.429719	-3.418870	-2.393360
H	-5.035299	-2.072420	-1.422931
H	-3.960276	-1.768495	-2.791360
H	-0.201968	-2.363928	-0.655649
H	-0.266049	-0.809273	-2.041430

R^1=R^3=Ph, R^2=H

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.085211	-0.300534	-0.301196
N	0.053137	1.167754	1.273853
C	2.833892	1.591645	0.451914
H	3.768287	1.558053	1.023768
H	3.027135	2.232988	-0.415950
C	-2.856789	0.642720	1.159077
C	0.167510	-1.550281	-1.545362
O	0.235760	-2.382860	-2.361937
P	-2.158999	-0.622950	0.035116
P	2.367990	-0.052419	-0.212169
Si	-1.429286	1.553070	2.040811
Si	1.337694	2.293657	1.404274
C	-1.485060	1.112217	3.878940
H	-0.805240	1.750025	4.457693
H	-2.489790	1.231410	4.305848
H	-1.165354	0.075282	4.044237
C	1.853400	2.672744	3.186224
H	2.784065	3.254131	3.224154
H	1.084726	3.261941	3.703074
H	2.001645	1.754216	3.767148
H	-3.367773	1.377009	0.526124
H	-3.616865	0.238925	1.836848
P	-0.183485	1.481555	-1.700215
C	-1.350236	2.858331	-1.305635
H	-1.388993	3.518751	-2.181526
H	-2.354579	2.426877	-1.209622
Si	-0.964963	3.970779	0.211789
C	-1.574311	5.689519	-0.283811
H	-1.039467	6.070115	-1.163073
H	-2.645058	5.677492	-0.525386

H	-1.429108	6.410573	0.530178
C	-1.827418	3.393508	1.784294
H	-2.911784	3.563180	1.753546
H	-1.438164	4.010784	2.607785
C	0.876540	3.961263	0.589142
H	1.462097	4.137237	-0.323042
H	1.102021	4.794416	1.270331
H	0.276502	-1.161574	1.267290
H	0.311545	-1.751164	0.753774
C	-2.462392	-2.226768	0.881605
C	-2.590154	-2.320958	2.269373
C	-2.443457	-3.403732	0.123712
C	-2.708951	-3.564563	2.886875
H	-2.591935	-1.425199	2.883474
C	-2.564799	-4.644464	0.739738
H	-2.333522	-3.350929	-0.956402
C	-2.698342	-4.728684	2.124700
H	-2.810877	-3.620659	3.967002
H	-2.553671	-5.548130	0.136944
H	-2.792704	-5.697544	2.606387
C	-3.373603	-0.711857	-1.342373
C	-2.946822	-0.727235	-2.671595
C	-4.747415	-0.765104	-1.072340
C	-3.872179	-0.788923	-3.713386
H	-1.885817	-0.701797	-2.896243
C	-5.670626	-0.825745	-2.108850
H	-5.095816	-0.764752	-0.042549
C	-5.233445	-0.835670	-3.433772
H	-3.524440	-0.802240	-4.742378
H	-6.732921	-0.868274	-1.885947
H	-5.956244	-0.882559	-4.243245
C	3.450594	-0.230101	-1.686129
C	4.843113	-0.303387	-1.551449
C	2.896259	-0.225122	-2.967597
C	5.659562	-0.370797	-2.674598
H	5.290126	-0.315325	-0.560813
C	3.713703	-0.288636	-4.095230
H	1.818422	-0.181396	-3.089441
C	5.094961	-0.362464	-3.950097
H	6.737416	-0.433104	-2.555729
H	3.266548	-0.287410	-5.084934
H	5.733020	-0.416386	-4.827573
C	3.101672	-1.263383	0.953437
C	3.275718	-2.586307	0.527476

C	3.363598	-0.943445	2.287013
C	3.717174	-3.561731	1.414185
H	3.064032	-2.854036	-0.504990
C	3.800668	-1.923022	3.177228
H	3.222465	0.071206	2.646729
C	3.980079	-3.232516	2.743522
H	3.853169	-4.582346	1.067981
H	3.999211	-1.659000	4.212076
H	4.321007	-3.995222	3.437562
H	-0.487512	1.273939	-3.068549
H	0.980383	2.252271	-1.938727

TSA5-1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.011429	0.432563	-0.013392
N	-0.004366	-0.957238	-1.740146
C	2.776600	-0.277832	-1.781424
H	2.599987	0.401185	-2.626675
H	3.839316	-0.540108	-1.802712
C	-2.855373	-1.213401	-0.986589
C	-0.037391	1.792011	1.103110
O	-0.040147	2.707034	1.830258
P	-2.295269	0.245041	-0.009671
P	2.261727	0.656595	-0.288484
Si	-1.435734	-1.857274	-2.081299
Si	1.536825	-1.693796	-1.992506
C	-1.992814	-1.716812	-3.875959
H	-1.218150	-2.068068	-4.568417
H	-2.902494	-2.300033	-4.068684
H	-2.208914	-0.669675	-4.124964
C	1.761155	-2.413293	-3.724752
H	2.780524	-2.795892	-3.865340
H	1.074378	-3.246991	-3.917856
H	1.582994	-1.651403	-4.493372
H	-3.137729	-2.027065	-0.312083
H	-3.747197	-0.973619	-1.575369
P	0.125066	-1.139128	1.619154
C	-0.534462	-2.841561	1.328419
H	-0.340828	-3.441410	2.226271
H	-1.624641	-2.759890	1.249037

Si	0.118492	-3.793337	-0.192696
C	0.296497	-5.594387	0.342766
H	1.044114	-5.704735	1.138316
H	-0.653053	-5.994974	0.720356
H	0.609938	-6.227816	-0.496429
C	-1.121997	-3.666522	-1.610051
H	-2.060581	-4.176358	-1.351769
H	-0.709244	-4.209095	-2.473595
C	1.784509	-3.100200	-0.747459
H	2.331625	-2.758041	0.141018
H	2.388694	-3.901618	-1.195167
H	-0.137641	1.388332	-1.454374
H	-0.098256	0.483356	-1.771062
C	-3.121875	0.109866	1.636567
C	-3.081336	1.239425	2.466126
C	-3.711571	-1.054956	2.131294
C	-3.608666	1.200871	3.751079
H	-2.635600	2.160300	2.102283
C	-4.236414	-1.097240	3.422939
H	-3.780103	-1.948175	1.518843
C	-4.184673	0.028112	4.237373
H	-3.567751	2.089242	4.374647
H	-4.689696	-2.014642	3.787682
H	-4.595350	-0.004728	5.242249
C	-3.279965	1.628775	-0.728450
C	-4.670376	1.517052	-0.859540
C	-2.660864	2.819202	-1.110348
C	-5.419964	2.565867	-1.377904
H	-5.172340	0.606162	-0.541774
C	-3.412117	3.875139	-1.625929
H	-1.586449	2.920328	-1.000857
C	-4.789813	3.748790	-1.764702
H	-6.496795	2.463633	-1.477225
H	-2.915790	4.796288	-1.917542
H	-5.375276	4.570067	-2.168116
C	2.964852	2.334420	-0.581447
C	4.340240	2.572093	-0.470193
C	2.129024	3.381471	-0.976763
C	4.865424	3.829977	-0.745113
H	5.006260	1.772658	-0.156537
C	2.654894	4.641673	-1.254756
H	1.061623	3.207268	-1.065537
C	4.022556	4.868535	-1.138085
H	5.933761	4.001408	-0.649112

H	1.991180	5.446678	-1.557279
H	4.433261	5.851996	-1.348167
C	3.342612	0.074576	1.076129
C	4.239398	-0.989773	0.970761
C	3.202591	0.715832	2.315016
C	4.979017	-1.407406	2.078338
H	4.369813	-1.508622	0.026445
C	3.943492	0.305372	3.416012
H	2.501049	1.539660	2.418975
C	4.833606	-0.762579	3.301245
H	5.672280	-2.237751	1.978543
H	3.821807	0.815271	4.367202
H	5.409870	-1.087848	4.162490
H	-0.495543	-0.844160	2.855247
H	1.386627	-1.485309	2.153943

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.001827	-0.295150	0.329797
N	0.062744	0.843756	-1.654668
C	-2.635059	-0.006285	-1.767122
H	-2.236512	-0.738324	-2.480932
H	-3.699506	0.106756	-1.991053
C	2.815721	1.394351	-0.705723
C	-0.059918	-1.317707	1.762688
O	-0.120027	-2.016283	2.696025
P	2.302899	-0.050024	0.320979
P	-2.265881	-0.667556	-0.097227
Si	1.500234	1.816600	-2.001148
Si	-1.533404	1.489310	-2.069812
C	2.121169	1.409377	-3.725577
H	1.436202	1.797386	-4.489062
H	3.111999	1.840039	-3.916610
H	2.179707	0.323818	-3.867402
C	-1.653275	1.944436	-3.892089
H	-2.690273	2.181790	-4.163114
H	-1.043557	2.820304	-4.146199
H	-1.327014	1.111260	-4.525746
H	2.892728	2.240858	-0.013996
H	3.812664	1.271096	-1.143205

P	-0.310657	1.579765	1.602550
C	0.304800	3.268403	1.164558
H	-0.006275	3.966450	1.951032
H	1.400872	3.255845	1.181827
Si	-0.303656	3.924437	-0.513550
C	-0.634022	5.768173	-0.324546
H	-1.425722	5.957734	0.410877
H	0.265985	6.299044	0.010139
H	-0.949362	6.216638	-1.274532
C	1.027227	3.629587	-1.817679
H	1.921256	4.220084	-1.573308
H	0.660464	4.015008	-2.780126
C	-1.880712	3.018685	-1.034087
H	-2.477680	2.773176	-0.145772
H	-2.497003	3.700846	-1.636584
C	3.161240	-1.485719	-0.432231
C	3.735496	-1.463940	-1.702806
C	3.141351	-2.689986	0.282036
C	4.288967	-2.622336	-2.248921
H	3.746189	-0.551363	-2.290614
C	3.699910	-3.840819	-0.256520
H	2.664306	-2.730407	1.257620
C	4.275092	-3.810172	-1.527551
H	4.728439	-2.590582	-3.241732
H	3.674712	-4.768031	0.308613
H	4.704888	-4.712196	-1.953605
C	3.309694	0.197328	1.845271
C	2.742098	0.037543	3.110546
C	4.662985	0.550498	1.755624
C	3.501411	0.240782	4.262626
H	1.703159	-0.254789	3.204668
C	5.421043	0.755919	2.902101
H	5.130477	0.661300	0.780736
C	4.839328	0.604523	4.160822
H	3.041407	0.112185	5.238130
H	6.468781	1.029090	2.814737
H	5.430238	0.766355	5.057757
C	-3.502400	0.117427	1.015935
C	-4.592599	0.866776	0.565775
C	-3.317941	-0.020009	2.399436
C	-5.474705	1.457807	1.469347
H	-4.767405	1.005596	-0.495733
C	-4.207405	0.552422	3.302295
H	-2.461575	-0.572743	2.776890

C	-5.288576	1.298658	2.838607
H	-6.312331	2.040568	1.096974
H	-4.047118	0.424658	4.368818
H	-5.979537	1.755054	3.541324
C	-2.853939	-2.417726	-0.162448
C	-3.443774	-3.033192	0.945897
C	-2.636772	-3.187686	-1.311186
C	-3.810900	-4.376119	0.906494
H	-3.633620	-2.469152	1.852862
C	-3.005930	-4.528118	-1.352304
H	-2.167530	-2.755067	-2.188165
C	-3.593329	-5.129203	-0.242644
H	-4.269372	-4.830682	1.780096
H	-2.826612	-5.103047	-2.256360
H	-3.878028	-6.177031	-0.274102
C	0.417678	-2.345718	-1.988617
O	0.288945	-2.067747	-0.766178
O	0.275376	-1.585509	-2.971593
H	0.673282	-3.404984	-2.194847
H	0.158329	-0.050241	-2.191919
H	-1.632547	1.950725	1.935456
H	0.151045	1.508335	2.938439

A7

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.126194	0.319427	0.362478
N	0.032405	-0.848093	-1.556396
C	2.514031	-1.980633	-0.423185
H	3.482783	-2.074045	-0.925763
H	2.503253	-2.748911	0.358783
C	-2.347902	0.755829	-1.836644
C	0.215195	1.373308	1.778219
O	0.235996	2.072903	2.708091
P	-2.019700	1.087226	-0.075040
P	2.331705	-0.367598	0.445712
Si	-1.583227	-0.895691	-2.313206
Si	1.053516	-2.302887	-1.593826
C	-1.411047	-0.955347	-4.181398
H	-1.144910	-1.955876	-4.541786
H	-2.348464	-0.665029	-4.672098

H	-0.626344	-0.260465	-4.499775
C	1.706374	-2.594736	-3.327992
H	2.513854	-3.337791	-3.326085
H	0.926234	-2.960290	-4.005943
H	2.086502	-1.652937	-3.740314
H	-3.383578	0.920273	-2.151070
H	-1.709205	1.475353	-2.376120
P	-0.464683	-1.486247	1.652865
C	-1.783095	-2.705823	1.261389
H	-1.758247	-3.494989	2.022535
H	-2.754685	-2.208686	1.355083
Si	-1.704204	-3.503682	-0.456330
C	-2.632924	-5.136798	-0.315760
H	-2.122134	-5.831162	0.362791
H	-3.646430	-4.978742	0.074044
H	-2.725758	-5.632542	-1.289751
C	-2.550087	-2.398440	-1.716572
H	-3.522028	-2.093643	-1.310027
H	-2.769996	-3.013814	-2.601002
C	0.077486	-3.805224	-0.990378
H	0.621709	-4.308600	-0.179439
H	0.046582	-4.528390	-1.818774
H	0.297859	1.612653	-0.841015
H	1.010004	1.547756	-0.495255
C	-2.295977	2.898048	0.132467
C	-3.220901	3.426536	1.037026
C	-1.513196	3.776063	-0.630200
C	-3.357750	4.805336	1.185330
H	-3.847541	2.770148	1.631760
C	-1.658773	5.151678	-0.482427
H	-0.801566	3.397602	-1.361479
C	-2.575889	5.671447	0.428581
H	-4.081269	5.197947	1.894306
H	-1.049362	5.818013	-1.086085
H	-2.683360	6.746158	0.544709
C	-3.400309	0.357826	0.884372
C	-3.273356	0.308906	2.279736
C	-4.549234	-0.177274	0.298065
C	-4.257194	-0.281303	3.065128
H	-2.395281	0.737988	2.755222
C	-5.528567	-0.785407	1.082356
H	-4.689121	-0.129770	-0.776929
C	-5.382605	-0.843969	2.465140
H	-4.140250	-0.310062	4.144405

H	-6.409512	-1.209204	0.609172
H	-6.145782	-1.318775	3.074621
C	3.215265	-0.677272	2.031678
C	4.549272	-1.106533	2.004742
C	2.587871	-0.510384	3.266570
C	5.232436	-1.370983	3.185117
H	5.058844	-1.224204	1.051709
C	3.272442	-0.773586	4.452866
H	1.562405	-0.161230	3.314601
C	4.593327	-1.205332	4.414001
H	6.266801	-1.700359	3.148305
H	2.770154	-0.634070	5.405661
H	5.127849	-1.407982	5.337541
C	3.497379	0.792350	-0.364427
C	3.741800	2.005898	0.292944
C	4.075388	0.568151	-1.612921
C	4.566828	2.965484	-0.278999
H	3.283061	2.200776	1.259902
C	4.904481	1.531820	-2.185382
H	3.870155	-0.342424	-2.164261
C	5.153423	2.727830	-1.522019
H	4.749168	3.900464	0.242648
H	5.344177	1.347466	-3.161057
H	5.796733	3.477963	-1.972756
C	1.179134	1.877065	-3.442962
O	0.143978	2.435155	-3.026193
O	1.529976	0.677053	-3.287760
H	1.885876	2.507975	-4.034256
H	0.565309	-0.166305	-2.166087
H	-0.753529	-1.211439	3.008709
H	0.582754	-2.402972	1.907598

A8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.079571	0.252455	0.500675
N	0.074592	-0.985600	-1.461067
C	2.441797	-2.077311	-0.093857
H	3.439921	-2.332684	-0.464344
H	2.258978	-2.721816	0.774277
C	-2.266499	0.639164	-1.844660

C	0.116462	1.318412	1.880030
O	0.088265	2.040153	2.804850
P	-1.964354	1.021151	-0.070505
P	2.290496	-0.354942	0.538766
Si	-1.522610	-1.043274	-2.243867
Si	1.089135	-2.440440	-1.363247
C	-1.337566	-1.206014	-4.108309
H	-0.987529	-2.204372	-4.397883
H	-2.299064	-1.039618	-4.611001
H	-0.617605	-0.476333	-4.494884
C	1.862682	-2.780900	-3.042819
H	2.660450	-3.531443	-2.975303
H	1.120695	-3.156737	-3.757398
H	2.286777	-1.864251	-3.469361
H	-3.303941	0.778657	-2.167737
H	-1.666000	1.374167	-2.398183
P	-0.523920	-1.472260	1.830129
C	-1.835028	-2.713993	1.429844
H	-1.857746	-3.480224	2.214337
H	-2.801654	-2.196299	1.468953
Si	-1.720240	-3.558204	-0.258694
C	-2.675403	-5.177328	-0.115817
H	-2.218871	-5.853014	0.618084
H	-3.708621	-4.991327	0.203577
H	-2.715950	-5.707720	-1.075182
C	-2.518118	-2.497982	-1.592229
H	-3.497321	-2.164318	-1.229900
H	-2.719946	-3.158785	-2.447986
C	0.056384	-3.909576	-0.789346
H	0.587481	-4.436998	0.014889
H	-0.004144	-4.623736	-1.624170
H	0.837868	2.160406	-1.545625
H	0.512769	1.460813	-0.466307
C	-2.309709	2.835125	-0.012081
C	-3.616001	3.314043	-0.173390
C	-1.270815	3.756462	0.137834
C	-3.875999	4.679619	-0.189702
H	-4.440914	2.614292	-0.278497
C	-1.530748	5.125546	0.124361
H	-0.255192	3.397699	0.262043
C	-2.831532	5.590496	-0.040240
H	-4.895437	5.033693	-0.315731
H	-0.711621	5.828871	0.244281
H	-3.033456	6.657951	-0.049571

C	-3.448530	0.389603	0.822385
C	-3.410311	0.466179	2.221659
C	-4.568235	-0.187188	0.218693
C	-4.450183	-0.038076	2.993760
H	-2.551154	0.920368	2.708826
C	-5.607388	-0.706951	0.991362
H	-4.644815	-0.239787	-0.862864
C	-5.548698	-0.638555	2.379525
H	-4.399435	0.031545	4.076501
H	-6.465343	-1.161327	0.503759
H	-6.356798	-1.044193	2.981276
C	3.319095	-0.409039	2.074470
C	4.346537	-1.345710	2.239171
C	3.105506	0.528942	3.089334
C	5.129763	-1.352397	3.389339
H	4.547032	-2.080363	1.465664
C	3.894721	0.529194	4.237630
H	2.318732	1.267157	2.993112
C	4.906075	-0.413503	4.393495
H	5.918132	-2.091916	3.498451
H	3.710913	1.267308	5.013077
H	5.516471	-0.417769	5.292095
C	3.395884	0.631946	-0.556370
C	3.515259	2.000141	-0.281303
C	4.079727	0.108489	-1.654295
C	4.310438	2.818271	-1.073287
H	2.962020	2.430513	0.549902
C	4.864071	0.931541	-2.461989
H	3.998864	-0.943795	-1.906950
C	4.984481	2.285959	-2.172387
H	4.391123	3.876935	-0.844422
H	5.376858	0.507741	-3.320857
H	5.597767	2.926637	-2.799666
C	1.468109	2.013308	-3.348457
O	1.119577	2.754622	-2.329458
O	1.356258	0.803131	-3.436037
H	1.879229	2.621869	-4.166422
H	0.605114	-0.280001	-1.993319
H	0.474505	-2.394086	2.246826
H	-0.932046	-1.129004	3.140720

TSA7-8

	Coordinates (Angstroms)		
	X	Y	Z
Mn	0.101052	0.310466	0.458848
N	0.121596	-0.971961	-1.430789
C	2.515914	-1.999631	-0.048293
H	3.517480	-2.257630	-0.406433
H	2.332982	-2.626002	0.832573
C	-2.291287	0.543727	-1.865231
C	0.095080	1.385991	1.844917
O	0.036309	2.093003	2.774161
P	-2.023338	0.984198	-0.106656
P	2.350093	-0.267248	0.532679
Si	-1.473500	-1.115955	-2.215390
Si	1.178643	-2.400569	-1.324735
C	-1.273694	-1.319945	-4.072293
H	-0.919823	-2.323793	-4.336817
H	-2.230954	-1.165433	-4.586430
H	-0.549504	-0.596821	-4.463217
C	1.976202	-2.719412	-2.993205
H	2.782431	-3.460137	-2.918033
H	1.249826	-3.098028	-3.722045
H	2.387778	-1.788564	-3.399621
H	-3.327151	0.640686	-2.207965
H	-1.698617	1.284464	-2.421721
P	-0.454966	-1.407104	1.846703
C	-1.702120	-2.718249	1.486207
H	-1.671922	-3.465802	2.288301
H	-2.694210	-2.251997	1.532436
Si	-1.578344	-3.598298	-0.186248
C	-2.481875	-5.239501	0.021401
H	-1.973933	-5.888523	0.745518
H	-3.505436	-5.079067	0.382838
H	-2.546298	-5.786422	-0.927179
C	-2.420068	-2.590368	-1.529853
H	-3.409661	-2.285465	-1.171311
H	-2.600844	-3.273443	-2.372744
C	0.198859	-3.902251	-0.736237
H	0.758250	-4.417810	0.056176
H	0.143527	-4.614720	-1.573077
H	0.524222	1.814786	-1.284748
H	0.647485	1.604295	-0.429088
C	-2.439086	2.779601	-0.061441
C	-3.767356	3.205459	-0.186190

C	-1.430340	3.739617	0.045561
C	-4.078976	4.560139	-0.204704
H	-4.567705	2.474206	-0.260733
C	-1.742674	5.097335	0.029281
H	-0.395774	3.428313	0.133898
C	-3.065198	5.510296	-0.094973
H	-5.114485	4.874094	-0.301928
H	-0.947200	5.832095	0.112715
H	-3.307023	6.569361	-0.106819
C	-3.445993	0.289903	0.825996
C	-3.399387	0.400576	2.222381
C	-4.543400	-0.346598	0.242137
C	-4.408682	-0.135179	3.013797
H	-2.560964	0.907462	2.693152
C	-5.551984	-0.894607	1.034754
H	-4.625601	-0.421419	-0.837425
C	-5.483896	-0.795802	2.420810
H	-4.353144	-0.040203	4.094240
H	-6.394655	-1.392935	0.564027
H	-6.268662	-1.223467	3.037862
C	3.357692	-0.253542	2.078251
C	4.353095	-1.208363	2.315344
C	3.156210	0.751597	3.029558
C	5.116376	-1.168638	3.478275
H	4.544995	-1.992157	1.589378
C	3.923169	0.795594	4.191401
H	2.396016	1.507343	2.870378
C	4.901781	-0.167176	4.421565
H	5.881755	-1.921373	3.644696
H	3.749032	1.581963	4.920059
H	5.494587	-0.137174	5.331222
C	3.408583	0.729508	-0.593507
C	3.349641	2.121690	-0.459412
C	4.242091	0.184350	-1.570806
C	4.107245	2.947275	-1.280629
H	2.685671	2.562886	0.279119
C	4.994870	1.011230	-2.402206
H	4.304214	-0.889543	-1.713799
C	4.929203	2.392804	-2.260406
H	4.042650	4.025315	-1.165927
H	5.627219	0.570359	-3.167468
H	5.512825	3.036846	-2.911859
C	1.184585	1.802185	-3.376520
O	0.530015	2.454060	-2.500561

O	1.465136	0.593937	-3.365273
H	1.518165	2.407398	-4.243515
H	0.645463	-0.307802	-2.042853
H	-0.870982	-1.031125	3.144065
H	0.599320	-2.248830	2.281754

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.097141	-0.031743	0.339016
N	0.006633	1.005154	-1.407742
C	-2.932873	1.010459	-1.303866
H	-3.411031	0.507868	-2.151507
H	-3.670700	1.684137	-0.854769
C	2.915413	0.960143	-0.842315
C	-0.199515	-1.316071	1.547835
O	-0.267734	-2.185296	2.326865
P	2.145013	-0.344228	0.178960
P	-2.341475	-0.189454	-0.041726
Si	1.521956	1.627018	-1.961889
Si	-1.372206	1.977168	-1.787285
C	1.943197	1.144552	-3.735602
H	1.180442	1.482868	-4.446890
H	2.904855	1.569037	-4.051538
H	2.015474	0.052548	-3.821304
C	-1.526193	2.442279	-3.614542
H	-2.482149	2.949963	-3.798931
H	-0.731275	3.119741	-3.949452
H	-1.497590	1.551496	-4.254459
H	3.244207	1.781074	-0.196965
H	3.793494	0.603227	-1.391137
P	0.024531	1.629613	1.820146
C	0.922693	3.169438	1.326843
H	0.826154	3.899489	2.140646
H	1.989143	2.916740	1.275563
Si	0.424034	4.030912	-0.309159
C	0.609851	5.881525	0.018345
H	-0.088485	6.226761	0.791108
H	1.625931	6.127076	0.353142
H	0.412647	6.464200	-0.890099
C	1.550282	3.514052	-1.733418

H	2.577660	3.873462	-1.583676
H	1.179293	4.018751	-2.638253
C	-1.344009	3.588570	-0.778593
H	-1.948176	3.476784	0.133177
H	-1.797173	4.408080	-1.354016
C	3.159719	-0.524193	1.699357
C	3.170381	-1.755781	2.366055
C	3.820269	0.559832	2.284557
C	3.829517	-1.899137	3.582135
H	2.660678	-2.611064	1.931830
C	4.477959	0.417269	3.504703
H	3.834071	1.528259	1.792803
C	4.484488	-0.811892	4.156850
H	3.828655	-2.863108	4.082489
H	4.986854	1.270839	3.943539
H	4.996900	-0.923451	5.107958
C	2.552020	-1.878959	-0.747955
C	3.877184	-2.217587	-1.048896
C	1.523953	-2.721150	-1.175919
C	4.165443	-3.371722	-1.767634
H	4.688845	-1.578378	-0.709577
C	1.811033	-3.877374	-1.899771
H	0.489641	-2.483088	-0.943015
C	3.130269	-4.203299	-2.196140
H	5.197564	-3.625188	-1.992137
H	0.998564	-4.520926	-2.224472
H	3.355772	-5.106370	-2.756397
C	-3.647681	-0.245909	1.237936
C	-5.003113	-0.293664	0.886648
C	-3.296530	-0.246477	2.589625
C	-5.984837	-0.344189	1.869361
H	-5.289194	-0.300844	-0.162221
C	-4.280621	-0.296664	3.575594
H	-2.248889	-0.217484	2.872612
C	-5.623888	-0.344324	3.216893
H	-7.032836	-0.384933	1.586671
H	-3.994876	-0.298158	4.623428
H	-6.391336	-0.382512	3.984550
C	-2.488096	-1.815263	-0.888957
C	-3.042787	-2.936512	-0.264947
C	-1.903835	-1.961884	-2.154066
C	-3.029007	-4.175337	-0.901222
H	-3.489906	-2.846645	0.720750
C	-1.896420	-3.199747	-2.790128

H	-1.422124	-1.110533	-2.628803
C	-2.460031	-4.310520	-2.165107
H	-3.466781	-5.037560	-0.406362
H	-1.438316	-3.297186	-3.770309
H	-2.452283	-5.277837	-2.659202
H	0.605102	1.406762	3.092196
H	-1.174268	2.212863	2.300881

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.122848	-0.470557	-0.195287
N	0.203461	1.322617	1.303833
C	2.572409	1.775430	-0.421745
H	3.598953	2.100146	-0.216871
H	2.319897	2.090069	-1.440045
C	-2.249592	-0.007228	2.075555
C	0.192381	-1.898703	-1.202538
O	0.216149	-2.843070	-1.894599
P	-1.942714	-0.929350	0.507732
P	2.342667	-0.050714	-0.315853
Si	-1.401514	1.669618	1.991199
Si	1.323973	2.590669	0.742519
C	-1.207641	2.351255	3.735341
H	-0.743982	3.345325	3.727651
H	-2.181382	2.449091	4.231934
H	-0.582098	1.698618	4.357008
C	2.238860	3.316058	2.214857
H	2.963960	4.074093	1.893538
H	1.556889	3.787962	2.932184
H	2.795051	2.533672	2.747016
H	-3.301288	0.031032	2.381123
H	-1.723108	-0.585876	2.846130
P	-0.381306	0.771625	-2.000189
C	-1.594330	2.174810	-2.007819
H	-1.574711	2.666701	-2.987991
H	-2.594312	1.734277	-1.901659
Si	-1.433980	3.483590	-0.653554
C	-2.288952	5.037193	-1.293194
H	-1.800451	5.422907	-2.196441
H	-3.337161	4.832273	-1.544378

H	-2.277793	5.836097	-0.541721
C	-2.295828	2.928129	0.925253
H	-3.299550	2.567584	0.671444
H	-2.441278	3.828402	1.540084
C	0.345286	3.902794	-0.183796
H	0.912775	4.208689	-1.073347
H	0.283477	4.797606	0.454205
H	0.382513	-1.330484	1.137839
H	0.688525	0.704484	1.956903
C	-3.391758	-0.534527	-0.568581
C	-3.354117	-1.061749	-1.867479
C	-4.473464	0.275104	-0.213983
C	-4.355707	-0.773839	-2.786933
H	-2.523606	-1.699074	-2.161903
C	-5.474892	0.576191	-1.138199
H	-4.549400	0.685275	0.788191
C	-5.417069	0.056236	-2.426991
H	-4.305001	-1.194247	-3.787145
H	-6.302684	1.215919	-0.844701
H	-6.194956	0.292120	-3.147266
C	-2.390846	-2.655818	0.995992
C	-3.724209	-3.003705	1.246274
C	-1.400348	-3.626000	1.166462
C	-4.058170	-4.288553	1.660870
H	-4.512308	-2.267796	1.109592
C	-1.734757	-4.915307	1.576947
H	-0.364572	-3.362881	0.981073
C	-3.062291	-5.249594	1.826061
H	-5.097900	-4.540758	1.850294
H	-0.952922	-5.660046	1.697497
H	-3.322468	-6.255707	2.143305
C	3.330494	-0.737771	-1.703502
C	3.905504	0.044730	-2.707199
C	3.473769	-2.129880	-1.767711
C	4.605483	-0.550501	-3.756216
H	3.819177	1.126709	-2.677626
C	4.176947	-2.722785	-2.809372
H	3.027947	-2.753280	-0.996968
C	4.743008	-1.933473	-3.809604
H	5.045759	0.072192	-4.530135
H	4.278407	-3.803613	-2.844739
H	5.286720	-2.396940	-4.627831
C	3.476424	-0.410224	1.108541
C	2.988159	-0.950604	2.298645

C	4.839081	-0.091356	1.024854
C	3.835020	-1.151847	3.389403
H	1.938946	-1.229793	2.354669
C	5.685901	-0.296343	2.107409
H	5.245029	0.311373	0.099705
C	5.182874	-0.823410	3.297362
H	3.437035	-1.574515	4.307811
H	6.740399	-0.049068	2.023127
H	5.844470	-0.983631	4.144029
H	-0.878751	0.060188	-3.117510
H	0.646950	1.429086	-2.733364

R^1=H, R^2=R^3=Ph

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.057572	-0.290233	-1.263490
N	-0.006148	-2.107642	-0.076664
C	1.542719	-0.484248	1.795416
H	2.439803	-0.660305	2.398517
H	0.949663	0.279328	2.312507
C	-1.520210	-3.065198	-2.373505
C	0.266996	1.066133	-2.372130
O	0.429501	1.898701	-3.176111
P	-1.530890	-1.248539	-2.612246
P	1.884889	0.182162	0.135194
Si	-1.002736	-3.407253	-0.568556
Si	0.465767	-2.040821	1.565962
C	-0.169046	-5.105519	-0.610785
H	0.057889	-5.485503	0.391863
H	-0.813916	-5.846253	-1.102716
H	0.776592	-5.061736	-1.166001
C	1.434983	-3.554762	2.167633
H	1.940119	-3.355720	3.122382
H	0.760824	-4.403601	2.338247
H	2.188115	-3.877996	1.440021
H	-2.453839	-3.545408	-2.684177
H	-0.720097	-3.463181	-3.011493
P	-1.685398	0.669537	-0.028563
C	-2.972811	-0.498901	0.568683
H	-3.786698	0.079573	1.023902

H	-3.407399	-0.948555	-0.332645
Si	-2.620493	-2.012650	1.683805
C	-4.133556	-2.123344	2.813619
H	-4.190877	-1.269678	3.501763
H	-5.067959	-2.150540	2.238292
H	-4.098633	-3.033627	3.425345
C	-2.531920	-3.524793	0.563479
H	-3.462700	-3.619769	-0.013428
H	-2.464183	-4.428924	1.186216
C	-1.051365	-1.890108	2.706545
H	-1.035779	-0.953280	3.276865
H	-1.057981	-2.704945	3.445050
H	1.194766	-1.549552	-1.882122
H	1.211174	-1.021362	-2.459787
C	-2.703415	1.857865	-1.031042
C	-4.040998	1.619315	-1.363714
C	-2.102620	3.023579	-1.524342
C	-4.752791	2.512591	-2.163227
H	-4.552378	0.734222	-1.002192
C	-2.812247	3.919757	-2.315154
H	-1.062933	3.237690	-1.302502
C	-4.142630	3.666233	-2.641396
H	-5.790439	2.302028	-2.406522
H	-2.320171	4.814672	-2.684687
H	-4.697154	4.361661	-3.264716
C	-1.342540	1.700985	1.462496
C	-0.346707	2.677412	1.364347
C	-2.010469	1.557042	2.682838
C	-0.016921	3.483562	2.448486
H	0.197324	2.796492	0.434843
C	-1.675060	2.353219	3.776188
H	-2.795583	0.817783	2.798829
C	-0.677685	3.318051	3.662671
H	0.767690	4.226846	2.343374
H	-2.197923	2.217327	4.718552
H	-0.416182	3.936188	4.516694
C	2.659824	1.832079	0.427357
C	3.303807	2.130326	1.631923
C	2.634471	2.804134	-0.577777
C	3.902519	3.371345	1.830053
H	3.336066	1.393583	2.428347
C	3.232266	4.046668	-0.381614
H	2.131684	2.601209	-1.517372
C	3.866646	4.334137	0.824201

H	4.396858	3.585592	2.773384
H	3.197973	4.791358	-1.171635
H	4.332234	5.303220	0.978878
C	3.381961	-0.717667	-0.455243
C	3.889811	-0.364314	-1.712191
C	4.023821	-1.724881	0.265668
C	5.012401	-0.995617	-2.231658
H	3.397399	0.413015	-2.292705
C	5.145142	-2.368425	-0.259276
H	3.656602	-2.025099	1.241243
C	5.643295	-2.005610	-1.505344
H	5.394192	-0.702639	-3.205554
H	5.628423	-3.155189	0.313141
H	6.518395	-2.504292	-1.911805
H	-1.464970	-1.083207	-4.013996
H	-2.898831	-0.925244	-2.481376

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	-0.106320	-0.629526	-1.235965
N	-0.650480	-2.464818	-0.060781
C	2.057337	-2.240056	0.782104
H	2.317266	-3.002524	0.036101
H	2.847309	-2.253194	1.539105
C	-3.232285	-2.018848	-1.381692
C	0.512370	0.508077	-2.425487
O	0.948888	1.232844	-3.231542
P	-1.952388	-1.243859	-2.448991
P	1.959362	-0.653112	-0.142157
Si	-2.294548	-2.998840	-0.040748
Si	0.310052	-2.649490	1.363015
C	-2.491193	-4.829121	-0.446726
H	-1.949578	-5.459344	0.268894
H	-3.544800	-5.136568	-0.432893
H	-2.090674	-5.047942	-1.445058
C	0.305213	-4.399116	2.073268
H	1.025475	-4.487642	2.897059
H	-0.676477	-4.685096	2.471278
H	0.583379	-5.134468	1.308965
H	-3.811068	-1.206068	-0.927104

H	-3.930544	-2.637549	-1.955300
P	-1.328168	0.957034	-0.062680
C	-2.459403	0.377247	1.291151
H	-2.681822	1.233590	1.939032
H	-3.408379	0.136873	0.795742
Si	-2.143776	-1.117248	2.427840
C	-2.974608	-0.659929	4.060938
H	-2.488433	0.203504	4.533075
H	-4.031930	-0.406342	3.911946
H	-2.934204	-1.491400	4.775678
C	-3.011477	-2.612086	1.668500
H	-4.094478	-2.433872	1.614774
H	-2.875495	-3.479140	2.331340
C	-0.316551	-1.473484	2.702298
H	0.226772	-0.520939	2.675581
H	-0.159599	-1.900848	3.702266
H	0.615512	-1.997524	-2.011073
H	0.132311	-2.378530	-1.271346
C	3.463624	-0.766639	-1.216291
C	4.743242	-0.609919	-0.666646
C	3.354834	-1.095724	-2.569832
C	5.879828	-0.769221	-1.451482
H	4.856507	-0.356549	0.383454
C	4.493780	-1.253585	-3.357939
H	2.375942	-1.232155	-3.014690
C	5.758032	-1.089044	-2.802517
H	6.862564	-0.641813	-1.006339
H	4.386420	-1.501038	-4.410202
H	6.645985	-1.209087	-3.416692
C	2.546763	0.614940	1.049973
C	2.762499	0.370385	2.407710
C	2.862945	1.878866	0.536151
C	3.296752	1.360721	3.232072
H	2.528817	-0.597045	2.839678
C	3.413512	2.857823	1.352034
H	2.694774	2.089426	-0.516826
C	3.634596	2.600903	2.704322
H	3.459740	1.151532	4.285577
H	3.660090	3.828501	0.933241
H	4.061045	3.369027	3.343127
C	-0.484766	2.387416	0.752426
C	-0.078897	3.472464	-0.033270
C	-0.264781	2.444311	2.130754
C	0.483852	4.602829	0.548783

H	-0.225495	3.448361	-1.109317
C	0.310934	3.570596	2.713771
H	-0.550249	1.613769	2.769227
C	0.671364	4.660011	1.927599
H	0.772974	5.441757	-0.078096
H	0.474206	3.593920	3.787294
H	1.108793	5.542970	2.384694
C	-2.543435	1.958804	-1.065576
C	-3.664270	2.562022	-0.477923
C	-2.319009	2.188841	-2.426509
C	-4.535510	3.345884	-1.227691
H	-3.865039	2.433135	0.580279
C	-3.184685	2.979346	-3.179856
H	-1.454333	1.755342	-2.911619
C	-4.300759	3.556177	-2.584304
H	-5.398062	3.799018	-0.747171
H	-2.981543	3.140376	-4.234719
H	-4.979271	4.169873	-3.169791
H	-2.695264	-0.410319	-3.311555
H	-1.714232	-2.283029	-3.375416

A6

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.172918	-0.250989	-1.113085
N	0.805327	-1.984190	0.269303
C	1.266544	0.342887	2.035552
H	2.075764	0.572593	2.737417
H	0.369201	0.857159	2.400752
C	-0.048958	-3.502118	-2.073230
C	-0.071757	1.013477	-2.319702
O	-0.156032	1.779497	-3.193518
P	-0.708337	-1.837910	-2.511107
P	1.541761	0.985722	0.339681
Si	0.250902	-3.608413	-0.208640
Si	0.867432	-1.510964	1.975113
C	1.587605	-4.890981	0.096317
H	1.755429	-5.070072	1.164860
H	1.316474	-5.850925	-0.361585
H	2.531168	-4.552538	-0.344882
C	2.197560	-2.495531	2.873435

H	2.425667	-2.057188	3.853331
H	1.868309	-3.527181	3.047941
H	3.128109	-2.544244	2.296021
H	-0.666029	-4.316941	-2.466389
H	0.938849	-3.583549	-2.542689
P	-1.936034	0.068507	-0.140651
C	-2.823028	-1.470567	0.340025
H	-3.865568	-1.239377	0.589025
H	-2.870116	-2.094272	-0.560333
Si	-2.099927	-2.622073	1.668894
C	-3.546530	-3.226734	2.715350
H	-4.010227	-2.406238	3.277385
H	-4.325759	-3.685746	2.094292
H	-3.217152	-3.977854	3.443636
C	-1.297899	-4.061425	0.765564
H	-2.033512	-4.538807	0.103993
H	-1.014210	-4.822120	1.506983
C	-0.801850	-1.838641	2.781320
H	-1.194644	-0.918281	3.229933
H	-0.642109	-2.539680	3.613929
C	-3.132338	0.809340	-1.352907
C	-4.133776	0.061193	-1.979370
C	-3.002032	2.158851	-1.704042
C	-4.979868	0.642742	-2.922805
H	-4.276341	-0.986877	-1.738745
C	-3.849918	2.743084	-2.637213
H	-2.226292	2.768156	-1.251941
C	-4.843595	1.986040	-3.253415
H	-5.750028	0.039334	-3.395046
H	-3.727870	3.793028	-2.886987
H	-5.504681	2.440216	-3.985706
C	-2.268581	1.157829	1.319873
C	-1.631681	2.401221	1.364944
C	-3.120606	0.818578	2.377279
C	-1.825650	3.279130	2.426984
H	-0.958869	2.686504	0.565435
C	-3.309365	1.687552	3.449784
H	-3.648447	-0.129085	2.382086
C	-2.662484	2.920136	3.479548
H	-1.309513	4.234426	2.430247
H	-3.969209	1.398270	4.262834
H	-2.811713	3.596400	4.316237
C	1.519989	2.820868	0.532232
C	1.798211	3.440561	1.754394

C	1.235189	3.622933	-0.577946
C	1.779551	4.828095	1.867673
H	2.024978	2.843151	2.632100
C	1.218655	5.011156	-0.466451
H	1.008424	3.165316	-1.534446
C	1.485774	5.617418	0.757760
H	1.992652	5.293304	2.825915
H	0.990090	5.616462	-1.338957
H	1.466732	6.699690	0.847881
C	3.341036	0.759620	0.036605
C	3.861953	1.267249	-1.159766
C	4.196051	0.087064	0.909005
C	5.205772	1.106381	-1.471430
H	3.204972	1.769386	-1.864063
C	5.543344	-0.082331	0.594075
H	3.823955	-0.324282	1.841609
C	6.051238	0.426136	-0.595266
H	5.593387	1.504043	-2.405077
H	6.192106	-0.618704	1.280591
H	7.100225	0.291132	-0.842764
C	2.876196	-1.504231	-2.166793
O	1.877068	-0.741606	-2.317705
O	3.126505	-2.265253	-1.213759
H	3.603116	-1.479613	-3.005019
H	1.769212	-1.965057	-0.136435
H	-0.416446	-1.728350	-3.885202
H	-2.087726	-2.115021	-2.654581

A7

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.172323	-0.234178	-1.095069
N	1.162637	-1.694381	0.334599
C	1.030182	0.748430	2.016222
H	1.733192	1.200651	2.723506
H	0.021449	1.031215	2.339990
C	0.683133	-3.481345	-1.893246
C	-0.340049	0.877858	-2.370295
O	-0.609155	1.562437	-3.271537
P	-0.357855	-2.060409	-2.382554
P	1.189331	1.364299	0.305543

Si	0.960126	-3.435612	-0.030820
Si	1.134226	-1.147431	2.025117
C	2.514125	-4.397357	0.386086
H	2.626037	-4.548546	1.466307
H	2.487841	-5.388297	-0.084673
H	3.394744	-3.857115	0.025254
C	2.716382	-1.696948	2.873419
H	2.877691	-1.172387	3.823344
H	2.697610	-2.771675	3.091257
H	3.573836	-1.512445	2.215393
H	0.322369	-4.438719	-2.282382
H	1.673407	-3.259624	-2.322757
P	-1.970930	-0.317002	-0.139716
C	-2.503736	-1.958109	0.485488
H	-3.562059	-1.910233	0.768864
H	-2.462222	-2.642976	-0.369120
Si	-1.532964	-2.883081	1.836237
C	-2.820515	-3.727087	2.923358
H	-3.446568	-3.001735	3.458324
H	-3.485015	-4.365458	2.327996
H	-2.339539	-4.363023	3.676770
C	-0.481225	-4.155466	0.948594
H	-1.114849	-4.764417	0.289085
H	-0.062887	-4.848135	1.692704
C	-0.390094	-1.832681	2.896107
H	-0.947861	-1.017877	3.374017
H	-0.050059	-2.488705	3.711263
H	1.646019	-0.700516	-2.014477
H	1.762277	0.016309	-1.689776
C	-3.293276	0.042143	-1.392147
C	-4.116846	-0.959625	-1.916422
C	-3.455986	1.346474	-1.876012
C	-5.070244	-0.669069	-2.890869
H	-4.033369	-1.983353	-1.568927
C	-4.411781	1.639975	-2.841478
H	-2.830850	2.151738	-1.506458
C	-5.223467	0.631906	-3.355642
H	-5.696966	-1.466332	-3.280190
H	-4.517374	2.660788	-3.196828
H	-5.967505	0.860414	-4.112902
C	-2.500766	0.801594	1.232359
C	-2.226222	2.167742	1.119569
C	-3.171931	0.358192	2.377763
C	-2.605727	3.066439	2.111514

H	-1.691119	2.539550	0.254282
C	-3.541323	1.251671	3.380539
H	-3.418757	-0.689690	2.507313
C	-3.261473	2.609055	3.250589
H	-2.372342	4.120000	1.992500
H	-4.053977	0.881436	4.263645
H	-3.553234	3.304937	4.031569
C	0.766489	3.154301	0.386950
C	0.812707	3.865737	1.588691
C	0.431336	3.835457	-0.787876
C	0.521005	5.226747	1.617755
H	1.066929	3.359849	2.514819
C	0.140108	5.196698	-0.759552
H	0.383894	3.304436	-1.732878
C	0.181665	5.895541	0.444327
H	0.558637	5.763851	2.561194
H	-0.119858	5.709751	-1.680843
H	-0.046446	6.957166	0.467820
C	2.998575	1.517988	0.000738
C	3.409565	1.849954	-1.295877
C	3.966757	1.337928	0.987165
C	4.757735	1.986163	-1.599837
H	2.671706	1.990127	-2.083094
C	5.319575	1.470144	0.682780
H	3.684959	1.073150	2.000853
C	5.718675	1.791405	-0.609194
H	5.058211	2.233200	-2.613740
H	6.062250	1.311216	1.459272
H	6.774096	1.887049	-0.846744
C	4.086919	-1.638303	-1.704663
O	3.334673	-1.901458	-2.665651
O	3.794843	-1.545483	-0.481314
H	5.164710	-1.464029	-1.944605
H	2.151612	-1.536922	-0.012319
H	-0.178999	-1.966550	-3.777058
H	-1.660312	-2.605843	-2.413011

A8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.122744	-0.195085	-1.062247

N	1.204427	-1.695863	0.367310
C	0.944767	0.686339	2.075985
H	1.633355	1.124412	2.806361
H	-0.069490	0.975721	2.376076
C	0.908544	-3.323351	-2.007720
C	-0.293246	0.938416	-2.326733
O	-0.466530	1.646231	-3.242849
P	-0.216850	-1.926098	-2.440123
P	1.141625	1.308341	0.359033
Si	1.063126	-3.400510	-0.129091
Si	1.025609	-1.204495	2.065133
C	2.597129	-4.384667	0.326187
H	2.705482	-4.490622	1.412252
H	2.539737	-5.395569	-0.097955
H	3.503405	-3.901850	-0.052848
C	2.515889	-1.794058	3.052138
H	2.583470	-1.287112	4.022982
H	2.459261	-2.871416	3.250177
H	3.448970	-1.610055	2.506695
H	0.604854	-4.271379	-2.464396
H	1.900015	-3.068796	-2.402906
P	-2.003457	-0.345208	-0.191315
C	-2.557411	-2.036180	0.285493
H	-3.625827	-2.043256	0.533838
H	-2.461903	-2.649377	-0.618419
Si	-1.586997	-2.997426	1.602034
C	-2.846679	-3.975240	2.607535
H	-3.503192	-3.313591	3.186732
H	-3.483025	-4.594880	1.963418
H	-2.348153	-4.644018	3.320238
C	-0.433604	-4.181510	0.702235
H	-1.008863	-4.760456	-0.033167
H	-0.056433	-4.912113	1.432688
C	-0.552661	-1.944904	2.770244
H	-1.174604	-1.152225	3.204028
H	-0.270085	-2.601739	3.606288
H	2.724477	-0.654903	-2.329635
H	1.533562	-0.268942	-1.834625
C	-3.283400	0.104789	-1.460033
C	-4.096795	-0.845669	-2.084325
C	-3.406117	1.441261	-1.861883
C	-5.005171	-0.473178	-3.074743
H	-4.038344	-1.892534	-1.806623
C	-4.318335	1.816774	-2.840419

H	-2.777182	2.204723	-1.415919
C	-5.122701	0.858879	-3.454033
H	-5.624661	-1.231666	-3.545437
H	-4.395004	2.861262	-3.128670
H	-5.832629	1.150376	-4.222593
C	-2.633226	0.661813	1.235065
C	-2.288755	2.016642	1.277400
C	-3.430981	0.156984	2.268021
C	-2.718635	2.843701	2.310483
H	-1.657927	2.431074	0.499682
C	-3.855486	0.976987	3.311871
H	-3.732873	-0.884840	2.276465
C	-3.502383	2.323320	3.336606
H	-2.428371	3.890256	2.312564
H	-4.469246	0.559661	4.105288
H	-3.835341	2.961605	4.149988
C	0.746965	3.108832	0.487899
C	0.809432	3.799598	1.701919
C	0.390628	3.813602	-0.666938
C	0.513304	5.158698	1.762911
H	1.080936	3.278539	2.614575
C	0.098400	5.174170	-0.607727
H	0.323194	3.298816	-1.619179
C	0.155307	5.850041	0.607970
H	0.563078	5.677253	2.716318
H	-0.178528	5.703234	-1.515119
H	-0.076643	6.910131	0.656297
C	2.970034	1.457438	0.141385
C	3.434213	1.874922	-1.111589
C	3.903940	1.201985	1.147029
C	4.793369	2.035683	-1.350582
H	2.723632	2.053774	-1.914417
C	5.269232	1.346185	0.905019
H	3.583872	0.876821	2.131614
C	5.718164	1.764660	-0.342396
H	5.132216	2.358873	-2.330739
H	5.980676	1.127924	1.696443
H	6.781722	1.881459	-0.530302
C	4.401827	-1.335677	-1.728752
O	3.641650	-0.894569	-2.703417
O	4.046431	-1.579983	-0.591538
H	5.437837	-1.484513	-2.065432
H	2.137302	-1.408175	0.038379
H	0.033211	-1.743610	-3.817039

H	-1.435356	-2.638739	-2.606658

TSA7-8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.130953	-0.213352	-1.092090
N	1.209439	-1.669811	0.317535
C	0.989555	0.737471	2.022441
H	1.678172	1.193210	2.741570
H	-0.026638	1.006396	2.334103
C	0.822511	-3.396854	-1.971512
C	-0.390870	0.906306	-2.346888
O	-0.652903	1.602027	-3.245270
P	-0.308709	-2.018082	-2.415897
P	1.159876	1.354358	0.307634
Si	1.048063	-3.401146	-0.099172
Si	1.120146	-1.153542	2.018718
C	2.591893	-4.367291	0.350999
H	2.694634	-4.482272	1.436705
H	2.549157	-5.374643	-0.082866
H	3.489331	-3.861800	-0.017595
C	2.689098	-1.691806	2.901486
H	2.811332	-1.181160	3.864858
H	2.682661	-2.770249	3.100870
H	3.567341	-1.480121	2.280280
H	0.511494	-4.360028	-2.388909
H	1.798162	-3.132966	-2.401254
P	-1.991660	-0.346022	-0.140249
C	-2.520335	-2.009135	0.435746
H	-3.575180	-1.984145	0.734826
H	-2.481112	-2.662725	-0.443378
Si	-1.509248	-2.952668	1.738382
C	-2.751051	-3.886133	2.805231
H	-3.391027	-3.205339	3.380872
H	-3.404795	-4.519301	2.192572
H	-2.238692	-4.537970	3.523605
C	-0.418282	-4.162915	0.805089
H	-1.031672	-4.742004	0.101319
H	-0.015599	-4.890408	1.524510
C	-0.402896	-1.899856	2.835932
H	-0.990742	-1.110109	3.319790

H	-0.059179	-2.562916	3.643749
H	2.187251	-0.661949	-2.140347
H	1.574236	-0.079710	-1.926887
C	-3.321022	0.042129	-1.378650
C	-4.136556	-0.947009	-1.937813
C	-3.490304	1.360179	-1.821618
C	-5.089753	-0.630652	-2.904756
H	-4.046190	-1.981326	-1.624586
C	-4.446266	1.679595	-2.778393
H	-2.866011	2.155061	-1.428609
C	-5.251008	0.683884	-3.326765
H	-5.710078	-1.418841	-3.322088
H	-4.556920	2.710983	-3.100318
H	-5.995038	0.932426	-4.077757
C	-2.539629	0.727901	1.264792
C	-2.254019	2.095691	1.201921
C	-3.223480	0.251599	2.389124
C	-2.636347	2.963049	2.220358
H	-1.707128	2.492898	0.355046
C	-3.596156	1.113227	3.418657
H	-3.476395	-0.798974	2.481953
C	-3.305944	2.472137	3.337454
H	-2.394931	4.018536	2.139616
H	-4.118463	0.716918	4.284716
H	-3.599681	3.143377	4.139138
C	0.748495	3.148285	0.405989
C	0.789589	3.854181	1.611524
C	0.411706	3.835427	-0.765104
C	0.492181	5.213887	1.647949
H	1.043672	3.344574	2.535651
C	0.116385	5.195805	-0.729900
H	0.366137	3.308559	-1.712375
C	0.152866	5.888281	0.477596
H	0.525605	5.745844	2.594578
H	-0.144354	5.712623	-1.648956
H	-0.079731	6.948864	0.506829
C	2.976139	1.494572	0.031199
C	3.412218	1.811896	-1.260101
C	3.927685	1.330826	1.038595
C	4.765937	1.953699	-1.537308
H	2.688060	1.926130	-2.061965
C	5.286242	1.462216	0.760080
H	3.627415	1.083489	2.051485
C	5.709161	1.771469	-0.527471

H	5.084904	2.191131	-2.548016
H	6.014080	1.315758	1.553079
H	6.768662	1.870496	-0.745565
C	4.172319	-1.504895	-1.707150
O	3.336798	-1.304168	-2.646134
O	3.942128	-1.553816	-0.488805
H	5.217250	-1.661771	-2.045620
H	2.178829	-1.452665	-0.003639
H	-0.135584	-1.890928	-3.809679
H	-1.559747	-2.676615	-2.465830

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.082599	-0.488186	-1.105942
N	0.086514	-2.146452	0.105694
C	1.760815	-0.415658	1.843483
H	2.737822	-0.585093	2.309163
H	1.208731	0.312018	2.450234
C	-1.981871	-3.113939	-1.774894
C	0.423947	0.671765	-2.385779
O	0.659676	1.386015	-3.284006
P	-1.054242	-1.775481	-2.593853
P	1.878797	0.263200	0.157566
Si	-1.005842	-3.461939	-0.172677
Si	0.687229	-1.979942	1.723541
C	-0.144819	-5.125942	-0.409076
H	0.410860	-5.433587	0.484122
H	-0.866426	-5.920217	-0.639848
H	0.575106	-5.076432	-1.236620
C	1.724167	-3.449099	2.303874
H	2.182408	-3.244720	3.280266
H	1.124369	-4.361052	2.413377
H	2.531298	-3.664427	1.592615
H	-2.972574	-2.722847	-1.516107
H	-2.123073	-3.995516	-2.408154
P	-1.653020	0.588561	-0.149445
C	-2.828951	-0.486129	0.803006
H	-3.551912	0.176207	1.297464
H	-3.411017	-0.995615	0.021438
Si	-2.391844	-1.871095	2.058875

C	-3.826046	-1.818759	3.288058
H	-3.853496	-0.867669	3.835620
H	-4.793458	-1.935536	2.782969
H	-3.741978	-2.623012	4.029436
C	-2.299980	-3.549699	1.209174
H	-3.268364	-3.876643	0.808404
H	-2.011566	-4.284077	1.975627
C	-0.746445	-1.731596	2.950650
H	-0.630562	-0.791139	3.500877
H	-0.736659	-2.532868	3.704654
C	-2.885763	1.518932	-1.173897
C	-3.912386	2.255649	-0.566726
C	-2.822121	1.490992	-2.567283
C	-4.854298	2.930807	-1.333512
H	-3.968215	2.317629	0.517349
C	-3.764678	2.168630	-3.340688
H	-2.020839	0.951786	-3.057399
C	-4.784554	2.885564	-2.726028
H	-5.641934	3.497779	-0.845313
H	-3.692610	2.137322	-4.424168
H	-5.518489	3.416041	-3.326032
C	-1.220914	1.923287	1.041218
C	-0.648107	3.090499	0.519854
C	-1.404643	1.826765	2.421361
C	-0.268039	4.131591	1.356800
H	-0.494894	3.181803	-0.552523
C	-1.006531	2.863593	3.265960
H	-1.868258	0.946170	2.853077
C	-0.438157	4.016769	2.735723
H	0.182150	5.023871	0.932949
H	-1.152601	2.768214	4.338277
H	-0.128530	4.824331	3.392850
C	2.451776	1.994728	0.358315
C	2.842311	2.503819	1.599287
C	2.510412	2.832990	-0.761849
C	3.269913	3.823768	1.723365
H	2.812552	1.874106	2.482494
C	2.939067	4.150337	-0.639117
H	2.217282	2.459198	-1.737013
C	3.317017	4.651084	0.605581
H	3.564394	4.204162	2.697289
H	2.975179	4.787279	-1.518259
H	3.648312	5.681146	0.702129
C	3.380504	-0.562018	-0.532275

C	4.644799	0.035952	-0.515750
C	3.246971	-1.840264	-1.091162
C	5.748136	-0.625608	-1.048938
H	4.773891	1.025690	-0.088667
C	4.352414	-2.502050	-1.619230
H	2.273595	-2.324605	-1.093844
C	5.605173	-1.894889	-1.603455
H	6.722136	-0.144870	-1.031096
H	4.230801	-3.492961	-2.047855
H	6.466712	-2.406604	-2.022845
H	-1.888335	-1.328920	-3.643508
H	-0.151135	-2.508414	-3.399336

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.050768	-0.212472	-1.229941
N	0.706084	-2.152906	-0.078823
C	1.526019	-0.017979	1.761029
H	2.388689	0.084233	2.427432
H	0.711762	0.576131	2.189132
C	-0.489948	-3.261258	-2.490830
C	-0.057650	1.162691	-2.305990
O	-0.063567	2.024537	-3.098137
P	-1.071092	-1.511747	-2.630111
P	1.772917	0.604264	0.047216
Si	-0.093806	-3.621228	-0.683975
Si	0.945459	-1.811492	1.651024
C	1.092345	-5.078590	-0.596207
H	1.333332	-5.345922	0.439523
H	0.660736	-5.966759	-1.074956
H	2.036292	-4.853724	-1.108187
C	2.267976	-2.947801	2.356579
H	2.496801	-2.687124	3.397907
H	1.945722	-3.996297	2.346455
H	3.200551	-2.879525	1.782890
H	-1.190650	-3.979473	-2.931001
H	0.451171	-3.327269	-3.050928
P	-1.824190	0.289835	-0.025674
C	-2.879359	-1.150746	0.441479
H	-3.831772	-0.818485	0.872602

H	-3.139424	-1.643507	-0.502908
Si	-2.158142	-2.546226	1.503491
C	-3.551198	-3.150866	2.619406
H	-3.871330	-2.368729	3.319390
H	-4.429657	-3.451718	2.034926
H	-3.237960	-4.016951	3.215468
C	-1.618071	-3.948456	0.364037
H	-2.457988	-4.234016	-0.284401
H	-1.410139	-4.826437	0.993200
C	-0.679501	-2.060355	2.559881
H	-0.916681	-1.156044	3.134541
H	-0.539247	-2.864698	3.296777
H	1.139910	-0.774372	-2.271740
H	1.597781	-2.070460	-0.572849
C	-3.022809	1.293288	-1.031201
C	-4.191853	0.754922	-1.577567
C	-2.720680	2.631442	-1.315153
C	-5.032295	1.527724	-2.378488
H	-4.467866	-0.276272	-1.386013
C	-3.561755	3.406804	-2.103924
H	-1.811725	3.078743	-0.926663
C	-4.723254	2.856929	-2.642289
H	-5.933155	1.083717	-2.793369
H	-3.303646	4.442647	-2.304844
H	-5.378025	3.460453	-3.264344
C	-1.844391	1.293611	1.536293
C	-1.012756	2.417867	1.592786
C	-2.622780	0.995594	2.659927
C	-0.962737	3.224072	2.725637
H	-0.376821	2.654710	0.745270
C	-2.564549	1.790176	3.803694
H	-3.287501	0.137638	2.660138
C	-1.735978	2.908112	3.839993
H	-0.304645	4.088153	2.737662
H	-3.172532	1.533587	4.666918
H	-1.692677	3.527403	4.731404
C	2.171515	2.391384	0.253778
C	2.402480	2.984168	1.498505
C	2.246005	3.186864	-0.895304
C	2.690848	4.343933	1.593755
H	2.343663	2.392567	2.406937
C	2.537298	4.544403	-0.800761
H	2.067832	2.745470	-1.870449
C	2.756417	5.127953	0.444849

H	2.861444	4.791016	2.569303
H	2.587062	5.146497	-1.703421
H	2.976721	6.188895	0.520597
C	3.479996	-0.024821	-0.345140
C	3.819718	-0.300884	-1.673397
C	4.467905	-0.176083	0.636629
C	5.101460	-0.732016	-2.008787
H	3.060911	-0.190794	-2.441659
C	5.745355	-0.619368	0.306245
H	4.254092	0.057089	1.674985
C	6.065583	-0.901307	-1.019801
H	5.342229	-0.938884	-3.047852
H	6.493103	-0.737301	1.085594
H	7.062805	-1.245429	-1.279480
H	-0.954124	-1.266047	-4.014410
H	-2.478095	-1.745349	-2.651168

$R^1=R^2=R^3=F$

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.370849	0.160044	-0.282341
N	-0.571513	-0.209312	-0.998760
C	0.104879	-2.991792	-0.384841
H	0.166448	-3.828553	-1.088565
H	-0.029331	-3.401177	0.621796
C	-0.727427	2.733673	-0.836849
C	3.025211	0.410295	0.349589
O	4.088920	0.560699	0.771241
P	0.968538	2.293616	-0.479745
P	1.607394	-2.022231	-0.416255
Si	-1.607000	1.116557	-1.385022
Si	-1.305385	-1.759625	-0.787129
C	-1.997313	1.300335	-3.215093
H	-2.501868	0.412805	-3.614303
H	-2.644257	2.166018	-3.405556
H	-1.073602	1.438187	-3.791610
C	-2.224358	-2.392961	-2.302602
H	-2.583249	-3.417749	-2.142438
H	-3.103056	-1.777479	-2.533596
H	-1.576880	-2.395268	-3.187799

H	-1.194759	3.103443	0.082960
H	-0.780929	3.536485	-1.580120
P	0.472043	0.085937	1.685940
C	-1.161306	0.730501	2.107719
H	-1.279705	0.559702	3.186245
H	-1.128660	1.820572	1.981494
Si	-2.742174	0.044157	1.246306
C	-4.096761	0.210174	2.543674
H	-3.892984	-0.419234	3.418652
H	-4.196186	1.245272	2.893750
H	-5.067341	-0.095423	2.134237
C	-3.159038	1.023614	-0.308811
H	-3.545609	2.026359	-0.085930
H	-3.970587	0.485637	-0.821009
C	-2.500150	-1.731529	0.690894
H	-2.130235	-2.352911	1.514946
H	-3.478567	-2.139640	0.400337
H	1.491402	0.162669	-2.069568
H	2.246939	0.243611	-1.870695
F	2.611314	-2.788548	0.571278
F	2.269997	-2.502120	-1.801161
F	0.299288	-1.399004	2.312068
F	1.336604	0.694417	2.898264
F	1.399898	3.295109	0.700250
F	1.766545	3.019730	-1.670996

TSA5-1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.276402	0.034349	-0.349050
N	-0.727488	0.179248	-1.186341
C	-0.198457	-2.555179	-1.816559
H	0.034953	-2.314278	-2.861944
H	-0.450991	-3.617688	-1.746051
C	-0.452859	2.902694	-0.136564
C	3.033929	0.001561	-0.052649
O	4.176670	-0.011470	0.103611
P	1.192238	2.210872	-0.306919
P	1.214153	-2.114740	-0.805949
Si	-1.655344	1.617726	-0.893771
Si	-1.553112	-1.346400	-1.238328

C	-2.380222	2.364602	-2.454606
H	-3.049309	1.659074	-2.961585
H	-2.955778	3.273610	-2.239246
H	-1.583892	2.630728	-3.160767
C	-2.984376	-1.399248	-2.454844
H	-3.394185	-2.414397	-2.530887
H	-3.807413	-0.742415	-2.146877
H	-2.666614	-1.090926	-3.457715
H	-0.658384	3.018553	0.934214
H	-0.526492	3.893955	-0.597226
P	0.762002	-0.143366	1.734197
C	-0.845999	0.318007	2.416977
H	-0.875120	-0.067217	3.444498
H	-0.863373	1.411809	2.505412
Si	-2.448412	-0.211984	1.511297
C	-3.732970	-0.493479	2.856748
H	-3.455943	-1.331020	3.508483
H	-3.852644	0.396346	3.486926
H	-4.712279	-0.722366	2.418911
C	-2.984095	1.203863	0.382167
H	-3.248610	2.089484	0.976234
H	-3.907887	0.899881	-0.132177
C	-2.182462	-1.776316	0.490145
H	-1.485082	-2.440313	1.018257
H	-3.132932	-2.322303	0.414531
H	1.515075	0.156027	-2.037358
H	0.566486	0.224952	-1.916590
F	1.128718	-3.228540	0.343373
F	2.479615	-2.731552	-1.574157
F	0.918150	-1.584304	2.434756
F	1.730268	0.647353	2.753608
F	2.087495	3.053062	0.721310
F	1.690726	2.940148	-1.648992

A6

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.170834	-0.362439	-0.026880
N	-0.468110	0.902549	0.837074
C	0.381510	2.648499	-1.351152
H	0.691929	3.674628	-1.123847

H	0.128076	2.606605	-2.416574
C	-0.438668	-1.302706	2.696921
C	2.628299	-1.245844	-0.587016
O	3.588049	-1.794335	-0.907178
P	0.517706	-1.963827	1.332365
P	1.744960	1.496787	-1.051848
Si	-1.561937	0.027800	1.938197
Si	-1.112709	2.122816	-0.294225
C	-2.174463	1.140544	3.313384
H	-2.912354	1.867929	2.957251
H	-2.649330	0.549916	4.106673
H	-1.341932	1.696964	3.759260
C	-1.741661	3.620603	0.639859
H	-1.935553	4.450725	-0.051200
H	-2.676880	3.415204	1.173178
H	-1.002505	3.961062	1.374469
H	-0.968244	-2.078961	3.259199
H	0.256632	-0.790843	3.374236
P	0.043856	-1.068796	-1.738027
C	-1.661318	-1.641412	-1.692230
H	-1.967505	-1.875078	-2.719520
H	-1.680881	-2.578267	-1.123942
Si	-2.926836	-0.447124	-0.920403
C	-4.594365	-0.887244	-1.664765
H	-4.603851	-0.719500	-2.748546
H	-4.839494	-1.941427	-1.487172
H	-5.396851	-0.281104	-1.227499
C	-2.975669	-0.707057	0.946767
H	-3.057991	-1.783197	1.149313
H	-3.909065	-0.258438	1.316286
C	-2.486033	1.343578	-1.316864
H	-2.259596	1.421804	-2.387684
H	-3.392868	1.943899	-1.155181
C	2.298982	1.116042	2.409936
O	2.313888	0.092085	1.658016
O	1.458295	2.031508	2.435655
H	3.140773	1.160583	3.126692
H	0.209668	1.408813	1.456972
F	-0.463719	-3.151079	0.845819
F	1.614361	-2.901887	2.019396
F	2.842558	2.440845	-0.367896
F	2.449508	1.391211	-2.488785
F	-0.092105	-0.061837	-3.004687
F	0.726634	-2.279877	-2.551424

A7

	Coordinates (Angstroms)		
	X	Y	Z
Mn	1.176482	-0.389976	0.292490
N	-0.338965	1.141102	-0.153170
C	0.640690	0.838772	-2.833603
H	1.085306	1.830060	-2.988518
H	0.492314	0.366255	-3.810089
C	-0.469999	1.143265	2.724739
C	2.584045	-1.445905	0.672882
O	3.503387	-2.087909	0.926568
P	0.466769	-0.323805	2.382354
P	1.792735	-0.104841	-1.824756
Si	-1.485647	1.512771	1.165373
Si	-0.950201	1.111044	-1.832111
C	-1.951628	3.320876	1.216648
H	-2.589847	3.624068	0.380440
H	-2.492834	3.543146	2.145186
H	-1.039010	3.927136	1.205461
C	-1.675236	2.768373	-2.310556
H	-1.796772	2.835958	-3.398950
H	-2.662098	2.933488	-1.862811
H	-1.008258	3.577446	-1.992659
H	-1.025380	1.104719	3.666625
H	0.250331	1.978041	2.733047
P	-0.037927	-2.144029	-0.158744
C	-1.779946	-2.328708	0.225604
H	-2.116037	-3.278176	-0.209452
H	-1.880711	-2.415762	1.312386
Si	-2.916090	-0.923887	-0.383527
C	-4.612653	-1.685801	-0.635509
H	-4.589657	-2.454700	-1.417002
H	-4.979222	-2.154863	0.285512
H	-5.345638	-0.927792	-0.936821
C	-2.994651	0.409873	0.946164
H	-3.254528	-0.067746	1.900939
H	-3.843041	1.067416	0.704142
C	-2.245958	-0.237346	-2.010146
H	-1.878934	-1.070918	-2.621452
H	-3.087244	0.198088	-2.567465

H	2.044205	0.931262	1.072043
H	2.222405	1.032507	0.294272
C	1.838077	3.632682	0.382670
O	1.423858	3.372837	1.528349
O	1.534421	3.041539	-0.695008
H	2.567395	4.469027	0.278891
H	0.357012	1.939785	-0.199333
F	-0.501925	-1.477848	2.952306
F	1.568386	-0.427443	3.536735
F	0.557030	-3.504902	0.450950
F	-0.082821	-2.622343	-1.696546
F	2.081267	-1.405534	-2.708451
F	3.205245	0.599865	-2.073456

A8

Coordinates (Angstroms)

	X	Y	Z
Mn	-0.806926	-0.876255	-0.193173
N	-0.021659	1.223532	-0.039479
C	-0.631269	0.673864	2.759225
H	-1.226239	1.330196	3.403667
H	-0.047714	0.004224	3.400440
C	0.052537	0.804048	-2.878851
C	-1.761199	-2.367349	-0.339765
O	-2.429504	-3.304332	-0.436461
P	-0.231039	-0.858885	-2.244735
P	-1.680563	-0.366835	1.716423
Si	0.931556	1.715908	-1.472363
Si	0.542152	1.630307	1.610859
C	0.808728	3.566604	-1.734205
H	1.440788	4.120887	-1.030981
H	1.131072	3.836812	-2.747444
H	-0.222755	3.913089	-1.602865
C	0.344990	3.466885	1.915441
H	0.524241	3.706667	2.970823
H	1.044861	4.062030	1.317783
H	-0.670328	3.793504	1.661913
H	0.604176	0.802932	-3.824622
H	-0.922477	1.279764	-3.040127
P	0.875185	-1.916271	0.618069
C	2.584599	-1.575574	0.158618

H	3.245581	-2.216872	0.754871
H	2.700017	-1.870385	-0.891568
Si	3.141685	0.234426	0.319011
C	5.006979	0.204596	0.542975
H	5.289393	-0.322918	1.462155
H	5.497043	-0.303941	-0.296397
H	5.418809	1.219456	0.602943
C	2.710407	1.162405	-1.264952
H	3.010233	0.545439	-2.122614
H	3.340945	2.062342	-1.303989
C	2.330948	1.084924	1.796297
H	2.433508	0.438270	2.677203
H	2.923499	1.986104	2.012615
H	-3.174817	0.629729	-0.900685
H	-1.952160	-0.160726	-1.038199
C	-3.573240	2.464939	-0.647857
O	-3.952725	1.252612	-0.970635
O	-2.441471	2.816053	-0.366916
H	-4.417263	3.166272	-0.669834
H	-0.935028	1.687988	-0.163983
F	-3.048910	0.488976	1.751896
F	-2.170485	-1.516109	2.724681
F	0.858459	-3.518309	0.430132
F	1.088742	-1.953396	2.233062
F	1.110658	-1.580579	-2.810435
F	-1.219701	-1.520028	-3.321151

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.024957	-0.625658	0.253049
N	-0.196307	1.240127	0.280062
C	1.119844	1.711336	-2.182192
H	1.724698	2.500218	-1.716944
H	1.136270	1.849870	-3.267627
C	-0.634564	0.399450	2.963187
C	2.262975	-1.916717	0.384642
O	3.087384	-2.710779	0.504566
P	0.207126	-1.009522	2.246449
P	1.818299	0.130977	-1.690543
Si	-1.461132	1.339973	1.534120

Si	-0.590514	1.791741	-1.367495
C	-1.738672	3.099750	2.105092
H	-2.329335	3.682358	1.389636
H	-2.276014	3.110024	3.061806
H	-0.777643	3.607229	2.243035
C	-1.210689	3.557675	-1.387896
H	-1.204408	3.955570	-2.410190
H	-2.239076	3.632805	-1.015067
H	-0.575304	4.201510	-0.769366
H	-1.290439	0.120115	3.794015
H	0.136528	1.082781	3.345748
P	-0.358295	-2.060508	-0.626734
C	-2.149033	-2.008452	-0.472053
H	-2.572671	-2.767721	-1.140539
H	-2.402440	-2.299532	0.553101
Si	-2.927200	-0.307040	-0.815908
C	-4.652174	-0.600315	-1.495185
H	-4.611835	-1.118732	-2.460648
H	-5.253485	-1.212273	-0.812049
H	-5.183055	0.347311	-1.647861
C	-3.036693	0.583942	0.847029
H	-3.475665	-0.116153	1.571427
H	-3.765323	1.402081	0.751342
C	-1.882734	0.636105	-2.085132
H	-1.426389	-0.093602	-2.767419
H	-2.558465	1.240393	-2.706193
H	2.413081	0.833250	0.758514
H	2.050863	0.227462	1.273776
C	2.675449	3.097794	0.890127
O	3.218116	2.067017	0.398698
O	1.483784	3.225656	1.242584
H	3.340148	3.977591	1.009928
H	0.528735	1.914750	0.631396
F	1.209014	-1.513931	3.387353
F	-0.910162	-2.151483	2.469644
F	1.551528	-0.726552	-3.017806
F	3.394741	0.272405	-1.888939
F	-0.267649	-2.385236	-2.199486
F	-0.063938	-3.561308	-0.125944

A2

Coordinates (Angstroms)

	X	Y	Z
Mn	-1.214317	-0.119696	-0.195799
N	0.519760	0.116793	-1.087512
C	-0.076725	2.989987	-0.886889
H	-0.182519	3.557566	-1.817534
H	0.099382	3.696050	-0.068283
C	0.700049	-2.812303	-0.737992
C	-2.951591	-0.334522	0.163046
O	-4.076974	-0.472281	0.390758
P	-0.974442	-2.260898	-0.459474
P	-1.542082	2.015279	-0.554776
Si	1.617271	-1.230284	-1.307741
Si	1.306248	1.676991	-0.953524
C	2.143269	-1.489551	-3.090130
H	2.683492	-0.626186	-3.493444
H	2.795626	-2.366468	-3.185919
H	1.262979	-1.654168	-3.723553
C	2.456282	2.084451	-2.383785
H	2.779677	3.131326	-2.318876
H	3.364061	1.468594	-2.380705
H	1.956677	1.948054	-3.349988
H	1.120806	-3.147926	0.217016
H	0.756681	-3.643396	-1.448363
P	-0.591683	-0.042977	1.820327
C	1.050034	-0.663408	2.256082
H	1.186399	-0.494457	3.332493
H	1.031263	-1.752385	2.116112
Si	2.596406	0.041367	1.354265
C	3.955122	0.048461	2.654046
H	3.716389	0.736610	3.474282
H	4.103101	-0.948548	3.087519
H	4.910922	0.367173	2.220634
C	3.075874	-1.031542	-0.121286
H	3.453090	-2.014745	0.189611
H	3.915828	-0.524695	-0.619906
C	2.274486	1.762663	0.672502
H	1.739590	2.367610	1.414983
H	3.241240	2.257190	0.500979
F	-1.475112	-0.710369	2.987596
F	-0.489426	1.426932	2.490114
F	-1.601049	-3.327935	0.560119
F	-1.713029	-2.774872	-1.791550
F	-2.442825	2.928273	0.402885

F	-2.391441	2.209793	-1.906082

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-1.270147	-0.236376	-0.279062
N	0.636017	0.596834	-1.188253
C	-0.436828	2.941892	0.191237
H	-0.535859	3.949833	-0.226467
H	-0.480007	3.011942	1.283641
C	0.639682	-2.091751	-2.201857
C	-2.930991	-0.742202	0.085965
O	-4.029414	-1.051055	0.267324
P	-0.667780	-2.154665	-0.957526
P	-1.780533	1.848718	-0.328586
Si	1.789648	-0.704777	-1.630923
Si	1.174475	2.077358	-0.320891
C	2.878608	-0.145447	-3.050835
H	3.626008	0.587669	-2.726340
H	3.419871	-0.998601	-3.478192
H	2.289423	0.308988	-3.856452
C	2.122469	3.183191	-1.499234
H	2.383392	4.131949	-1.014214
H	3.055224	2.718625	-1.839154
H	1.523791	3.421233	-2.387128
H	1.140092	-3.057392	-2.329372
H	0.188626	-1.801219	-3.158245
P	-0.671572	-0.371673	1.757804
C	0.915612	-1.037545	2.304640
H	0.990727	-0.939950	3.394776
H	0.907197	-2.109170	2.070899
Si	2.448552	-0.277495	1.486773
C	3.888853	-0.526859	2.667444
H	3.719682	-0.007900	3.618640
H	4.036743	-1.590643	2.889936
H	4.824424	-0.143727	2.241743
C	2.807314	-1.175659	-0.132706
H	2.720294	-2.255880	0.043920
H	3.862517	-0.992536	-0.381142
C	2.223461	1.566630	1.147375
H	1.835680	2.046622	2.055306

H	3.228031	1.985948	0.990140
H	-1.696836	-0.361449	-1.813896
H	0.182371	0.877926	-2.061035
F	-1.651728	-1.231841	2.711688
F	-0.678015	0.957487	2.703201
F	-0.020718	-3.288996	0.015253
F	-1.761963	-3.135616	-1.601272
F	-3.067166	2.454480	0.413598
F	-2.077385	2.506410	-1.775644

$R^1=R^2=R^3=NH_2$

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.341277	0.167087	-0.388730
N	-0.632513	-0.363046	-1.061462
C	0.170793	-3.039777	-0.141515
H	0.189643	-3.957068	-0.742119
H	0.078552	-3.314690	0.913098
C	-0.692406	2.467821	-1.767832
C	2.989829	0.525707	0.085876
O	4.087367	0.751565	0.434653
P	0.810959	2.355200	-0.749763
P	1.685844	-2.064627	-0.355568
Si	-1.717660	0.882620	-1.496798
Si	-1.278984	-1.881574	-0.612334
C	-2.640186	0.623617	-3.131936
H	-3.391128	-0.173062	-3.076808
H	-3.161441	1.542512	-3.433811
H	-1.938315	0.358911	-3.932942
C	-2.275455	-2.756805	-1.964387
H	-2.487940	-3.797660	-1.684710
H	-3.241626	-2.270565	-2.146066
H	-1.725789	-2.768155	-2.913667
H	-1.245087	3.404547	-1.621437
H	-0.359260	2.447670	-2.812937
P	0.616504	0.259282	1.764095
C	-1.067689	0.824154	2.212276
H	-1.175677	0.694806	3.300040
H	-1.104284	1.904747	2.032605
Si	-2.620661	0.097076	1.378703

C	-3.991263	0.286352	2.672133
H	-3.794836	-0.328941	3.559739
H	-4.094061	1.327255	3.005415
H	-4.961350	-0.025902	2.265115
C	-3.028008	1.142299	-0.134781
H	-3.116293	2.199251	0.154185
H	-4.017282	0.845990	-0.514194
C	-2.426072	-1.709922	0.903493
H	-2.018200	-2.258239	1.762166
H	-3.417571	-2.136027	0.692456
H	1.639561	-0.261250	-2.095573
H	1.729544	0.523639	-2.095575
N	2.254308	-2.677443	-1.844534
H	3.047101	-2.168937	-2.221682
H	2.415045	-3.679756	-1.893312
N	2.684025	-2.645805	0.928427
H	2.855469	-3.648680	0.920545
H	3.568388	-2.148220	0.983669
N	1.989836	3.125741	-1.726133
H	1.856619	4.131101	-1.810835
H	2.929882	2.943335	-1.387469
N	0.492938	3.427870	0.538911
H	0.784780	3.057176	1.444280
H	-0.429638	3.845118	0.570184
N	1.495360	1.456383	2.654306
H	1.288989	1.488834	3.649786
H	2.499387	1.386571	2.516471
N	0.634460	-1.206613	2.621050
H	1.438355	-1.800036	2.416228
H	0.404087	-1.175774	3.608815

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	-1.282248	-0.179936	-0.374485
N	0.688759	0.458152	-1.181557
C	-0.248359	3.037861	-0.043475
H	-0.290695	3.989515	-0.587010
H	-0.177004	3.246715	1.028440
C	0.733107	-2.320645	-1.978359
C	-2.953403	-0.597932	-0.099412

O	-4.081287	-0.871993	0.079316
P	-0.701124	-2.306120	-0.852549
P	-1.722370	2.017929	-0.339393
Si	1.806474	-0.822803	-1.517009
Si	1.251828	1.972146	-0.554532
C	2.944873	-0.454128	-2.979477
H	3.704287	0.296526	-2.729750
H	3.477089	-1.360694	-3.297124
H	2.377225	-0.078505	-3.839329
C	2.257625	2.960879	-1.810374
H	2.482575	3.966072	-1.430007
H	3.214110	2.480212	-2.047532
H	1.701044	3.071127	-2.749228
H	1.282577	-3.269921	-1.957175
H	0.350526	-2.168399	-2.995024
P	-0.715356	-0.334301	1.800803
C	0.958709	-0.831171	2.353232
H	1.041460	-0.623362	3.430656
H	1.029024	-1.917370	2.228436
Si	2.495490	-0.128485	1.485384
C	3.891390	-0.292572	2.752739
H	3.713446	0.343962	3.628993
H	3.991980	-1.326227	3.107947
H	4.856187	0.003311	2.321805
C	2.887494	-1.203462	-0.011003
H	2.766473	-2.256503	0.276801
H	3.945360	-1.067180	-0.277725
C	2.327403	1.678672	0.984777
H	1.923125	2.240487	1.837046
H	3.337835	2.073698	0.801693
H	-1.452705	-0.059556	-2.077473
H	-0.543698	0.256477	-1.898334
N	-2.813531	2.578760	0.873767
H	-3.010631	3.576623	0.848896
H	-3.687377	2.059689	0.865633
N	-2.203558	2.599564	-1.866472
H	-2.841697	1.979962	-2.352362
H	-2.503599	3.568054	-1.925584
N	-1.883761	-3.147299	-1.760742
H	-1.685470	-4.127365	-1.942907
H	-2.820412	-3.042225	-1.385254
N	-0.141886	-3.305161	0.414603
H	-0.705194	-3.191440	1.257497
H	0.004164	-4.284980	0.188486

N	-1.606296	-1.601882	2.575732
H	-1.471310	-1.666028	3.582406
H	-2.599357	-1.542426	2.369965
N	-0.861980	1.100725	2.708520
H	-1.663027	1.673936	2.444329
H	-0.747424	1.030510	3.714836

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	-1.227301	-0.272292	-0.072902
N	0.485670	1.026943	0.683693
C	0.297260	-0.884357	2.880163
H	-0.337179	-0.251798	3.511524
H	0.821391	-1.602487	3.523816
C	-0.053494	2.344849	-1.940935
C	-2.642180	-1.145990	-0.611429
O	-3.590060	-1.728852	-0.980735
P	-1.582264	1.464006	-1.473210
P	-0.789348	-1.693323	1.655701
Si	1.235955	2.026006	-0.581023
Si	1.476919	0.261319	1.956038
C	1.766292	3.679300	0.142873
H	2.563016	3.572977	0.887828
H	2.132102	4.355065	-0.640964
H	0.916363	4.167112	0.636265
C	2.119191	1.567346	3.147645
H	2.488797	1.101596	4.070362
H	2.945851	2.147682	2.720737
H	1.314143	2.260460	3.415776
H	0.324172	1.920758	-2.876433
H	-0.235932	3.416105	-2.089320
P	0.031876	-1.460134	-1.558877
C	1.789114	-1.930031	-1.332480
H	1.809739	-2.749097	-0.604911
H	2.163782	-2.333499	-2.285025
Si	3.014002	-0.645718	-0.680177
C	4.723448	-1.205272	-1.251793
H	4.933770	-2.235769	-0.938790
H	4.808830	-1.166713	-2.345272
H	5.512555	-0.565826	-0.837039

C	2.710481	1.104002	-1.304878
H	2.617078	1.078955	-2.398293
H	3.619864	1.682825	-1.084436
C	2.928073	-0.665106	1.197500
H	2.902811	-1.710918	1.530816
H	3.853258	-0.226940	1.597827
C	-2.317438	1.519867	2.266612
O	-2.523783	0.704699	1.319965
O	-1.265464	2.113394	2.563173
H	-3.213950	1.724109	2.891964
H	-0.176549	1.606742	1.243292
N	-2.463276	2.708695	-0.740379
H	-2.795836	3.479072	-1.309640
H	-3.154360	2.363718	-0.084123
N	-2.244657	1.091120	-3.022484
H	-3.095837	0.540952	-2.943492
H	-2.413392	1.893657	-3.624749
N	-2.149552	-2.104352	2.594989
H	-2.993571	-2.243736	2.052010
H	-2.025938	-2.839357	3.283850
N	0.115567	-3.100751	1.311084
H	0.206984	-3.775341	2.065494
H	-0.191875	-3.543603	0.444767
N	-0.593734	-3.069713	-1.701775
H	-1.598979	-3.084820	-1.846809
H	-0.140260	-3.635821	-2.415226
N	0.172029	-0.772819	-3.114128
H	0.570962	-1.360262	-3.840353
H	-0.673846	-0.294668	-3.426786

A7

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-1.051470	-0.684482	-0.112982
N	0.134279	1.071441	0.648504
C	0.493410	-0.848560	2.917219
H	0.310466	-0.638556	3.977998
H	1.215967	-1.666084	2.839715
C	-0.577050	2.082989	-1.981085
C	-2.146819	-1.964759	-0.615253
O	-2.860491	-2.833425	-0.927234

P	-1.122364	0.348098	-2.145600
P	-1.030851	-1.336024	2.055798
Si	0.716411	2.195129	-0.626594
Si	1.210240	0.660077	2.009489
C	0.782609	3.943245	0.056228
H	1.632530	4.098570	0.731199
H	0.871786	4.673207	-0.758698
H	-0.141426	4.152696	0.606592
C	1.298547	2.104091	3.205521
H	1.832866	1.825421	4.122687
H	1.812791	2.969458	2.772448
H	0.288575	2.427101	3.485481
H	-0.247496	2.515136	-2.934119
H	-1.462291	2.626751	-1.627241
P	0.718626	-1.991384	-0.708329
C	2.302331	-1.352836	-1.358948
H	3.016665	-2.188583	-1.392543
H	2.121327	-1.042260	-2.394241
Si	3.131586	0.125571	-0.514510
C	4.970251	-0.010854	-0.913125
H	5.411692	-0.911487	-0.467985
H	5.142378	-0.056600	-1.995805
H	5.524143	0.853721	-0.527065
C	2.420413	1.696484	-1.251201
H	2.385327	1.594470	-2.343641
H	3.110072	2.524015	-1.032417
C	2.916165	0.204814	1.352997
H	3.230098	-0.747274	1.798892
H	3.629926	0.962881	1.709378
H	-2.342574	0.530618	-0.058945
H	-2.356806	0.101341	0.623437
C	-3.137855	2.852293	0.550004
O	-3.456480	2.255509	-0.504249
O	-2.096259	2.730844	1.242344
H	-3.881682	3.595809	0.934222
H	-0.707049	1.582599	1.006014
N	-2.166971	-0.523732	3.015747
H	-3.092892	-0.409821	2.621834
H	-2.198206	-0.732544	4.008234
N	-1.093233	-3.032765	2.338753
H	-1.107929	-3.308781	3.317820
H	-1.864825	-3.474896	1.847015
N	1.342870	-2.980711	0.529176
H	0.627390	-3.369248	1.144287

H	2.026964	-3.677703	0.250182
N	0.287821	-2.961840	-2.068215
H	0.995232	-3.633947	-2.354631
H	-0.607034	-3.429828	-1.964513
N	-2.703848	0.394232	-2.803138
H	-3.323362	0.784494	-2.088285
H	-2.763205	1.010385	-3.613313
N	-0.129984	-0.229047	-3.394928
H	-0.099622	-1.248928	-3.409473
H	-0.322247	0.150767	-4.317716

A8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.852876	-0.901795	0.138504
N	0.069020	1.253468	-0.008104
C	0.439449	0.604412	-2.878280
H	0.967499	1.223139	-3.614654
H	-0.263025	-0.046688	-3.407706
C	0.076665	0.838700	2.856756
C	1.718984	-2.408552	0.192408
O	2.334646	-3.409938	0.187611
P	0.351703	-0.891115	2.303504
P	1.577989	-0.455339	-1.918412
Si	-0.811483	1.745360	1.463240
Si	-0.536913	1.652399	-1.636213
C	-0.662470	3.603699	1.723571
H	-1.278434	4.165757	1.011027
H	-0.995860	3.881491	2.732007
H	0.375042	3.934321	1.603459
C	-0.224113	3.473750	-1.985377
H	-0.451014	3.720208	-3.030470
H	-0.835084	4.125583	-1.349983
H	0.827637	3.721896	-1.799268
H	-0.453844	0.900901	3.815814
H	1.061529	1.308777	2.978161
P	-1.029439	-1.961829	-0.482787
C	-2.743775	-1.419348	-0.103899
H	-3.443370	-2.004158	-0.718813
H	-2.937926	-1.680918	0.942719
Si	-3.163536	0.414537	-0.251298

C	-5.040622	0.528200	-0.418209
H	-5.388256	0.032887	-1.333711
H	-5.545296	0.049166	0.430372
H	-5.378581	1.571303	-0.458535
C	-2.626478	1.281436	1.331028
H	-2.894843	0.637966	2.179119
H	-3.214431	2.204520	1.433143
C	-2.373762	1.259310	-1.738352
H	-2.560109	0.646607	-2.629724
H	-2.911875	2.206343	-1.892983
H	3.149262	0.683771	0.842470
H	2.160323	-0.179822	0.770815
C	3.617791	2.540913	0.696127
O	3.971975	1.296297	0.908339
O	2.488245	2.952417	0.515845
H	4.489990	3.211922	0.709338
H	1.001090	1.679752	0.084349
N	1.749453	-1.810972	-2.972160
H	2.139479	-1.609198	-3.889658
H	2.276913	-2.561081	-2.534008
N	2.977976	0.518519	-2.000752
H	3.708555	0.235444	-1.357724
H	3.355981	0.711520	-2.924082
N	-1.234300	-2.219709	-2.163380
H	-0.351058	-2.395944	-2.642267
H	-1.947715	-2.889792	-2.437213
N	-1.123675	-3.485132	0.335548
H	-1.881652	-4.089180	0.026244
H	-0.245647	-3.994523	0.308963
N	1.581407	-1.526002	3.318906
H	2.491806	-1.435643	2.879530
H	1.612442	-1.134545	4.256713
N	-1.079195	-1.627699	2.878168
H	-1.208907	-2.523769	2.406165
H	-1.123030	-1.753667	3.886430

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	0.916093	-0.840720	0.151518
N	0.020777	1.241560	0.072337

C	0.477667	0.724566	-2.825988
H	0.960815	1.376479	-3.564835
H	-0.198014	0.040839	-3.348093
C	-0.102355	0.700403	2.915166
C	1.846609	-2.315682	0.191772
O	2.484400	-3.300355	0.204691
P	0.265622	-0.979350	2.305593
P	1.695268	-0.257507	-1.885210
Si	-0.960766	1.628823	1.515313
Si	-0.527189	1.716633	-1.559376
C	-0.918012	3.475994	1.858700
H	-1.547795	4.037550	1.157939
H	-1.288243	3.687984	2.870184
H	0.105873	3.856738	1.778095
C	-0.204657	3.550426	-1.805869
H	-0.409300	3.852229	-2.840896
H	-0.826033	4.170675	-1.149680
H	0.843519	3.781622	-1.582596
H	-0.671870	0.706465	3.853325
H	0.862321	1.191272	3.092640
P	-0.875965	-1.980273	-0.631835
C	-2.629229	-1.520110	-0.342636
H	-3.255766	-2.087962	-1.045543
H	-2.886398	-1.863858	0.665908
Si	-3.153163	0.296464	-0.382106
C	-5.024101	0.282624	-0.630989
H	-5.293233	-0.150321	-1.602757
H	-5.522100	-0.311162	0.146011
H	-5.443937	1.295341	-0.591616
C	-2.741178	1.075491	1.278872
H	-3.002506	0.358874	2.067770
H	-3.385220	1.955364	1.417136
C	-2.356679	1.313772	-1.750442
H	-2.516657	0.817839	-2.716572
H	-2.911787	2.262900	-1.796476
H	2.789007	0.499111	0.887494
H	2.126210	-0.099542	1.013536
C	3.401284	2.558197	0.916831
O	3.831250	1.353230	0.886700
O	2.229734	2.942182	0.839446
H	4.202336	3.317338	1.025811
H	0.910531	1.746535	0.249928
N	2.995618	0.807610	-1.877216
H	3.618979	0.821084	-1.077618

H	3.373809	1.199983	-2.729817
N	1.993379	-1.565384	-2.971779
H	2.366092	-1.287485	-3.876945
H	2.612038	-2.257479	-2.556951
N	-0.950775	-2.195570	-2.322229
H	-0.031623	-2.299389	-2.754311
H	-1.616803	-2.879741	-2.668688
N	-0.945429	-3.532150	0.136851
H	-1.672556	-4.144917	-0.225789
H	-0.052863	-4.016458	0.111252
N	1.503453	-1.495564	3.363298
H	1.229497	-1.677141	4.324095
H	2.052116	-2.264554	2.994597
N	-1.182189	-1.800052	2.694430
H	-1.245792	-2.684882	2.190212
H	-1.378221	-1.920947	3.684417

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.192339	0.147554	-0.345836
N	-0.585252	-0.423769	-1.112594
C	0.237594	-3.088211	-0.115439
H	0.270551	-4.002216	-0.719888
H	0.167693	-3.364661	0.941248
C	-0.737740	2.347075	-1.989320
C	2.885550	0.548506	-0.154888
O	4.026168	0.808233	-0.021289
P	0.701758	2.300687	-0.882128
P	1.690266	-2.033560	-0.346132
Si	-1.738917	0.801566	-1.520992
Si	-1.224684	-1.939682	-0.566890
C	-2.827266	0.403913	-3.017409
H	-3.612087	-0.327435	-2.794577
H	-3.326304	1.316913	-3.369483
H	-2.229386	0.009658	-3.848057
C	-2.277820	-2.863233	-1.837962
H	-2.469589	-3.889682	-1.497578
H	-3.252972	-2.391892	-2.004675
H	-1.764550	-2.921263	-2.805576
H	-1.301340	3.285802	-1.931572

H	-0.379255	2.214571	-3.017218
P	0.740492	0.354544	1.814809
C	-0.938963	0.861302	2.337197
H	-1.033804	0.677321	3.418034
H	-1.007444	1.944798	2.187548
Si	-2.470801	0.132559	1.471268
C	-3.863984	0.304734	2.741630
H	-3.677842	-0.316890	3.626947
H	-3.972758	1.342769	3.081436
H	-4.827502	-0.006296	2.318456
C	-2.877210	1.174025	-0.045988
H	-2.810595	2.236253	0.226302
H	-3.923316	0.987363	-0.329519
C	-2.279557	-1.679855	0.996813
H	-1.835300	-2.216626	1.845262
H	-3.282073	-2.106820	0.845022
N	1.632472	1.626052	2.578124
H	1.489959	1.710872	3.582082
H	2.626494	1.559722	2.378830
N	0.883202	-1.079773	2.719820
H	1.665235	-1.672177	2.443917
H	0.772614	-1.017398	3.726780
N	0.213307	3.338988	0.379314
H	0.773100	3.203994	1.221482
H	0.108385	4.322219	0.146022
N	1.917021	3.050884	-1.827543
H	1.728926	4.008458	-2.112586
H	2.843517	2.980740	-1.419148
N	2.201894	-2.485969	-1.903828
H	2.860783	-1.841663	-2.326173
H	2.471927	-3.452492	-2.058108
N	2.794889	-2.608222	0.846162
H	3.028251	-3.596471	0.784835
H	3.648404	-2.056341	0.866557

A1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.309861	0.126224	-0.351777
N	-0.741342	-0.534850	-1.206037
C	0.131534	-3.021547	0.150657

H	0.126044	-4.029561	-0.283605
H	0.110298	-3.107886	1.241582
C	-0.569111	2.217215	-2.127419
C	2.964584	0.459287	0.026545
O	4.101078	0.668406	0.260392
P	0.856091	2.195008	-0.974903
P	1.617391	-2.062538	-0.320789
Si	-1.767912	0.874863	-1.577311
Si	-1.364313	-2.001015	-0.402203
C	-2.940754	0.462261	-2.994228
H	-3.720027	-0.245598	-2.686907
H	-3.444991	1.367463	-3.356211
H	-2.405515	0.020103	-3.843601
C	-2.381636	-3.011032	-1.621864
H	-2.712467	-3.952831	-1.165315
H	-3.276394	-2.475817	-1.960860
H	-1.786921	-3.263790	-2.508747
H	-1.044384	3.203636	-2.205991
H	-0.180047	1.949043	-3.117046
P	0.710455	0.379084	1.780718
C	-0.927554	0.965278	2.380624
H	-1.014533	0.764048	3.458539
H	-0.939523	2.054496	2.253254
Si	-2.477434	0.337498	1.505726
C	-3.920286	0.630326	2.688258
H	-3.799607	0.057554	3.616350
H	-3.998876	1.690438	2.960726
H	-4.875515	0.333266	2.237696
C	-2.762047	1.349673	-0.057919
H	-2.562295	2.402736	0.180003
H	-3.828273	1.280881	-0.316796
C	-2.416822	-1.494032	1.070574
H	-2.083690	-2.053029	1.954656
H	-3.451891	-1.810178	0.873827
H	1.737949	0.078744	-1.913152
H	-0.239863	-0.801039	-2.056917
N	1.646389	1.648157	2.507381
H	1.528859	1.737588	3.514336
H	2.634239	1.556952	2.288364
N	0.840311	-1.017664	2.770423
H	1.626900	-1.607189	2.500631
H	0.821487	-0.868039	3.775807
N	0.314669	3.328474	0.194827
H	0.840848	3.222861	1.062477

H	0.273751	4.301988	-0.095294
N	2.084075	2.967167	-1.892458
H	2.070657	3.982475	-1.874502
H	3.007008	2.623308	-1.650439
N	1.864118	-2.734089	-1.875962
H	2.484345	-2.163356	-2.439991
H	2.108941	-3.719436	-1.927831
N	2.781448	-2.679975	0.787760
H	2.960518	-3.679641	0.729650
H	3.658868	-2.170289	0.731341

$R^1=R^2=R^3=H$

A5

	Coordinates (Angstroms)		
	X	Y	Z

Mn	1.757004	-0.002050	0.228591
N	-0.234807	0.115954	1.038148
C	0.274344	2.962815	0.969705
H	0.535155	3.050008	2.032022
H	-0.018673	3.951955	0.604309
C	-0.183915	-2.807707	0.712943
C	3.432440	-0.119731	-0.340852
O	4.526718	-0.205092	-0.728426
P	1.555010	-2.257821	0.483069
P	1.726262	2.278258	0.092076
Si	-1.215433	-1.272858	1.208751
Si	-1.047832	1.602657	0.819311
C	-1.849668	-1.596856	2.959322
H	-2.459853	-0.763735	3.328301
H	-2.464330	-2.505606	3.007542
H	-1.012280	-1.722120	3.658218
C	-2.396266	1.995168	2.087728
H	-2.779107	3.014950	1.949711
H	-3.253636	1.315691	2.003911
H	-2.009604	1.918558	3.111316
H	-0.548262	-3.211051	-0.238373
H	-0.247720	-3.617548	1.447241
P	0.969737	-0.166467	-1.901979
C	-0.684297	-0.857952	-2.328751
H	-0.813636	-0.771788	-3.414687
H	-0.659750	-1.933188	-2.111661

Si	-2.221706	-0.101809	-1.471800
C	-3.590350	-0.123395	-2.772185
H	-3.350521	0.531556	-3.619534
H	-3.755521	-1.133697	-3.167774
H	-4.540443	0.223199	-2.346621
C	-2.690847	-1.171167	0.007089
H	-3.018776	-2.168334	-0.318039
H	-3.557294	-0.713581	0.507641
C	-1.866276	1.661075	-0.900843
H	-1.220162	2.159896	-1.638370
H	-2.800708	2.238851	-0.870024
H	2.255002	0.528980	1.836781
H	2.197425	-0.262407	1.912777
H	1.593203	2.851185	-1.193910
H	2.816937	3.070127	0.516370
H	1.783252	-0.870660	-2.821432
H	0.912540	1.039211	-2.642956
H	2.059698	-3.129261	-0.510087
H	2.215340	-2.865806	1.572837

TSA5-1

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-1.709431	-0.005999	-0.172113
N	0.286355	0.106167	-1.138250
C	-0.292180	2.927053	-1.072285
H	-0.577717	2.938389	-2.131897
H	-0.013959	3.944558	-0.781529
C	0.165264	-2.825193	-0.755641
C	-3.433087	-0.095877	0.196424
O	-4.575412	-0.159277	0.414560
P	-1.564084	-2.244470	-0.469239
P	-1.715417	2.263926	-0.119217
Si	1.255490	-1.326308	-1.209349
Si	1.066188	1.623527	-0.851608
C	1.986973	-1.637808	-2.918273
H	2.659769	-0.825693	-3.219252
H	2.559952	-2.573408	-2.951962
H	1.194113	-1.702880	-3.674281
C	2.476155	1.998407	-2.047824
H	2.866167	3.012266	-1.890342

H	3.317514	1.305600	-1.921689
H	2.138983	1.928403	-3.088970
H	0.536027	-3.275055	0.172605
H	0.195846	-3.608727	-1.520093
P	-1.046013	-0.164705	1.973230
C	0.612081	-0.858150	2.397524
H	0.755259	-0.794315	3.483145
H	0.586547	-1.928716	2.155532
Si	2.131492	-0.087250	1.531067
C	3.506630	-0.039282	2.821080
H	3.253092	0.634081	3.649724
H	3.696206	-1.033178	3.245681
H	4.446607	0.317572	2.382024
C	2.640442	-1.176334	0.077376
H	2.953946	-2.167654	0.433476
H	3.529951	-0.729476	-0.391483
C	1.760357	1.658407	0.911870
H	1.059944	2.148048	1.604129
H	2.683498	2.254639	0.939447
H	-1.974071	0.132988	-1.874868
H	-1.000354	0.131842	-1.774459
H	-2.818413	3.017127	-0.577201
H	-1.557796	2.922286	1.123555
H	-2.245789	-2.803096	-1.571596
H	-2.048985	-3.153899	0.499287
H	-1.856180	-0.900770	2.871352
H	-1.003052	1.021934	2.749106

A6

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-1.472882	-0.592090	-0.018982
N	0.177615	0.991145	-0.022332
C	-0.474335	1.011527	2.773356
H	-1.087368	1.904818	2.596847
H	-0.189285	0.994189	3.829722
C	0.257780	0.200715	-2.874349
C	-2.846782	-1.704741	-0.075907
O	-3.752748	-2.432260	-0.123630
P	-1.425638	-0.249555	-2.267475
P	-1.473305	-0.446829	2.259396

Si	1.156564	1.148257	-1.496079
Si	0.969247	1.075897	1.559875
C	1.275024	2.957853	-1.973573
H	1.783761	3.542452	-1.198185
H	1.826224	3.091181	-2.912635
H	0.273632	3.386106	-2.100570
C	1.923129	2.681568	1.772780
H	2.293359	2.787816	2.800365
H	2.793815	2.736036	1.107433
H	1.281784	3.544603	1.558331
H	0.787981	-0.735282	-3.085571
H	0.220117	0.768417	-3.810390
P	-0.078695	-2.388424	-0.043480
C	1.686282	-2.408016	-0.601906
H	2.121500	-3.383872	-0.355529
H	1.693451	-2.338842	-1.697090
Si	2.802039	-1.029990	0.085857
C	4.528468	-1.747096	0.307001
H	4.534576	-2.538993	1.066068
H	4.905506	-2.178065	-0.628706
H	5.240039	-0.976173	0.627096
C	2.842133	0.386838	-1.157124
H	3.284698	0.035241	-2.099367
H	3.517975	1.166745	-0.776466
C	2.140100	-0.388611	1.736983
H	1.658834	-1.213811	2.280819
H	2.990294	-0.075144	2.358982
C	-2.805794	2.229038	0.058735
O	-2.892382	0.972288	0.157693
O	-1.785955	2.924490	-0.121222
H	-3.775747	2.761713	0.151638
H	-0.525686	1.767694	-0.055132
H	-2.683436	-0.291461	2.966047
H	-0.911525	-1.463722	3.067259
H	-2.190762	0.847765	-2.719637
H	-1.854909	-1.181267	-3.238983
H	0.099927	-3.033622	1.206749
H	-0.542690	-3.537055	-0.728663

A7

Coordinates (Angstroms)		
X	Y	Z

Mn	-1.351588	-0.941185	0.006204
N	-0.047438	0.878269	0.185914
C	-0.405580	0.442115	2.975077
H	-1.098610	1.293190	2.996591
H	-0.030285	0.264886	3.987140
C	-0.348078	0.866344	-2.734258
C	-2.551305	-2.241761	-0.127673
O	-3.330821	-3.095773	-0.228070
P	-1.192752	-0.686309	-2.260241
P	-1.335083	-0.983541	2.294116
Si	0.729375	1.464520	-1.303311
Si	0.897338	0.897208	1.688890
C	0.781156	3.336742	-1.378633
H	1.393620	3.776457	-0.584157
H	1.196423	3.666866	-2.339889
H	-0.235789	3.734032	-1.293700
C	1.583842	2.600261	2.076211
H	1.976105	2.633415	3.100765
H	2.405923	2.878587	1.405730
H	0.797489	3.358423	1.990382
H	0.163371	0.789609	-3.698643
H	-1.137384	1.624063	-2.804129
P	0.288799	-2.507133	-0.087298
C	1.916403	-2.202641	-0.881836
H	2.534721	-3.102813	-0.789090
H	1.738259	-2.051882	-1.954438
Si	2.859847	-0.689681	-0.221117
C	4.696624	-1.097110	-0.284381
H	4.948146	-1.924438	0.390628
H	5.004071	-1.385908	-1.297177
H	5.303681	-0.232155	0.010511
C	2.487970	0.774955	-1.341278
H	2.760168	0.508123	-2.372345
H	3.165040	1.595762	-1.061040
C	2.325680	-0.323604	1.555718
H	2.101191	-1.267256	2.072286
H	3.180570	0.111508	2.091979
H	-2.549970	0.299317	-0.367835
H	-2.618335	0.182318	0.424443
C	-2.689600	2.934871	0.002537
O	-2.537922	2.515875	-1.163521
O	-2.019823	2.629159	1.026949
H	-3.519682	3.664430	0.174643

H	-0.837274	1.548205	0.395006
H	-0.693040	-2.082396	2.909027
H	-2.522334	-1.017613	3.054013
H	-2.351838	-0.702766	-3.061603
H	-0.473062	-1.664713	-2.984268
H	0.712206	-3.098100	1.126268
H	-0.092071	-3.706449	-0.730497

A8

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-1.121537	-1.106875	-0.086652
N	-0.050066	0.927949	-0.228044
C	-0.968964	1.173957	2.465721
H	-1.700337	1.953358	2.217814
H	-0.763757	1.249042	3.538270
C	0.108385	0.105144	-2.995173
C	-2.216983	-2.479648	-0.074378
O	-2.966833	-3.373357	-0.090843
P	-0.531339	-1.440558	-2.221349
P	-1.692950	-0.463403	1.997445
Si	0.971712	1.126643	-1.664213
Si	0.532346	1.460431	1.361282
C	0.987771	2.919000	-2.232114
H	1.554174	3.564221	-1.551398
H	1.442990	3.009939	-3.226706
H	-0.032242	3.316532	-2.293823
C	0.971631	3.288993	1.364360
H	1.083501	3.660690	2.391040
H	1.917768	3.483420	0.844757
H	0.188173	3.880030	0.876264
H	0.713859	-0.079978	-3.888511
H	-0.768845	0.688636	-3.305057
P	0.558688	-2.380518	0.679525
C	2.319500	-2.150928	0.170084
H	2.963031	-2.856254	0.709100
H	2.391330	-2.409503	-0.894472
Si	2.956231	-0.379564	0.391515
C	4.799462	-0.466827	0.767494
H	4.989769	-0.995105	1.709883
H	5.342171	-0.995073	-0.026393

H	5.237211	0.535244	0.857077
C	2.713031	0.562566	-1.227786
H	3.125317	-0.051081	-2.041058
H	3.344137	1.462852	-1.189197
C	2.054416	0.460048	1.829986
H	1.797215	-0.305211	2.575458
H	2.758665	1.138701	2.331259
H	-3.214076	0.602107	-0.268918
H	-2.318816	-0.277892	-0.819835
C	-3.458792	2.505337	-0.133361
O	-3.931921	1.291142	-0.016178
O	-2.322163	2.816520	-0.444875
H	-4.228318	3.258998	0.089974
H	-0.921667	1.444789	-0.408421
H	-1.483246	-1.886397	-3.163412
H	0.491330	-2.348804	-2.602256
H	0.425478	-3.766309	0.420761
H	0.762004	-2.523298	2.079469
H	-1.233197	-1.258688	3.077000
H	-3.024197	-0.336997	2.455605

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	Coordinates (Angstroms)		
	X	Y	Z

Mn	-1.199117	-1.108603	-0.066836
N	-0.116765	0.884021	0.124749
C	-0.306000	0.169378	2.964568
H	-0.666975	0.853736	3.739276
H	0.296999	-0.596880	3.465415
C	-0.442568	0.706033	-2.762416
C	-2.208171	-2.552693	-0.149465
O	-2.879383	-3.502840	-0.184244
P	-0.774544	-1.039395	-2.297289
P	-1.705835	-0.681745	2.107031
Si	0.635571	1.427907	-1.396100
Si	0.753683	1.067478	1.671491
C	0.612560	3.302661	-1.504170
H	1.366844	3.762627	-0.855710
H	0.809573	3.637753	-2.530073
H	-0.365296	3.695607	-1.202709
C	0.878020	2.886147	2.116629

H	1.215720	3.017850	3.152345
H	1.586370	3.419113	1.471591
H	-0.100869	3.367672	2.010161
H	-0.017222	0.817181	-3.765428
H	-1.404984	1.232100	-2.731085
P	0.599079	-2.377925	0.447516
C	2.234211	-2.127748	-0.365889
H	2.948770	-2.873999	0.001609
H	2.107490	-2.315904	-1.439469
Si	2.975028	-0.395294	-0.136391
C	4.847028	-0.579862	-0.232129
H	5.228791	-1.215238	0.576603
H	5.152884	-1.034233	-1.182749
H	5.348130	0.392664	-0.153219
C	2.394914	0.766194	-1.501454
H	2.546152	0.277893	-2.474420
H	3.075907	1.630034	-1.495135
C	2.481274	0.320136	1.536838
H	2.628820	-0.442411	2.313822
H	3.196624	1.122208	1.770683
H	-2.747394	0.569912	-0.719002
H	-2.617498	-0.302645	-0.462089
C	-3.040496	2.667306	-0.258659
O	-3.203375	1.753158	-1.135042
O	-2.292474	2.633844	0.728365
H	-3.646167	3.577901	-0.435533
H	-0.965549	1.467702	0.264087
H	0.327381	-1.691812	-2.901123
H	-1.745992	-1.452119	-3.232998
H	1.048377	-2.454197	1.791673
H	0.436968	-3.771631	0.276059
H	-2.055386	-1.691499	3.030348
H	-2.776437	0.193638	2.374128

A2

	Coordinates (Angstroms)		
	X	Y	Z

Mn	-1.631209	-0.012452	-0.131219
N	0.154935	-0.004599	-1.076304
C	-0.290870	2.850132	-1.323315
H	-0.613734	2.785292	-2.369455

H	0.027650	3.875804	-1.115294
C	0.135624	-2.893843	-0.496006
C	-3.381462	-0.048632	0.147174
O	-4.536995	-0.077942	0.305967
P	-1.582459	-2.266748	-0.400741
P	-1.665919	2.276779	-0.259742
Si	1.172380	-1.407010	-1.096304
Si	1.007169	1.501561	-1.019146
C	1.846550	-1.852826	-2.800940
H	2.503203	-1.073618	-3.204418
H	2.422870	-2.786561	-2.766789
H	1.025460	-1.993793	-3.515413
C	2.383207	1.706349	-2.297013
H	2.769278	2.733914	-2.276270
H	3.234029	1.039110	-2.112958
H	2.015830	1.510854	-3.311540
H	0.448659	-3.176521	0.515766
H	0.230775	-3.781413	-1.129543
P	-1.077424	-0.033706	2.029699
C	0.615117	-0.628479	2.471447
H	0.776510	-0.450412	3.541921
H	0.610901	-1.718739	2.342144
Si	2.119298	0.052082	1.499119
C	3.515382	0.197795	2.761515
H	3.274665	0.931424	3.541233
H	3.711904	-0.761829	3.256209
H	4.447934	0.519232	2.281346
C	2.595083	-1.168570	0.141035
H	2.899847	-2.131194	0.574556
H	3.483002	-0.770846	-0.372659
C	1.773944	1.729187	0.704986
H	1.115367	2.324148	1.354276
H	2.716662	2.289686	0.630114
H	-2.802218	2.995946	-0.692928
H	-1.439359	3.010935	0.927513
H	-2.126292	-2.706283	-1.628433
H	-2.261788	-3.189382	0.426598
H	-1.844790	-0.752312	2.977951
H	-1.087000	1.199190	2.730055

A1

Coordinates (Angstroms)

	X	Y	Z
Mn	1.725991	0.007762	0.190879
N	-0.361261	0.141910	1.205110
C	0.252408	2.930094	1.076782
H	0.476637	2.944224	2.151315
H	0.013701	3.953932	0.772052
C	-0.081731	-2.803699	1.052806
C	3.430861	-0.083894	-0.214484
O	4.576326	-0.149873	-0.432816
P	1.595419	-2.192738	0.515483
P	1.726717	2.238082	0.199224
Si	-1.298791	-1.365692	1.234081
Si	-1.131060	1.686297	0.785343
C	-2.166380	-1.543340	2.894027
H	-2.898827	-0.745635	3.064309
H	-2.695917	-2.501936	2.963638
H	-1.440343	-1.510296	3.716464
C	-2.607562	2.054999	1.892098
H	-2.998537	3.061568	1.696701
H	-3.429572	1.348840	1.720634
H	-2.339521	2.005649	2.954269
H	-0.452354	-3.548316	0.339502
H	0.014681	-3.320001	2.014839
P	1.083523	-0.165944	-1.940800
C	-0.533700	-0.898178	-2.474076
H	-0.643323	-0.821396	-3.562655
H	-0.497549	-1.970860	-2.239800
Si	-2.058491	-0.157252	-1.623254
C	-3.463452	-0.110383	-2.876293
H	-3.227897	0.566617	-3.707012
H	-3.653628	-1.103625	-3.301485
H	-4.396635	0.239860	-2.418229
C	-2.546017	-1.258083	-0.168586
H	-2.768469	-2.266598	-0.543598
H	-3.491150	-0.877430	0.247130
C	-1.707603	1.596344	-1.000095
H	-0.974758	2.072089	-1.666627
H	-2.628825	2.188655	-1.090631
H	2.212042	0.145686	1.738233
H	0.174975	0.239817	2.069555
H	1.859886	-3.094716	-0.547769
H	2.429468	-2.842959	1.451835
H	1.942711	-0.893368	-2.802107

H	1.048438	1.007861	-2.744069
H	1.636236	2.963849	-1.019669
H	2.787940	2.988941	0.749901