Supporting Information

For

Theoretical study on the hydrogenation of CO_2 to methanol catalyzed by ruthenium pincer complexes

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Content

1. The Gibbs free energy of the by-product in the stage I

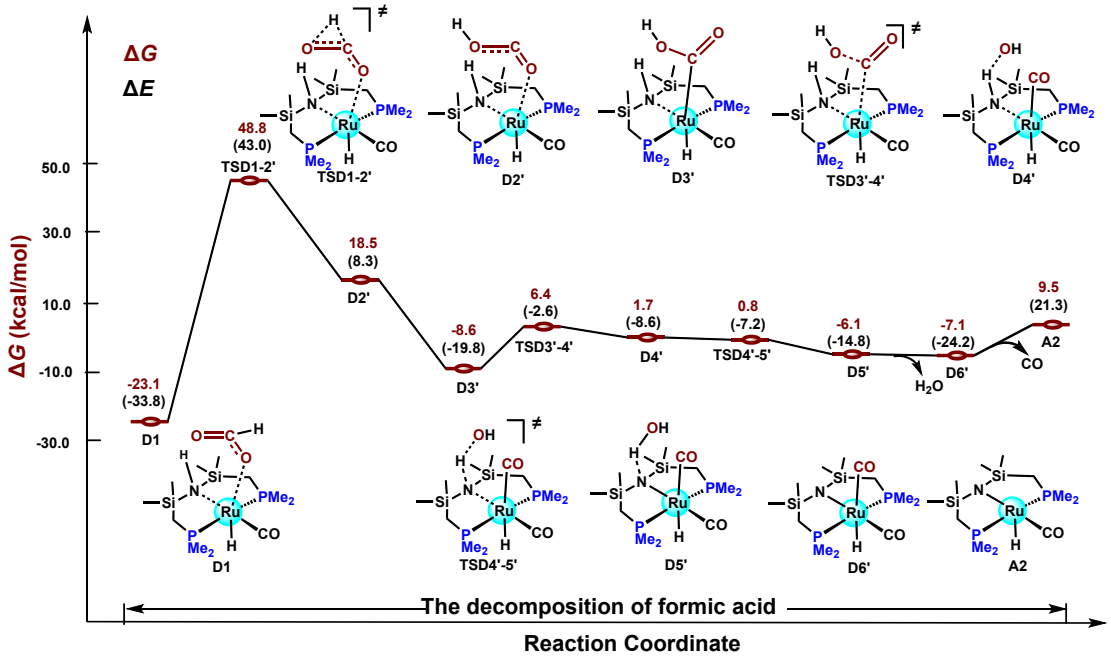


Figure S1. The Gibbs free energy profiles of the decomposition of formic acid to CO and H_2O by complex Ru-PNP (unit: kcal/mol).

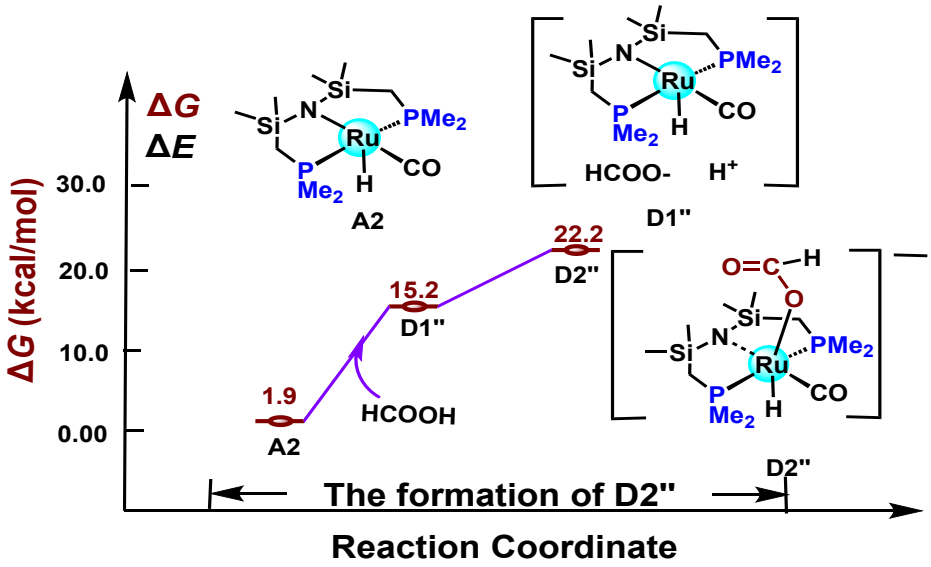


Figure S2. The Gibbs free energy profiles of **A2** with a formate anion (**D2''**) in stage I (unit: kcal/mol).

The relative free energy of the structure of **A2** with a formate anion (**D2''**), which is 20.3 kcal/mol higher than **A2** and 45.3 kcal/mol higher than **D1**. Note that the solvent free energy of a proton $G_{sol}(H^+)$ used in this study is an experimental value of -265.9 kcal/mol.[1]

2. Key scan curve

In the process of searching for transition states, the relaxed scan was used at the the LANL2DZ basis set for Ru center and the 6-31G* basis sets for all the other atoms (Figure S2). It was found that the dehydroxylation of gem-diolate (**B5→B6**) was an ascending process from the first point and the 12th point, then the HCHO turned over at the 13th point without transition state.

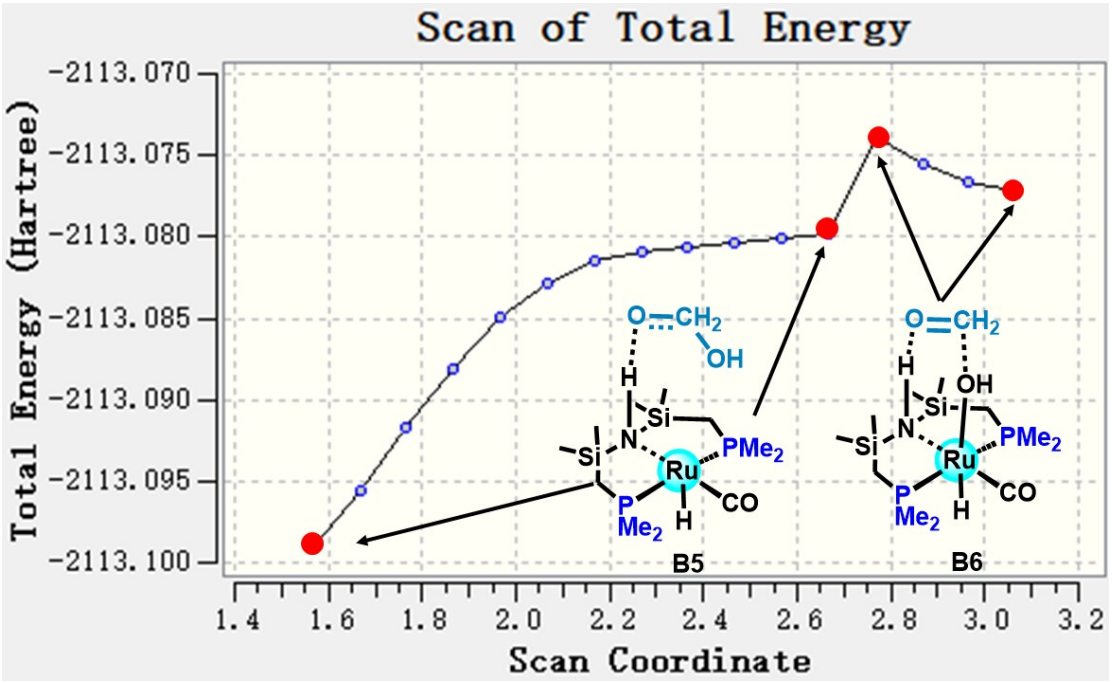


Figure S3. Scanning curve of formaldehyde hydrogenation process (**B5→B6**).

3. Effects of Ru-O bond

Considering that the formation of Ru-O band of intermediate **D1** is stable, the methanol moiety of **C3** could also turn over to form anther intermediate **C4**. But the free energy of **C4** is not different from that of **C3**.

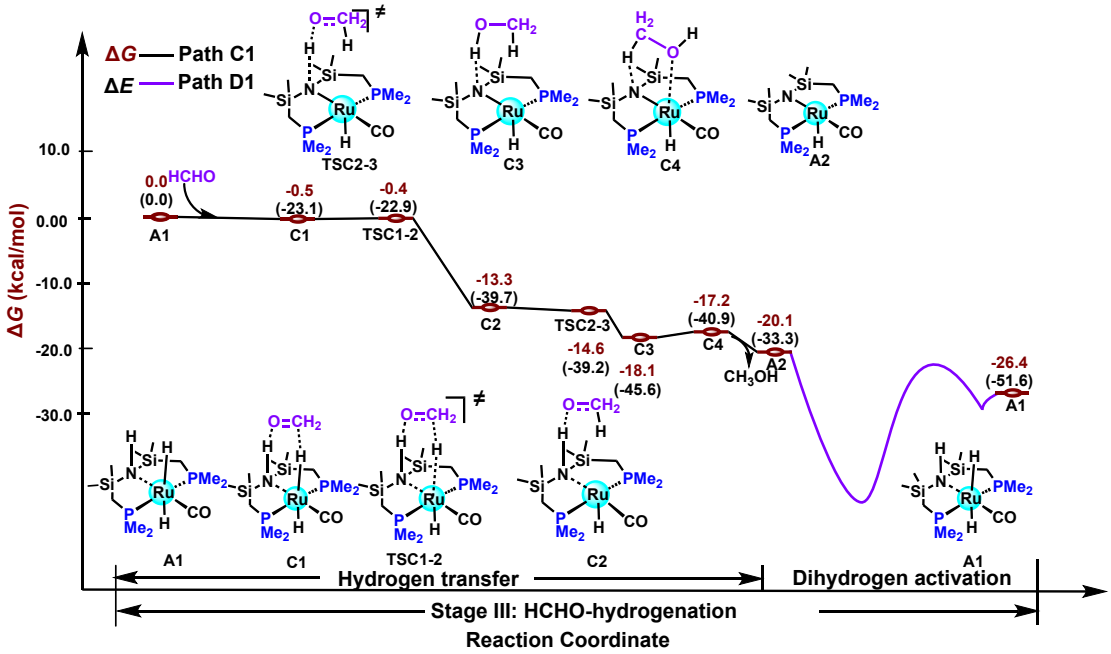
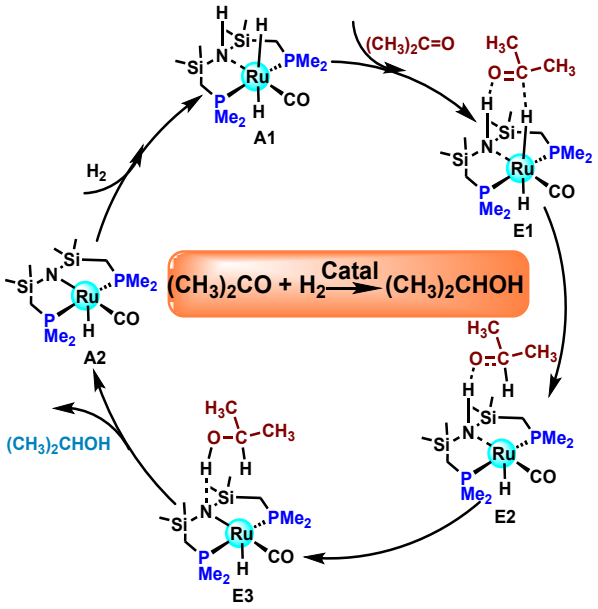


Figure S4. The free energy profiles of the hydrogenation of formaldehyde to methanol catalyzed by Ru-PNP complex (unit: kcal/mol).

4. The hydrogenation of acetone by Ru-PNP pincer complex



Scheme S1. Proposed reaction mechanisms of the acetone hydrogenation to isopropyl alcohol catalyzed by the Ru-PNP complex in this work.

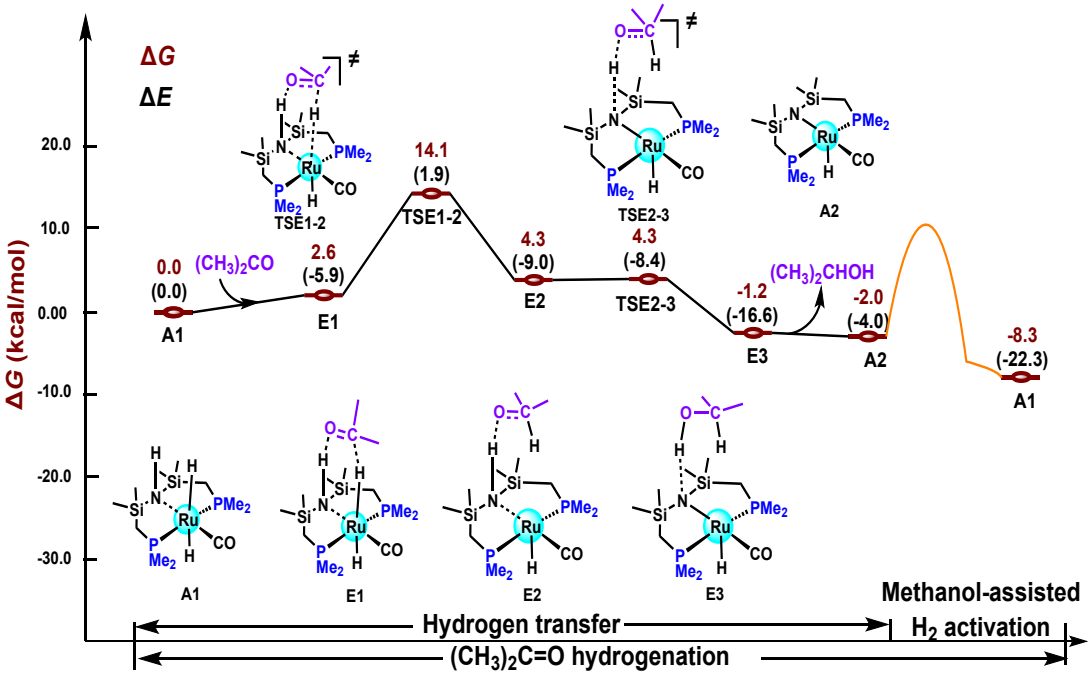


Figure S5. The free energy profiles of the hydrogenation of acetone to isopropyl alcohol catalyzed by Ru-PNP (unit: kcal/mol).

Scheme S1 explored the mechanism of hydrogenation of acetone, and the free energy profiles of the hydrogenation of acetone to isopropanol is shown in Figure S3. First, the acetone approaches the Ru-PNP species **A1** to form the intermediate **E1**. The next steps are the transfer of hydride and the regeneration of **A1**. Compared with the free energy barrier of hydride transfer (11.5 kcal/mol, **E1→TSE1-2**) to

intermediate **E2**, the energy barrier of H proton transfer from **E2** to **E3** is approximately 0.0 kcal/mol (**E2→TSE2-3**). Then, the removal of isopropanol generates the intermediate **A2**. The regeneration of **A1** considers the involvement of MeOH solvent with an energy span of 12.3 kcal/mol, due to the absence of formic acid. In addition, the regeneration of **A1** considers the isopropanol which is the reverse reaction of the hydrogenation of acetone with an energy span of 16.1 kcal/mol (**E3→TSE1-2**). This shows that the Ru-PNP catalyst is efficient for the transfer hydrogenation of C=O bonds using isopropanol as hydrogen resources.

5. Solvent effect

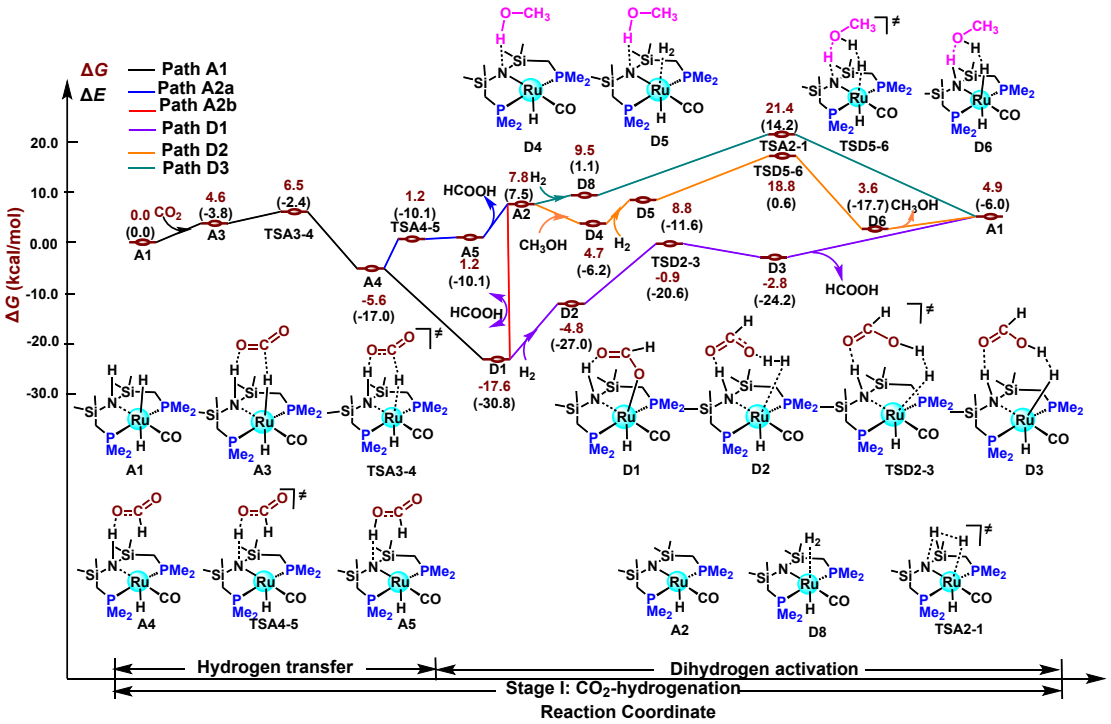


Figure S6. The Gibbs free energy profiles of the hydrogenation of CO_2 to HCOOH by Ru-PNP in toluene (unit: kcal/mol).

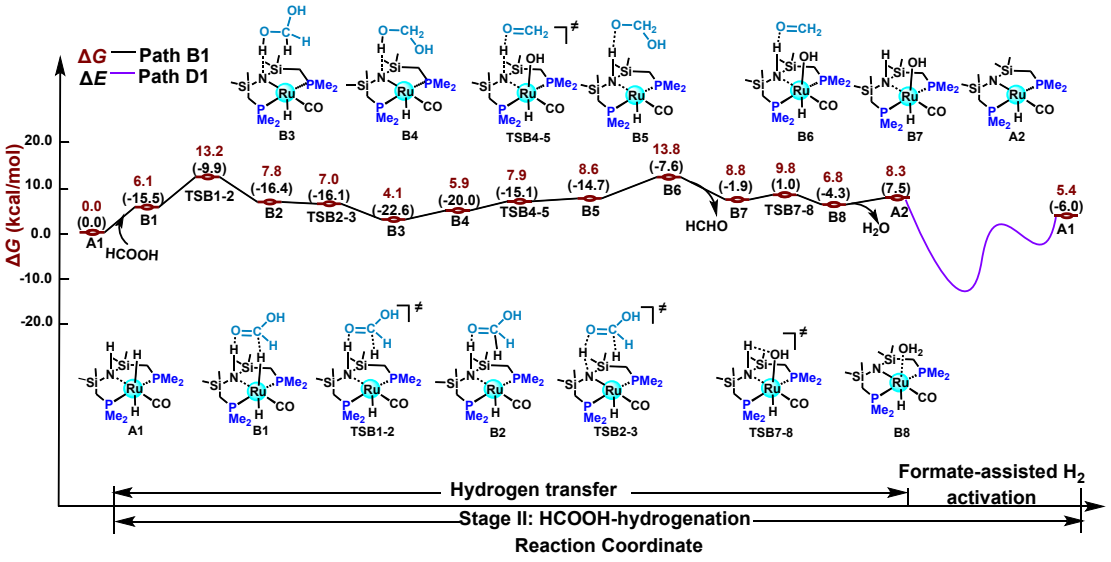


Figure S7. The Gibbs free energy profiles of the hydrogenation of HCOOH to HCHO by Ru-PNP in toluene (unit: kcal/mol).

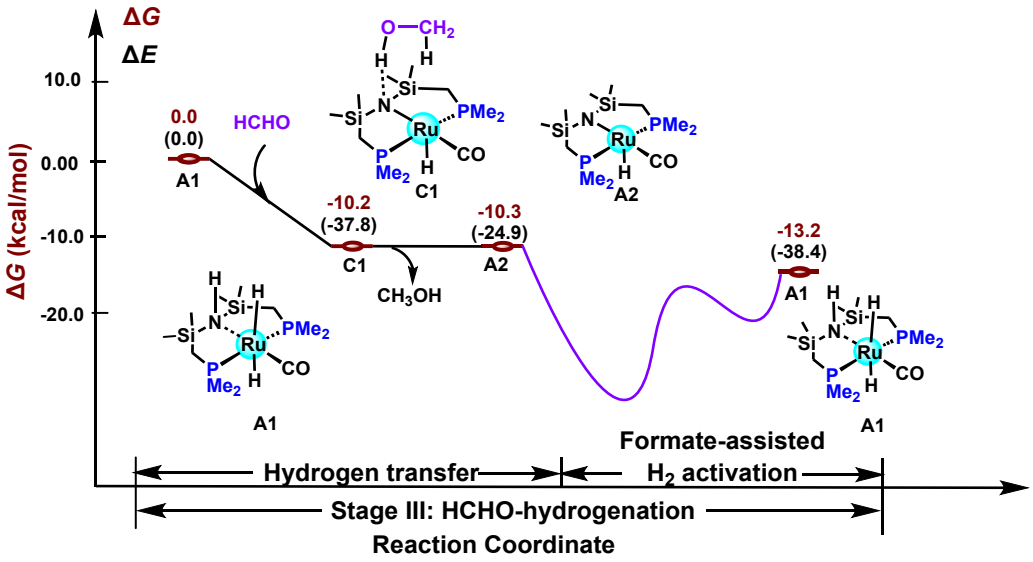


Figure S8. The Gibbs free energy profiles of the hydrogenation of HCHO to MeOH by Ru-PNP in toluene (unit: kcal/mol).

6. The $RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$, $RuH_2(Ph_2PCH_2SiMe_2)_2NH(CO)$ and $RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$ catalysts

Table S1 shows the Gibbs free energies of key processes for the CO_2 hydrogenation to methanol by three catalysts (Figure S4). It is found that the energy spans of the rate-determining processes (the formate-assisted H_2 activation) of the hydrogenation of CO_2 to methanol catalyzed by [$RuH_2(Ph_2PCH_2SiMe_2)_2NH(CO)$] and [$RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$] are 21.0 kcal/mol and 19.1 kcal/mol, respectively, which are relatively low as well. However, in the process of methanol-assisted dihydrogen activation, the rate-determining step of $RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$ was dihydrogen activation, while the rate-determining steps of $RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$ and $RuH_2(Ph_2PCH_2SiMe_2)_2NH(CO)$ were proton transfer. In order to better clarify the mechanism, HUMO-LUMO gap analysis (Table S2) and NBO charge analysis (Figure S10) for the intermediate **A2** for three catalysts. By means of NBO charge analysis, there is less negative charge on the N atom of the pincer ligand of $RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$, caused by the difference in the electronegativity of Si atom and C atom. As a result, the proton transfer from hydroxy group to N atom of $RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$ is much easier. Besides, the HOMO-LUMO gaps and the NBO charges on Ru center of the pincer complexes are similar. Therefore, there is little difference in the energy barrier of the dihydrogen activation assisted by MeOH on the Ru center (**D6→TSD6-7**).

Table S1. The calculated Gibbs free energies of key processes for the CO_2 hydrogenation to methanol by $RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$, $RuH_2(Ph_2PCH_2SiMe_2)_2NH(CO)$ and $RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$ catalysts (unit: kcal/mol)

Process	$RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$	$RuH_2(Ph_2PCH_2SiMe_2)_2NH(CO)$	$RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$
$\Delta G^{\neq}$ The formate-assisted H_2 activation (**D1→TSD2-3**)	20.2	21.0	19.1
$\Delta G^{\neq}$ The methanol-assisted H_2 activation (**D5→TSD5-6**)	5.7	2.5	2.3[a]
The energy span of stage I (**D1→TSD2-3**)	20.2	21.0	19.1
The energy span of hydride transfer of stage II (**B1→TSB1-2**)	8.0	9.9	8.8
The energy span of hydride transfer of stage III (**C1→TSC1-2**)	0.1	0.0	1.1

[a] the methanol-assisted H_2 activation catalyzed by $RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$ is **D6→TSD6-7**.

Table S2. The HUMO-LUMO gap analysis

catalysts	HOMO/eV	LUMO/eV	Gap/eV
$RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$	-7.288146	0.636052	7.924198
$RuH_2(Ph_2PCH_2SiMe_2)_2NH(CO)$	-7.275678	0.590953	7.866631
$RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$	-6.699172	0.704900	7.404072

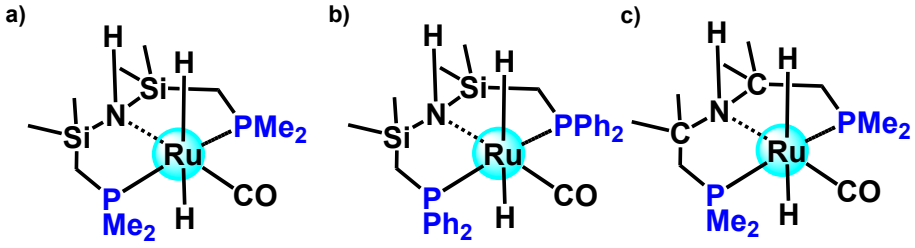


Figure S9. The pincer ruthenium catalysts (a) $RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$, (b) $RuH_2(Ph_2PCH_2SiMe_2)_2NH(CO)$, and (c) $RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$ for the CO_2 hydrogenation to methanol.

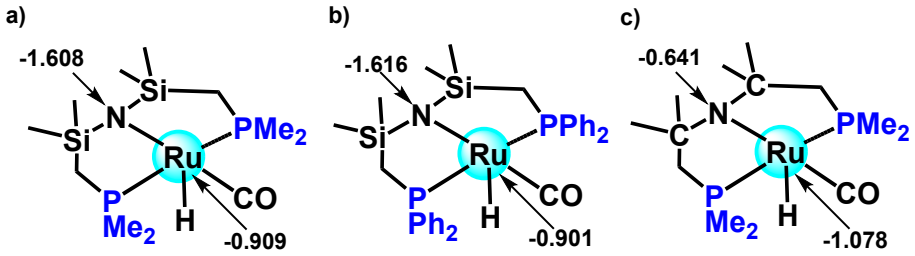


Figure S10. NBO charge analysis on Ru center and N atom of (a) $RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$, (b) $RuH_2(Ph_2PCH_2SiMe_2)_2NH(CO)$, and (c) $RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$.

7. The optimized geometry structures of transition states

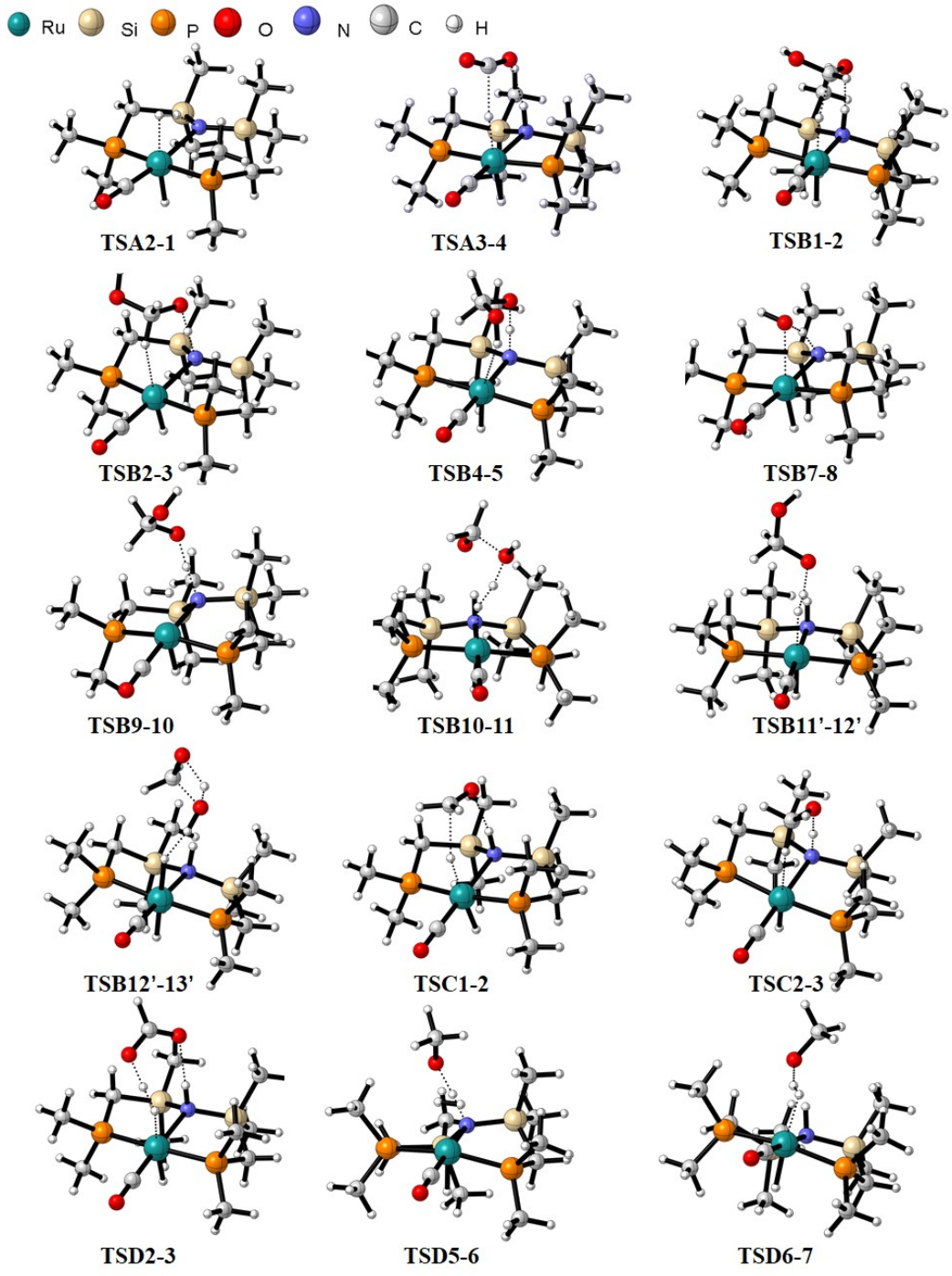


Figure S11. The optimized geometry structures of transition states for the CO_2 hydrogenation to methanol by $RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$.

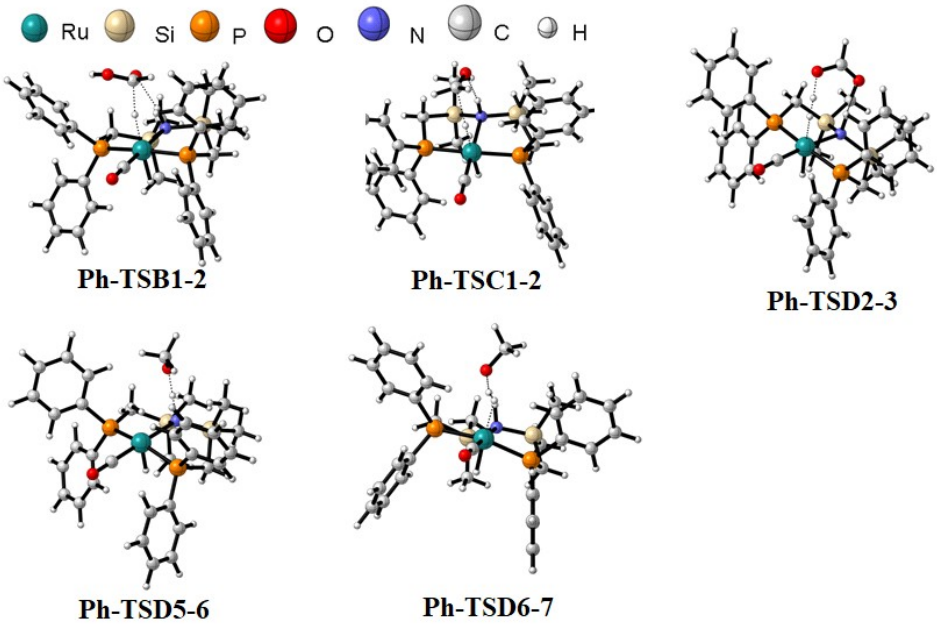


Figure S12. The optimized geometry structures of key transition states for the CO_2 hydrogenation to methanol by $RuH_2(Ph_2PCH_2SiMe_2)_2NH(CO)$.

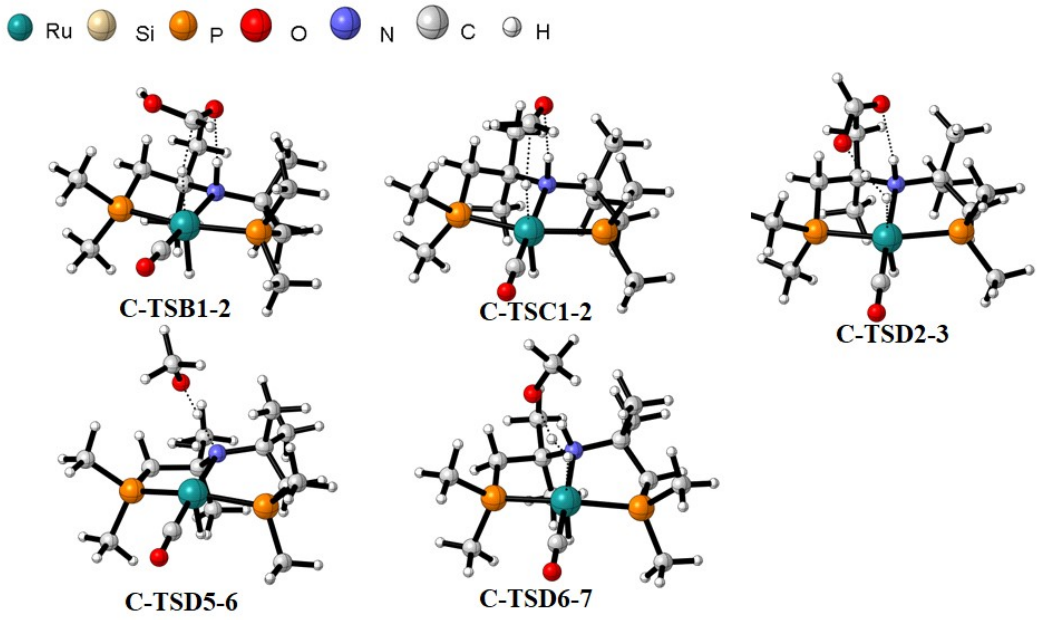


Figure S13. The optimized geometry structures of key transition states for the CO_2 hydrogenation to methanol by $RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$.

8. The NBO analysis of Ru-N bonds

Based on the NBO orbital analysis, there should be non-bonded interaction between Ru center and N atom of PNP ligand of **A1**, and there is a σ single bond between Ru center and N atom of **A2**. Similarly, there is a σ single bond between Ru center and N atom in **B8** and **D8**.

Table S3. The NBO analysis of Ru-N bonds of intermediates **A2**, **B8** and **D8**.

	(1.87517)	BD	(1) N 1 -Ru 46
	(84.26%)	0.9179*N	1 s(28.45%) p2.51(71.54%) d0.00(0.01%)
			0.0000 -0.5332 -0.0049 -0.0116 0.0428
			0.0007 -0.0004 0.8186 0.0047 -0.0018
			-0.2083 0.0029 -0.0045 0.0011 0.0002
			-0.0020 -0.0087 0.0029
A2	(15.74%)	0.3968*Ru	46 s(1.17%) p4.68(52.22%) d3.28(36.62%)
			0.0033 -0.3338 -0.0153 -0.0001 -0.0544
			-0.0019 -0.0019 -0.7129 0.0060 -0.0016
			-0.1041 0.0042 -0.0806 0.0073 -0.0185
			0.0031 -0.1495 -0.0037 0.5297 -0.0461
			0.2320 -0.0193
	(1.87359)	BD	(1) N 1 -Ru 47
	(84.34%)	0.9184* N	1 s(26.45%) p2.78(73.55%) d0.00(0.01%)
			0.0000 -0.5141 -0.0070 -0.0106 0.1157
			-0.0004 -0.0002 0.8290 0.0013 0.0001
			0.1866 -0.0011 0.0068 0.0019 -0.0003
			-0.0008 -0.0090 0.0002
B8	(15.66%)	0.3957*Ru	47 s(9.61%) p5.45(52.42%) d3.95(37.97%)
			0.0030 -0.3092 -0.0228 -0.0003 -0.0954
			0.0010 -0.0017 -0.7152 0.0047 0.0013
			0.0595 -0.0030 -0.1426 0.0156 0.0059
			0.0057 0.0649 0.0164 0.5185 -0.0446
			0.2884 -0.0218
	(1.87330)	BD	(1) N 1 -Ru 48
	(83.22%)	0.9122* N	1 s(28.03%) p2.57(71.96%) d0.00(0.01%)
			0.0000 -0.5292 -0.0034 -0.0127 0.0559
			0.0002 0.0002 0.8331 0.0050 -0.0001
			0.1498 0.0007 0.0040 0.0010 -0.0002
			0.0001 -0.0099 0.0026
D8	(16.78%)	0.4097*Ru	48 s(9.14%) p5.68(51.90%) d4.27(38.97%)
			0.0030 -0.3021 -0.0098 -0.0001 -0.0423
			-0.0010 -0.0017 -0.7160 -0.0106 0.0011
			0.0668 -0.0022 -0.0651 0.0066 0.0039
			0.0045 0.0623 0.0113 0.5334 -0.0445
			0.3076 -0.0160

9. The relative free energy profiles for the formate-assisted H_2 activation catalyzed by Ru-PNP complex using different density functionals

In view of the errors of the computational methods, the density functionals including dispersion corrected methods such as B3LYP-D3BJ, M06-D3 and M062X-D3 were used to calculate the relative free energy of the rate-determining states. As shown in Table S4, the relative free energy profiles for the formate-assisted H_2 activation catalyzed by Ru-PNP complex at B3LYP-D3BJ/BSI, M06-D3/BSI and M062X-D3/BSI levels were calculated and compared with those at ωB97X-D/BSI level. This proves the reliability of ωB97X-D method, which is very close to the M06-D3 method.

Table S4. The relative free energy profiles for the formate-assisted H_2 activation catalyzed by Ru-PNP complex using different density functionals (unit: kcal/mol).

Methods	ωB97X-D/BSI	B3LYP-D3BJ/BSI	M06-D3/BSI	M062X-D3/BSI
$\Delta G^{\neq}$ **(D1→TSD2-3)**	20.2	23.9	20.9	26.9

10. Energies of all the structures

Table S5. The calculated absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.) of $RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$ (Calculated at 298.15 K and 1 atm).

Complex	*E*	*G*
A1	-1923.449637	-1923.100478
TSA2-1	-1923.407612	-1923.064602
A2	-1922.245525	-1921.917051
A3	-2111.978288	-2111.625751
TSA3-4	-2111.972489	-2111.618893
A4	-2112.016613	-2111.652647
B1	-2113.180851	-2112.803419
TSB1-2	-2113.168888	-2112.790647
B2	-2113.186245	-2112.801762
TSB2-3	-2113.182442	-2112.798619
B3	-2113.189097	-2112.803382
B4	-2113.189191	-2112.800882
TSB4-5	-2113.18011	-2112.79668
B5	-2113.183481	-2112.795772
B6	-2113.167135	-2112.791052
B7	-1998.687754	-1998.333343
TSB7-8	-1998.676065	-1998.326934
B8	-1998.683852	-1998.331781
B9	-2114.367914	-2113.966713
TSB9-10	-2114.362742	-2113.965298
B10	-2114.367989	-2113.967474
TSB10-11	-2114.340555	-2113.9435
B11	-2114.363304	-2113.971232
B11'	-2114.382919	-2113.983442
TSB11'-12'	-2114.360589	-2113.964012
B12'	-2114.382979	-2113.983701
TSB12'-13'	-2114.315146	-2113.920521
B13'	-2114.361046	-2113.969366
C1	-2037.934282	-2037.558801
TSC1-2	-2037.934071	-2037.558632
C2	-2037.960884	-2037.579313
TSC2-3	-2037.960005	-2037.581381
C3	-2037.970184	-2037.586941
D1	-2112.025529	-2111.665369
D2	-2113.200643	-2112.822805
TSD2-3	-2113.180797	-2112.806565
D3	-2113.187184	-2112.811039
D4	-2037.966983	-2037.587335
D5	-2039.148855	-2038.754646
TSD5-6	-2039.13972	-2038.74551

D6	-2039.141154	-2038.750141
TSD6-7	-2039.137338	-2038.743804
D7	-2039.16467	-2038.769294
D8	-1923.083077	-1923.083077
TSD1-2'	-2111.903219	-2111.550846
D2'	-2111.958478	-2111.599209
D3'	-2112.003298	-2111.642359
TSD3'-4'	-2111.975765	-2111.618433
D4'	-2111.985319	-2111.625881
TSD4'-5'	-2111.983145	-2111.627358
D5'	-2111.995256	-2111.638372
D6'	-2035.556987	-2035.222668
E1	-2116.57844	-2116.57844
TSE1-2	-2116.566046	-2116.566046
E2	-2116.583368	-2116.583368
TSE2-3	-2116.582488	-2116.582488
E3	-2116.595516	-2116.595516

Table S6. The calculated absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.) of $RuH_2(Ph_2PCH_2SiMe_2)_2NH(CO)$ (Calculated at 298.15 K and 1 atm).

Complex	***E***	***G***
Ph-A2	-2688.96566529	-2688.439194
Ph-B1	-2879.897744	-2879.321867
Ph-TSB1-2	-2879.887574	-2879.306012
Ph-C1	-2804.651117	-2804.077709
Ph-TSC1-2	-2804.650655	-2804.07776
Ph-D1	-2878.743886	-2878.182623
Ph-TSD2-3	-2879.897833	-2879.322571
Ph-D5	-2805.866192	-2805.271248
Ph-TSD5-6	-2805.856076	-2805.267332
Ph-D6	-2805.855608	-2805.262335
Ph-TSD6-7	-2805.854997	-2805.262177

Table S7. The calculated absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.) of $RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$ (Calculated at 298.15 K and 1 atm)

Complex	***E***	***G***
C-A2	-1419.33914760	-1418.983956
C-B1	-1610.290986	-1609.886007
C-TSB1-2	-1610.27839	-1609.871927
C-C1	-1535.044369	-1534.64264
C-TSC1-2	-1535.043871	-1534.640843
C-D1	-1609.134429	-1608.744047
C-TSD2-3	-1610.288123	-1609.88702
C-D5	-1536.241399	-1535.81986

C-TSD5-6	-1536.240683	-1535.822173
C-D6	-1536.25307	-1535.83
C-TSD6-7	-1536.24949	-1535.83

Table S8. The calculated absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.) of $RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$ in toluene (Calculated at 298.15 K and 1 atm).

Complex	*E*	*G*
A1	-1923.437004	-1923.087646
TSA2-1	-1923.404805	-1923.061225
A2	-1922.240616	-1921.909861
A3	-2111.97023	-2111.613542
TSA3-4	-2111.967976	-2111.610523
A4	-2111.991361	-2111.629775
TSA4-5	-2111.980351	-2111.618914
A5	-2111.98033	-2111.618927
B1	-2113.163706	-2112.784283
TSB1-2	-2113.154838	-2112.773011
B2	-2113.165153	-2112.781569
TSB2-3	-2113.164627	-2112.782948
B3	-2113.174987	-2112.787557
B4	-2113.170946	-2112.784552
TSB4-5	-2113.163162	-2112.781457
B5	-2113.162459	-2112.780322
B6	-2113.151199	-2112.772052
B7	-1998.669779	-1998.316353
TSB7-8	-1998.665277	-1998.314692
B8	-1998.673739	-1998.31956
C1	-2037.959813	-2037.576221
D1	-2112.01331	-2111.648949
D2	-2113.181976	-2112.801674
TSD2-3	-2113.171921	-2112.795471
D3	-2113.177633	-2112.798566
D4	-2037.961103	-2037.581156
D5	-2039.144408	-2038.747866
TSD5-6	-2039.124987	-2038.731979
D6	-2039.154251	-2038.756103
D8	-1923.425599	-1923.080234

11. Imaginary frequencies of transition states

Table S9. Calculated imaginary frequencies of transition states at ωB97XD/BSI level of $RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$.

TSA2-1	1287.79*i*
TSA3-4	552.53*i*
TSB1-2	762.20*i*
TSB2-3	1140.64*i*
TSB4-5	1112.83*i*
TSB7-8	1304.58*i*
TSB9-10	1215.59*i*
TSB10-11	1165.66*i*
TSB11'-12'	552.84*i*
TSB12'-13'	1674.09*i*
TSC1-2	109.76*i*
TSC2-3	754.03*i*
TSD2-3	1281.57*i*
TSD5-6	1012.31*i*
TSD6-7	604.79*i*
TSD1-2'	2053.75*i*
TSD3'-4'	297.89*i*
TSD4'-5'	1039.51*i*
TSE1-2	615.37*i*
TSE2-3	185.05*i*

Table S10. Calculated imaginary frequencies of transition states at ωB97XD/BSI level of $RuH_2(Ph_2PCH_2SiMe_2)_2NH(CO)$.

Ph-TSB1-2	770.99*i*
Ph-TSC1-2	159.67*i*
Ph-TSD2-3	1208.02*i*
Ph-TSD5-6	928.20*i*
Ph-TSD6-7	596.17*i*

Table S11. Calculated imaginary frequencies of transition states at ωB97XD/BSI level of $RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$.

C-TSB1-2	757.55*i*
C-TSC1-2	167.45*i*
C-TSD2-3	1212.23*i*
C-TSD5-6	748.64*i*
C-TSD6-7	611.74*i*

Table S12. Calculated imaginary frequencies of transition states at ωB97XD/BSI level of $RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$ in toluene.

TSA2-1	1299.95*i*
TSA3-4	305.07*i*

TSA4-5	88.44*i*
TSB1-2	554.02*i*
TSB2-3	664.50*i*
TSB4-5	517.63*i*
TSB7-8	1079.04*i*
TSD2-3	978.89*i*
TSD5-6	164.01*i*

12. Cartesian coordinates of all the structures

Table S13. Atomic cartesian coordinates of intermediates and transition states (presented in Å) of $RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$.

A1

	Coordinates (Angstroms)		
	X	Y	Z
N	-0.435228	1.169755	-0.402041
C	0.954084	-2.732150	0.189103
O	1.339816	-3.827763	0.349137
C	2.404614	1.586108	-0.745356
H	3.314035	2.155523	-0.518067
H	2.288434	1.563191	-1.837021
C	-2.842675	-0.208333	0.719402
P	-1.919213	-1.636899	0.047859
P	2.537980	-0.150552	-0.182281
Si	-2.156332	1.422741	0.063529
Si	0.848979	2.365505	-0.021882
C	-3.045245	1.945170	-1.499327
H	-4.111738	2.112955	-1.308238
H	-2.621906	2.876755	-1.893996
H	-2.962188	1.180006	-2.280160
C	-2.351147	2.711362	1.406015
H	-1.969176	3.695612	1.115399
H	-3.423789	2.822346	1.610807
H	-1.868018	2.408011	2.340183
C	0.493607	3.985420	-0.897659
H	0.369490	3.828091	-1.975616
H	-0.416826	4.461827	-0.516308
H	1.321633	4.690900	-0.755882
C	1.017364	2.612854	1.824972
H	2.028078	2.977321	2.045234
H	0.308654	3.355935	2.203075
H	0.867269	1.677773	2.374292
H	-3.919687	-0.302278	0.531255
H	-2.692024	-0.220725	1.806223
H	-0.441453	1.086858	-1.421427
H	0.369288	-1.143617	-1.750013
C	3.527049	-0.069478	1.354219
H	3.672915	-1.087176	1.730237
H	4.503344	0.394059	1.176636
H	2.988717	0.499663	2.116567
C	3.714176	-0.929779	-1.346127

H	4.659499	-0.377450	-1.374533
H	3.908214	-1.961125	-1.034180
H	3.273550	-0.949783	-2.346525
C	-2.396173	-3.052164	1.101971
H	-3.484413	-3.165220	1.144222
H	-1.955753	-3.968613	0.696047
H	-2.004622	-2.899446	2.111559
C	-2.779063	-2.015640	-1.523363
H	-2.335030	-2.912020	-1.967142
H	-3.848312	-2.186741	-1.358592
H	-2.648706	-1.189336	-2.228049
Ru	0.357152	-1.033357	-0.048037
H	0.285810	-0.745680	1.629016

TSA2-1

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.188129	1.197831	-0.241561
C	0.403606	-2.891092	-0.146032
O	0.555384	-4.046409	-0.229979
C	2.663943	1.108108	-0.704206
H	3.654969	1.517496	-0.475147
H	2.567901	1.054168	-1.796905
C	-2.806171	0.360072	0.780803
P	-2.186418	-1.255409	0.204713
P	2.479082	-0.594890	-0.074395
Si	-1.812638	1.768988	-0.016936
Si	1.233704	2.173682	-0.055294
C	-2.589210	2.240444	-1.666905
H	-3.657725	2.467968	-1.565540
H	-2.093494	3.130450	-2.075224
H	-2.483653	1.437527	-2.406371
C	-1.940590	3.250627	1.139615
H	-1.446778	4.141148	0.734234
H	-2.997536	3.502688	1.296126
H	-1.502445	3.033743	2.120523
C	1.180582	3.753510	-1.079703
H	0.996037	3.533002	-2.138001
H	0.394929	4.436603	-0.735177
H	2.135364	4.290653	-1.009642
C	1.558880	2.643786	1.742056

H	2.615396	2.890146	1.906892
H	0.967327	3.521622	2.028606
H	1.291320	1.827073	2.422804
H	-3.890122	0.445966	0.635810
H	-2.607954	0.402656	1.860361
H	-0.092722	0.238150	-1.345547
H	-0.002142	-0.594144	-1.820984
C	3.366568	-0.609113	1.523419
H	3.302989	-1.611249	1.957895
H	4.419494	-0.340845	1.387095
H	2.900161	0.094405	2.217792
C	3.550270	-1.636913	-1.127287
H	4.558166	-1.213904	-1.193964
H	3.610276	-2.644449	-0.703531
H	3.120172	-1.707339	-2.130424
C	-2.838520	-2.496609	1.376178
H	-3.927818	-2.421044	1.458129
H	-2.571318	-3.500600	1.031037
H	-2.388303	-2.338166	2.360076
C	-3.133296	-1.608128	-1.319535
H	-2.816322	-2.575991	-1.720172
H	-4.209788	-1.633764	-1.119463
H	-2.925565	-0.841828	-2.071316
Ru	0.157475	-1.079006	-0.027833
H	0.242879	-1.210451	1.591463

A2

	Coordinates (Angstroms)		
	X	Y	Z

N	0.070599	1.094576	-0.034609
C	-0.207914	-2.864996	-0.292859
O	-0.295458	-4.012983	-0.519875
C	2.842358	0.514352	-0.715733
H	3.894425	0.729981	-0.493074
H	2.737955	0.430533	-1.805916
C	-2.722777	0.918559	0.772731
P	-2.406797	-0.783868	0.207147
P	2.306850	-1.082044	-0.017688
Si	-1.377548	2.035828	0.030696
Si	1.622721	1.847389	-0.128658
C	-1.938262	2.627302	-1.674675

H	-2.949496	3.052848	-1.639571
H	-1.263669	3.405203	-2.053767
H	-1.939720	1.809813	-2.405363
C	-1.264407	3.574048	1.122681
H	-0.535356	4.297422	0.737768
H	-2.237175	4.081541	1.164313
H	-0.978789	3.318858	2.150262
C	1.700573	3.268726	-1.371818
H	1.389562	2.942093	-2.371524
H	1.059422	4.108003	-1.075787
H	2.726168	3.653295	-1.449334
C	2.231840	2.532334	1.525176
H	3.300901	2.778490	1.483555
H	1.691965	3.448405	1.794680
H	2.083781	1.812106	2.338508
H	-3.750623	1.237477	0.562415
H	-2.583388	0.924221	1.861852
C	3.135029	-1.185921	1.609075
H	2.943779	-2.169712	2.048207
H	4.215544	-1.041078	1.504956
H	2.732783	-0.427023	2.285107
C	3.175022	-2.371473	-0.983786
H	4.252754	-2.177900	-1.011277
H	2.998874	-3.352655	-0.531372
H	2.785026	-2.385273	-2.005805
C	-3.315944	-1.884663	1.348218
H	-4.376658	-1.615753	1.391506
H	-3.220927	-2.921987	1.011732
H	-2.882424	-1.803930	2.349240
C	-3.352460	-0.950771	-1.350619
H	-3.232558	-1.968055	-1.736507
H	-4.416771	-0.749334	-1.189005
H	-2.964922	-0.251935	-2.097351
Ru	-0.072525	-1.062216	0.014626
H	-0.051462	-1.427635	1.538493

A3

	Coordinates (Angstroms)		
	X	Y	Z

N	0.591741	1.076413	-0.008451
C	-1.098016	-2.716749	-0.505610

O	-1.568663	-3.782345	-0.640456
C	-2.222173	1.759135	0.044128
H	-3.044781	2.390573	-0.313118
H	-2.231131	1.797210	1.141302
C	2.957109	-0.574163	-0.756137
P	1.838647	-1.845857	-0.065897
P	-2.462074	0.010041	-0.443052
Si	2.363627	1.160655	-0.311585
Si	-0.538419	2.358945	-0.550340
C	3.150642	1.751001	1.282789
H	4.231391	1.884359	1.154225
H	2.726431	2.713460	1.592781
H	2.996977	1.034623	2.097692
C	2.787951	2.310749	-1.723982
H	2.517821	3.352508	-1.520623
H	3.874785	2.275192	-1.873347
H	2.317248	2.001109	-2.662342
C	-0.110255	3.971889	0.304153
H	-0.084033	3.838300	1.392330
H	0.866292	4.352896	-0.016620
H	-0.857690	4.742044	0.077919
C	-0.521637	2.540220	-2.412973
H	-1.489332	2.938379	-2.741883
H	0.252606	3.237817	-2.746309
H	-0.364939	1.579290	-2.913960
H	3.997683	-0.744478	-0.452400
H	2.907943	-0.676036	-1.847682
H	0.501343	1.055843	1.009948
H	-0.564252	-1.061750	1.379166
C	-3.287648	0.087367	-2.073240
H	-3.512056	-0.934809	-2.394634
H	-4.218419	0.662488	-2.025202
H	-2.617659	0.535634	-2.811176
C	-3.807361	-0.599629	0.634629
H	-4.704299	0.020259	0.532354
H	-4.050894	-1.632176	0.364041
H	-3.471057	-0.585606	1.674950
C	2.338257	-3.404669	-0.878587
H	3.408464	-3.589999	-0.739234
H	1.771754	-4.237571	-0.450497
H	2.115974	-3.345755	-1.947928
C	2.445202	-2.083044	1.645104
H	1.897696	-2.911897	2.104392
H	3.518080	-2.303246	1.663086

H	2.249328	-1.182693	2.234369
Ru	-0.370507	-1.064452	-0.308416
H	-0.098420	-0.912830	-1.986811
C	-0.823950	0.594626	3.448126
O	0.189053	1.107311	3.180393
O	-1.837009	0.106323	3.748246

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

N	0.843110	0.954609	0.189898
C	-1.725051	-2.150709	-0.877986
O	-2.431546	-3.034054	-1.180468
C	-1.696244	2.293771	0.499766
H	-2.335953	3.166452	0.322257
H	-1.676173	2.107711	1.581852
C	2.727251	-1.078199	-0.920226
P	1.316470	-2.126827	-0.421859
P	-2.371813	0.789704	-0.294877
Si	2.579814	0.651500	-0.177943
Si	0.076802	2.554606	-0.082475
C	3.492690	0.756620	1.453934
H	4.565833	0.582458	1.311895
H	3.366315	1.746104	1.909713
H	3.123916	0.009652	2.166613
C	3.262823	1.877357	-1.414687
H	3.233017	2.911097	-1.054275
H	4.314417	1.623792	-1.600209
H	2.736925	1.823901	-2.373423
C	0.911901	3.854525	0.978172
H	0.874057	3.581518	2.039305
H	1.963067	3.990668	0.699267
H	0.410832	4.823567	0.863242
C	0.121751	3.021544	-1.894489
H	-0.702544	3.712071	-2.110301
H	1.053414	3.530126	-2.160076
H	0.008720	2.146093	-2.542184
H	3.686675	-1.550496	-0.674663
H	2.673307	-0.979727	-2.011917
H	0.748529	0.780937	1.196041
H	-0.795766	-1.010068	1.272216

C	-3.141050	1.379369	-1.845298
H	-3.642409	0.534425	-2.328330
H	-3.874329	2.168926	-1.649950
H	-2.375032	1.755128	-2.528304
C	-3.831012	0.336035	0.707820
H	-4.538182	1.170068	0.769418
H	-4.331234	-0.525345	0.253660
H	-3.508955	0.055292	1.714483
C	1.383808	-3.583158	-1.522211
H	2.366473	-4.063630	-1.474926
H	0.617188	-4.301970	-1.215759
H	1.176543	-3.273616	-2.550448
C	1.829002	-2.820730	1.192170
H	1.064358	-3.522710	1.538593
H	2.790035	-3.340049	1.113538
H	1.911589	-2.017446	1.930107
Ru	-0.615404	-0.780298	-0.425226
H	-0.329865	-0.427825	-2.040485
C	-0.704673	-0.638578	3.062198
O	0.181357	0.143164	3.095652
O	-1.568361	-1.343108	3.446771

A4

	Coordinates (Angstroms)		
	X	Y	Z

N	0.661435	1.054555	0.121402
C	-1.346288	-2.486065	-0.693429
O	-1.909036	-3.467303	-0.978355
C	-2.068790	2.025217	0.217197
H	-2.824117	2.751410	-0.105542
H	-2.069789	2.006648	1.315026
C	2.871364	-0.686677	-0.858432
P	1.670439	-1.946411	-0.317584
P	-2.469427	0.339490	-0.358880
Si	2.440702	1.008946	-0.144982
Si	-0.327685	2.475764	-0.349923
C	3.234742	1.273544	1.529013
H	4.326825	1.207703	1.458718
H	2.978265	2.265117	1.921397
H	2.897103	0.530132	2.259427
C	3.033421	2.286038	-1.377651

H	2.841012	3.317656	-1.066540
H	4.120151	2.170114	-1.479794
H	2.594061	2.130784	-2.368415
C	0.233654	3.998960	0.584187
H	0.222993	3.810487	1.664382
H	1.244554	4.313382	0.303372
H	-0.443033	4.839150	0.385173
C	-0.266883	2.723901	-2.204820
H	-1.178076	3.232858	-2.540608
H	0.584284	3.345002	-2.501093
H	-0.196258	1.768340	-2.735855
H	3.901844	-0.985598	-0.630286
H	2.779620	-0.614540	-1.950013
H	0.533444	0.985502	1.150996
H	-0.452671	-1.003408	2.066630
C	-3.262720	0.555574	-1.989154
H	-3.572555	-0.425856	-2.361813
H	-4.138603	1.208204	-1.915332
H	-2.551189	0.982981	-2.700471
C	-3.839411	-0.239820	0.700006
H	-4.652448	0.493197	0.715253
H	-4.217199	-1.192708	0.315921
H	-3.469244	-0.394604	1.717676
C	1.961929	-3.401673	-1.378965
H	3.012511	-3.706654	-1.336390
H	1.331879	-4.231201	-1.043775
H	1.696782	-3.157467	-2.411572
C	2.267939	-2.498301	1.320000
H	1.625347	-3.306897	1.681515
H	3.299739	-2.859880	1.256503
H	2.218401	-1.676430	2.039791
Ru	-0.462240	-0.931222	-0.312979
H	-0.319700	-0.763468	-1.861851
C	-0.646870	-0.319097	2.934305
O	-0.028073	0.776131	2.936575
O	-1.443558	-0.748803	3.799393

B1

	Coordinates (Angstroms)		
	X	Y	Z

N	0.543420	1.073284	-0.068952

C	-0.989658	-2.786407	-0.497746
O	-1.415500	-3.872878	-0.616089
C	-2.286493	1.632369	0.064078
H	-3.152976	2.231123	-0.241974
H	-2.230529	1.660354	1.160467
C	2.982871	-0.497867	-0.775418
P	1.904594	-1.775616	-0.035290
P	-2.470882	-0.122873	-0.423804
Si	2.296405	1.230857	-0.441695
Si	-0.654983	2.293336	-0.608342
C	3.110292	1.978979	1.071372
H	4.181297	2.136630	0.896781
H	2.660827	2.948080	1.318334
H	3.004217	1.324166	1.943633
C	2.603135	2.291824	-1.951346
H	2.260019	3.323894	-1.823539
H	3.686257	2.322589	-2.126460
H	2.136608	1.874158	-2.849195
C	-0.270697	3.955343	0.169247
H	-0.222058	3.877046	1.261512
H	0.685242	4.356716	-0.187465
H	-1.050184	4.685032	-0.082392
C	-0.713223	2.430622	-2.474994
H	-1.705486	2.789546	-2.774853
H	0.022369	3.148549	-2.850515
H	-0.540434	1.467628	-2.965927
H	4.019944	-0.600221	-0.431664
H	2.971209	-0.663696	-1.859932
H	0.485258	1.086617	0.955013
H	0.149035	-0.489773	3.751528
C	-3.356615	-0.078326	-2.023641
H	-3.559896	-1.108402	-2.333642
H	-4.303103	0.466335	-1.940932
H	-2.730740	0.388803	-2.787809
C	-3.749618	-0.801037	0.694465
H	-4.685721	-0.238576	0.613130
H	-3.935877	-1.849069	0.437725
H	-3.386437	-0.758405	1.725094
C	2.469032	-3.358357	-0.753064
H	3.543010	-3.501246	-0.594231
H	1.924135	-4.183588	-0.283464
H	2.255315	-3.367724	-1.825717
C	2.502090	-1.886922	1.691958
H	1.954092	-2.678027	2.212734

H	3.575101	-2.104355	1.727803
H	2.310785	-0.940954	2.207946
Ru	-0.333053	-1.101858	-0.327163
H	-0.068467	-0.967556	-2.014999
C	-0.359149	0.439004	3.476201
O	0.196209	1.403110	2.980862
O	-1.646666	0.395486	3.784555
H	-2.077078	1.231891	3.536335
H	-0.535102	-1.081289	1.350121

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	Coordinates (Angstroms)		
	X	Y	Z
N	0.664792	1.057805	0.126961
C	-1.313070	-2.494047	-0.720116
O	-1.863526	-3.503010	-0.943756
C	-2.077406	1.943397	0.356839
H	-2.855451	2.684357	0.137647
H	-2.041093	1.803799	1.445691
C	2.883615	-0.650837	-0.894322
P	1.687190	-1.907958	-0.323556
P	-2.461594	0.316332	-0.385833
Si	2.427187	1.058079	-0.231248
Si	-0.363704	2.485998	-0.209410
C	3.319018	1.404761	1.380030
H	4.397559	1.503826	1.207924
H	2.960915	2.338017	1.831178
H	3.167116	0.599946	2.107804
C	2.898613	2.330157	-1.520223
H	2.682011	3.357062	-1.207335
H	3.981686	2.257468	-1.683070
H	2.409391	2.145789	-2.481935
C	0.209357	3.944556	0.819305
H	0.233715	3.686111	1.884586
H	1.210744	4.280233	0.525684
H	-0.474754	4.793020	0.694597
C	-0.371237	2.902251	-2.035866
H	-1.314918	3.399465	-2.290784
H	0.441837	3.586071	-2.297591
H	-0.282724	2.006041	-2.658625
H	3.914120	-0.930264	-0.641801

H	2.804855	-0.617931	-1.988348
H	0.600438	0.917967	1.149760
H	0.057283	-1.603233	3.081991
C	-3.251637	0.698757	-1.990072
H	-3.574045	-0.239494	-2.452476
H	-4.121767	1.349829	-1.854434
H	-2.537013	1.181076	-2.660985
C	-3.872261	-0.335459	0.576754
H	-4.687850	0.394513	0.607158
H	-4.233648	-1.257858	0.111073
H	-3.550107	-0.564204	1.595674
C	2.004250	-3.379953	-1.358207
H	3.058599	-3.671252	-1.308880
H	1.384602	-4.212348	-1.010394
H	1.737078	-3.157442	-2.395171
C	2.327732	-2.426021	1.309716
H	1.704197	-3.236760	1.698895
H	3.362619	-2.776100	1.231883
H	2.284116	-1.590189	2.014027
Ru	-0.454449	-0.923818	-0.380187
H	-0.216619	-0.644576	-2.006344
C	-0.385556	-0.618204	2.913771
O	0.289685	0.433271	2.922526
O	-1.679822	-0.613598	3.341706
H	-2.005078	0.299564	3.319608
H	-0.627532	-1.031272	1.353107

B2

	Coordinates (Angstroms)		
	X	Y	Z

N	0.614734	1.056604	0.092473
C	-1.241850	-2.588710	-0.591709
O	-1.753692	-3.617404	-0.797167
C	-2.159140	1.896827	0.218073
H	-2.945666	2.600988	-0.078265
H	-2.151780	1.839117	1.314435
C	2.883893	-0.595606	-0.907786
P	1.748514	-1.886379	-0.302948
P	-2.487853	0.213016	-0.406598
Si	2.375122	1.103540	-0.251309
Si	-0.440440	2.433802	-0.342819

C	3.279669	1.488356	1.344055
H	4.354100	1.595315	1.150525
H	2.920246	2.428637	1.779058
H	3.147681	0.700900	2.093450
C	2.845063	2.368918	-1.550912
H	2.606380	3.396924	-1.257937
H	3.932481	2.312166	-1.690357
H	2.379826	2.164028	-2.520116
C	0.073168	3.968314	0.604289
H	0.089090	3.768525	1.682218
H	1.069301	4.315754	0.307270
H	-0.632299	4.788877	0.424582
C	-0.430268	2.738044	-2.193806
H	-1.383309	3.188291	-2.496384
H	0.366224	3.429389	-2.485121
H	-0.300728	1.808085	-2.757940
H	3.928402	-0.836526	-0.673957
H	2.782111	-0.576264	-2.000533
H	0.529109	0.975612	1.150751
H	0.177387	-1.072426	3.718840
C	-3.227494	0.434381	-2.062525
H	-3.497616	-0.549616	-2.458303
H	-4.124495	1.060229	-2.010500
H	-2.506577	0.890120	-2.745183
C	-3.894643	-0.417908	0.573584
H	-4.722504	0.298622	0.558254
H	-4.233176	-1.369975	0.152826
H	-3.577207	-0.582564	1.606609
C	2.104907	-3.369130	-1.304631
H	3.173079	-3.607438	-1.272885
H	1.533928	-4.219707	-0.920322
H	1.805346	-3.186571	-2.340451
C	2.381533	-2.337371	1.352168
H	1.774700	-3.153188	1.756767
H	3.426780	-2.659266	1.295681
H	2.303939	-1.484683	2.032814
Ru	-0.431296	-0.973609	-0.316065
H	-0.324487	-0.870454	-1.875683
C	-0.313424	-0.395743	2.990414
O	0.331860	0.764947	2.825963
O	-1.693486	-0.242965	3.426628
H	-1.668232	0.245777	4.259059
H	-0.439574	-0.997327	2.050662

TSB2-3

	Coordinates (Angstroms)		
	X	Y	Z
N	0.558194	1.038584	0.088739
C	-1.146784	-2.648458	-0.518204
O	-1.626833	-3.702053	-0.679180
C	-2.238502	1.793077	0.246000
H	-3.050805	2.468615	-0.047231
H	-2.225397	1.731112	1.341635
C	2.897761	-0.503768	-0.911465
P	1.820300	-1.824158	-0.273820
P	-2.495507	0.101218	-0.385445
Si	2.280612	1.180181	-0.293038
Si	-0.528931	2.368791	-0.323035
C	3.252545	1.665384	1.241416
H	4.305678	1.836624	0.985274
H	2.859940	2.589726	1.682124
H	3.217520	0.886913	2.010682
C	2.690149	2.422553	-1.644991
H	2.429005	3.452376	-1.377150
H	3.775382	2.392760	-1.809617
H	2.206569	2.177610	-2.596159
C	-0.069862	3.935509	0.611650
H	-0.014132	3.743937	1.689733
H	0.899630	4.331687	0.286494
H	-0.818403	4.721026	0.447989
C	-0.600533	2.736672	-2.169112
H	-1.571515	3.180204	-2.421690
H	0.173247	3.450228	-2.469119
H	-0.475161	1.829263	-2.770017
H	3.952384	-0.686405	-0.670048
H	2.796284	-0.516883	-2.004444
H	0.471896	0.938070	1.348163
H	0.266746	-0.872265	3.719156
C	-3.265568	0.295271	-2.031315
H	-3.468901	-0.698851	-2.441312
H	-4.203573	0.855568	-1.959444
H	-2.585968	0.813031	-2.711769
C	-3.857718	-0.618101	0.599576
H	-4.726093	0.049211	0.607389
H	-4.146572	-1.580748	0.165612

H	-3.519299	-0.783393	1.625721
C	2.223802	-3.323105	-1.234075
H	3.302419	-3.511457	-1.224786
H	1.704106	-4.185469	-0.804985
H	1.886458	-3.193929	-2.266392
C	2.482407	-2.204546	1.388824
H	1.906826	-3.024256	1.829333
H	3.537163	-2.494011	1.330930
H	2.386774	-1.330149	2.038887
Ru	-0.390915	-0.994360	-0.301606
H	-0.299729	-0.931304	-1.864384
C	-0.264703	-0.321485	2.925679
O	0.394778	0.817699	2.585944
O	-1.609797	-0.090074	3.371491
H	-1.561593	0.451808	4.169049
H	-0.396582	-1.028967	2.073915

B3

	Coordinates (Angstroms)		
	X	Y	Z

N	0.501419	1.020620	-0.033668
C	-1.055477	-2.675337	-0.510046
O	-1.508133	-3.748234	-0.639954
C	-2.305596	1.704139	0.275512
H	-3.137915	2.361747	-0.002423
H	-2.309644	1.592638	1.367451
C	2.920692	-0.385329	-0.948450
P	1.888076	-1.744949	-0.322099
P	-2.488233	0.033580	-0.431283
Si	2.202852	1.258401	-0.321918
Si	-0.599812	2.351656	-0.243390
C	3.137769	1.753451	1.241393
H	4.191336	1.957460	1.009970
H	2.712256	2.661946	1.685665
H	3.110588	0.965946	2.002293
C	2.627043	2.555902	-1.626830
H	2.352438	3.571645	-1.318498
H	3.712497	2.547157	-1.793521
H	2.142948	2.346647	-2.587319
C	-0.162740	3.825352	0.850703
H	-0.100657	3.534677	1.906161

H	0.800152	4.265393	0.563249
H	-0.922298	4.613034	0.763225
C	-0.737202	2.983883	-2.020450
H	-1.697283	3.494140	-2.171441
H	0.056407	3.702612	-2.252610
H	-0.671805	2.167828	-2.749196
H	3.980721	-0.526163	-0.703965
H	2.822043	-0.397005	-2.041888
H	0.431651	0.795742	1.748478
H	0.184943	-0.935295	3.953790
C	-3.234103	0.278819	-2.082597
H	-3.396778	-0.699351	-2.545609
H	-4.191381	0.804345	-2.001240
H	-2.560535	0.853662	-2.722661
C	-3.849969	-0.772476	0.487259
H	-4.750170	-0.148301	0.479866
H	-4.079213	-1.737592	0.024139
H	-3.541339	-0.947146	1.521544
C	2.338428	-3.227393	-1.289017
H	3.419179	-3.401213	-1.257777
H	1.821478	-4.102196	-0.881992
H	2.023692	-3.091395	-2.327628
C	2.563050	-2.125487	1.337001
H	2.046117	-2.999742	1.744576
H	3.636537	-2.336005	1.281867
H	2.398354	-1.282377	2.013738
Ru	-0.349530	-0.989059	-0.350906
H	-0.281784	-0.969286	-1.914890
C	-0.269088	-0.497455	3.058181
O	0.444298	0.654566	2.738729
O	-1.641475	-0.244407	3.290659
H	-1.725526	0.271191	4.102399
H	-0.242198	-1.234570	2.243400

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	Coordinates (Angstroms)		
	X	Y	Z

N	-0.022052	1.174064	0.003123
C	0.046438	-2.838106	-0.454371
O	0.060203	-4.002521	-0.579668
C	-2.841035	0.661872	0.461724

H	-3.881470	0.928308	0.240479
H	-2.746326	0.541804	1.549359
C	2.654394	0.916361	-1.157703
P	2.351957	-0.787824	-0.591891
P	-2.368345	-0.927431	-0.292528
Si	1.441884	2.072761	-0.265686
Si	-1.568629	1.959982	-0.084776
C	2.224516	2.657721	1.349158
H	3.133205	3.240359	1.149842
H	1.531023	3.301604	1.904718
H	2.498520	1.825209	2.006420
C	1.257290	3.602040	-1.357685
H	0.599686	4.359931	-0.916213
H	2.243202	4.065387	-1.495957
H	0.867051	3.348419	-2.349768
C	-1.712334	3.428191	1.092470
H	-1.485749	3.131101	2.123453
H	-1.028870	4.240777	0.818009
H	-2.730832	3.837475	1.077579
C	-2.026396	2.561212	-1.816971
H	-3.113001	2.675148	-1.920188
H	-1.573752	3.537098	-2.026390
H	-1.683706	1.863135	-2.589332
H	3.708431	1.200875	-1.053075
H	2.402596	0.942576	-2.226123
H	0.039034	0.824344	1.810209
C	-3.182102	-0.940121	-1.928643
H	-3.011146	-1.909525	-2.406635
H	-4.259620	-0.775515	-1.823584
H	-2.759978	-0.162124	-2.568920
C	-3.299027	-2.221416	0.606975
H	-4.370889	-1.996287	0.609203
H	-3.137769	-3.189780	0.122156
H	-2.944687	-2.288106	1.639767
C	3.135363	-1.882189	-1.828084
H	4.191490	-1.626226	-1.963368
H	3.057796	-2.923238	-1.498789
H	2.613994	-1.780340	-2.784046
C	3.444364	-0.996740	0.863092
H	3.394222	-2.033194	1.211017
H	4.481947	-0.759102	0.604298
H	3.121497	-0.343066	1.677424
Ru	0.016090	-1.005700	-0.305647
H	-0.037651	-0.987535	-1.868954

H	-1.034103	-1.046553	2.204906
C	-0.330598	-0.711568	2.977867
H	-0.785642	-0.803320	3.966232
O	0.011849	0.628283	2.786239
O	0.794521	-1.572771	2.977264
H	1.010329	-1.784306	2.057958

TSB4-5

	Coordinates (Angstroms)		
	X	Y	Z

N	0.431744	1.119885	0.146464
C	-1.008463	-2.671306	-0.482621
O	-1.421393	-3.752134	-0.646777
C	-2.421289	1.632005	0.473741
H	-3.289446	2.253065	0.221761
H	-2.387794	1.530185	1.566168
C	2.762715	-0.137324	-1.184643
P	1.899546	-1.604798	-0.536884
P	-2.560208	-0.045567	-0.231361
Si	2.114057	1.419181	-0.320704
Si	-0.781242	2.378588	-0.109362
C	3.143759	1.790701	1.206840
H	4.183760	1.997829	0.925506
H	2.752927	2.676504	1.723104
H	3.146019	0.963306	1.923485
C	2.360170	2.841424	-1.526744
H	2.015027	3.803244	-1.132009
H	3.437021	2.935208	-1.719313
H	1.868292	2.663985	-2.488472
C	-0.407113	3.904577	0.921968
H	-0.276046	3.641938	1.978214
H	0.508278	4.403451	0.582391
H	-1.224003	4.633957	0.854258
C	-0.966507	2.867529	-1.918884
H	-1.991684	3.207843	-2.109871
H	-0.292797	3.688926	-2.183884
H	-0.757944	2.028655	-2.592242
H	3.852076	-0.247466	-1.119270
H	2.498115	-0.057473	-2.247172
H	0.442082	0.912754	1.372162
C	-3.371045	0.164230	-1.854370

H	-3.522142	-0.823224	-2.301419
H	-4.338839	0.663870	-1.742506
H	-2.735872	0.750564	-2.522214
C	-3.843364	-0.908930	0.743371
H	-4.774232	-0.332114	0.757901
H	-4.034624	-1.891001	0.299282
H	-3.493577	-1.053493	1.769595
C	2.252401	-2.959325	-1.710620
H	3.330225	-3.073309	-1.865252
H	1.844770	-3.896635	-1.318812
H	1.769306	-2.745509	-2.668249
C	2.863504	-2.092011	0.940296
H	2.461442	-3.024006	1.349140
H	3.916800	-2.242949	0.680545
H	2.792296	-1.319785	1.710686
Ru	-0.367755	-0.969680	-0.263126
H	-0.392007	-0.866489	-1.823196
H	-1.262840	-0.375863	2.236960
C	-0.440865	-0.285937	2.971288
H	-0.873753	-0.118112	3.967702
O	0.440037	0.697007	2.631405
O	0.160436	-1.596974	3.062069
H	0.262656	-1.931425	2.160589

B5

	Coordinates (Angstroms)		
	X	Y	Z

N	0.495194	1.132454	0.166395
C	-1.130206	-2.589983	-0.587765
O	-1.589898	-3.642718	-0.793180
C	-2.332594	1.746331	0.522685
H	-3.177743	2.410852	0.306417
H	-2.287665	1.602161	1.609964
C	2.765722	-0.228183	-1.174790
P	1.829894	-1.664358	-0.553875
P	-2.560734	0.099768	-0.235451
Si	2.214630	1.352217	-0.298199
Si	-0.681359	2.461133	-0.051641
C	3.203579	1.655400	1.263337
H	4.258155	1.832040	1.019069
H	2.825067	2.544370	1.782724

H	3.154688	0.814731	1.962515
C	2.497700	2.774080	-1.484985
H	2.201163	3.744334	-1.072869
H	3.575716	2.820197	-1.687861
H	1.989263	2.628386	-2.442998
C	-0.215816	3.922205	1.026143
H	-0.083809	3.609424	2.068423
H	0.716273	4.390553	0.689237
H	-1.000066	4.688476	0.999617
C	-0.811611	2.960085	-1.855860
H	-1.818568	3.345331	-2.056229
H	-0.100050	3.752682	-2.106545
H	-0.632762	2.115210	-2.529858
H	3.847968	-0.394359	-1.109113
H	2.510631	-0.119861	-2.237085
H	0.510332	0.915488	1.210840
C	-3.376947	0.398407	-1.841032
H	-3.582854	-0.566831	-2.313583
H	-4.317501	0.941983	-1.704956
H	-2.719382	0.969675	-2.500191
C	-3.869301	-0.728764	0.734021
H	-4.779281	-0.119877	0.759028
H	-4.096035	-1.697712	0.278098
H	-3.520060	-0.897575	1.756716
C	2.136982	-3.012247	-1.746084
H	3.210682	-3.169353	-1.890504
H	1.685296	-3.936808	-1.373236
H	1.674375	-2.762153	-2.704798
C	2.755916	-2.213134	0.925596
H	2.324141	-3.145912	1.301420
H	3.808679	-2.383894	0.676844
H	2.690949	-1.459797	1.715211
Ru	-0.414745	-0.930336	-0.303457
H	-0.415648	-0.783992	-1.860867
H	-1.247417	-0.441155	2.147145
C	-0.492647	-0.502130	2.962818
H	-1.034115	-0.460683	3.925927
O	0.472578	0.429038	2.844595
O	-0.000913	-1.878285	2.926949
H	0.269991	-2.053068	2.015078

B6

	Coordinates (Angstroms)		
	X	Y	Z
N	0.510304	-1.111346	-0.049663
C	-1.349557	2.624386	-0.010596
O	-1.855756	3.678808	-0.072565
C	2.813272	0.552432	-0.515014
H	3.610556	0.888713	-1.188474
H	3.289127	0.288433	0.438198
C	-2.245282	-1.779591	-0.850666
P	-2.625267	-0.142846	-0.131837
P	1.613167	1.903732	-0.197170
Si	-0.670500	-2.460072	-0.072104
Si	1.917371	-0.981086	-1.150602
C	-0.930128	-2.956816	1.716211
H	-1.870805	-3.506905	1.836237
H	-0.115977	-3.610031	2.051430
H	-0.953199	-2.086254	2.381070
C	-0.103803	-3.942652	-1.068265
H	0.781875	-4.413828	-0.628854
H	-0.909015	-4.688576	-1.067846
H	0.113879	-3.696699	-2.113582
C	3.071905	-2.452471	-0.998316
H	3.255286	-2.708580	0.051388
H	2.679175	-3.339334	-1.505748
H	4.038394	-2.209962	-1.457834
C	1.340535	-0.806184	-2.921808
H	2.189700	-0.946302	-3.601820
H	0.589950	-1.565445	-3.171500
H	0.902381	0.176901	-3.115801
H	-3.090586	-2.473314	-0.764335
H	-2.048171	-1.620960	-1.919031
H	0.887878	-1.093253	0.904767
C	1.812467	3.033364	-1.619137
H	1.123740	3.876273	-1.504544
H	2.838323	3.410507	-1.685290
H	1.560027	2.503693	-2.542261
C	2.333754	2.861063	1.182943
H	3.359128	3.167513	0.950737
H	1.721135	3.749927	1.363883
H	2.337503	2.254038	2.092958
C	-3.886219	0.591832	-1.231556
H	-4.738623	-0.085092	-1.350380
H	-4.234635	1.538787	-0.807043

H	-3.441566	0.791943	-2.210210
C	-3.595106	-0.504539	1.376891
H	-3.931736	0.438845	1.818095
H	-4.469584	-1.119362	1.138593
H	-2.982086	-1.028088	2.114654
Ru	-0.561690	0.991320	0.044211
H	-0.617220	0.962553	-1.564244
H	1.862316	0.160521	3.121062
C	2.615186	-0.640974	3.055690
H	3.590904	-0.483822	3.544367
O	2.372549	-1.674886	2.460562
O	-0.334026	0.797079	2.300440
H	-1.184825	0.504299	2.640948

B7

	Coordinates (Angstroms)		
	X	Y	Z

N	0.465472	1.174587	0.307835
C	-1.035039	-2.665866	-0.256400
O	-1.467055	-3.741161	-0.425379
C	-2.363648	1.680318	0.641606
H	-3.247773	2.284379	0.403889
H	-2.276151	1.635422	1.735339
C	2.822312	-0.225341	-0.843406
P	1.885643	-1.664170	-0.216937
P	-2.541318	-0.038824	0.044802
Si	2.205617	1.384411	-0.069796
Si	-0.765237	2.426297	-0.029547
C	3.072444	1.743125	1.551155
H	4.159449	1.791789	1.417176
H	2.736279	2.704990	1.957735
H	2.856272	0.971476	2.298932
C	2.512755	2.757544	-1.304608
H	2.178179	3.738405	-0.950974
H	3.595180	2.821604	-1.475442
H	2.041342	2.553103	-2.271285
C	-0.380456	4.004428	0.907683
H	-0.254703	3.799330	1.977476
H	0.536479	4.482162	0.544461
H	-1.196616	4.729645	0.800477
C	-0.889210	2.731270	-1.872968

H	-1.880706	3.133537	-2.112949
H	-0.147169	3.459225	-2.215374
H	-0.751383	1.805752	-2.442432
H	3.903347	-0.361897	-0.715671
H	2.620872	-0.165694	-1.920978
H	0.395105	0.929427	1.308282
C	-3.451275	0.089149	-1.533190
H	-3.615088	-0.919189	-1.926027
H	-4.416918	0.585692	-1.391895
H	-2.859607	0.647726	-2.262657
C	-3.772420	-0.816181	1.149838
H	-4.696396	-0.229149	1.180888
H	-3.996631	-1.823480	0.784433
H	-3.363849	-0.898457	2.161228
C	2.290260	-3.037640	-1.351031
H	3.373513	-3.170823	-1.437421
H	1.844242	-3.962708	-0.972330
H	1.868810	-2.829293	-2.338458
C	2.751364	-2.142926	1.320305
H	2.290493	-3.048446	1.726337
H	3.811523	-2.334841	1.124425
H	2.662572	-1.351851	2.069441
Ru	-0.375439	-0.990673	-0.024428
H	-0.376589	-0.824110	-1.633177
O	-0.176877	-0.823539	2.225112
H	-1.054319	-0.780889	2.617595

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	Coordinates (Angstroms)		
	X	Y	Z

N	0.380483	1.144624	0.244757
C	-0.872918	-2.762353	-0.090499
O	-1.223859	-3.877644	-0.140637
C	-2.463411	1.539215	0.605602
H	-3.369872	2.095033	0.336971
H	-2.401954	1.515863	1.701793
C	2.837724	-0.079964	-0.843116
P	1.968335	-1.569114	-0.249840
P	-2.544904	-0.192019	0.029200
Si	2.074236	1.476235	-0.069630
Si	-0.870975	2.333347	-0.048300

C	2.943326	1.887521	1.546546
H	4.016989	2.052663	1.394101
H	2.520856	2.802688	1.980762
H	2.824818	1.087302	2.286239
C	2.381858	2.878985	-1.285844
H	2.015065	3.845787	-0.923426
H	3.463719	2.977952	-1.443942
H	1.923883	2.680189	-2.261048
C	-0.582714	3.932228	0.903307
H	-0.481351	3.735719	1.977505
H	0.324738	4.447633	0.567978
H	-1.423463	4.624123	0.766486
C	-1.078213	2.724866	-1.878137
H	-2.071188	3.149004	-2.071996
H	-0.336158	3.455644	-2.217914
H	-0.966268	1.823034	-2.490861
H	3.921027	-0.156692	-0.688159
H	2.657912	-0.021903	-1.924870
H	0.236146	0.579769	1.408112
C	-3.469173	-0.134014	-1.545187
H	-3.573106	-1.152161	-1.932818
H	-4.462756	0.302811	-1.399792
H	-2.918789	0.458561	-2.280396
C	-3.719014	-1.031313	1.151097
H	-4.663688	-0.480288	1.209440
H	-3.913100	-2.043541	0.782262
H	-3.280873	-1.105755	2.150744
C	2.435337	-2.921237	-1.385973
H	3.523675	-3.013845	-1.461836
H	2.019123	-3.863616	-1.015318
H	2.016289	-2.724552	-2.376815
C	2.834294	-2.024960	1.295578
H	2.392573	-2.940038	1.701779
H	3.900190	-2.192264	1.108176
H	2.721620	-1.232539	2.040134
Ru	-0.324013	-1.021428	-0.044900
H	-0.401152	-1.050659	-1.635895
O	0.036293	-0.316547	2.197285
H	-0.800872	-0.142943	2.642073

B8

Coordinates (Angstroms)

	X	Y	Z
N	0.170661	1.112081	0.083572
C	-0.390100	-2.887538	-0.018759
O	-0.549211	-4.048158	0.008087
C	-2.683536	1.092724	0.592803
H	-3.671224	1.498236	0.343078
H	-2.604088	1.057144	1.687646
C	2.828449	0.354940	-0.884278
P	2.202402	-1.242302	-0.270402
P	-2.475267	-0.611722	-0.020630
Si	1.766265	1.748830	-0.151273
Si	-1.227125	2.125527	-0.055589
C	2.536587	2.317213	1.476167
H	3.551895	2.706413	1.327364
H	1.933421	3.118353	1.922138
H	2.591846	1.502614	2.207324
C	1.877793	3.201949	-1.353387
H	1.360294	4.094605	-0.982663
H	2.931262	3.472264	-1.504025
H	1.457313	2.947059	-2.333072
C	-1.129506	3.681148	1.008601
H	-0.954454	3.432552	2.062445
H	-0.327385	4.354419	0.683216
H	-2.071327	4.242635	0.950399
C	-1.600820	2.668138	-1.827525
H	-2.661887	2.916696	-1.955784
H	-1.020095	3.559371	-2.094077
H	-1.348353	1.881274	-2.547888
H	3.904512	0.466639	-0.703858
H	2.665884	0.360100	-1.970367
H	0.142425	0.572627	1.861752
C	-3.342510	-0.639808	-1.630130
H	-3.255188	-1.638376	-2.068791
H	-4.401881	-0.391969	-1.505455
H	-2.882831	0.076377	-2.316328
C	-3.549923	-1.663584	1.021641
H	-4.557871	-1.240838	1.091329
H	-3.610228	-2.667687	0.589715
H	-3.122833	-1.743959	2.025665
C	2.889918	-2.520623	-1.381248
H	3.979920	-2.437196	-1.444279
H	2.625009	-3.514483	-1.006619
H	2.459900	-2.401578	-2.379950

C	3.105256	-1.543043	1.292559
H	2.805675	-2.515404	1.695756
H	4.188105	-1.537677	1.128398
H	2.849467	-0.775406	2.027657
Ru	-0.141369	-1.070665	-0.069300
H	-0.222874	-1.180640	-1.629200
O	0.101371	0.077133	2.719463
H	-0.830717	0.079007	2.965161

B9

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.083506	1.113223	-0.273237
C	0.366753	-2.932199	0.338206
O	0.474648	-4.087518	0.453029
C	-2.840200	0.364608	-0.525241
H	-3.760782	0.309082	-1.117974
H	-3.086571	0.830171	0.437910
C	2.726032	0.805899	-1.060796
P	2.509561	-0.804527	-0.241726
P	-2.167132	-1.293019	-0.188435
Si	1.410237	1.976341	-0.340368
Si	-1.445701	1.407639	-1.293249
C	1.984057	2.496998	1.383045
H	3.056556	2.730423	1.384771
H	1.448062	3.395351	1.712731
H	1.803387	1.716572	2.130796
C	1.406039	3.535806	-1.402204
H	0.715329	4.290438	-1.009364
H	2.410937	3.977808	-1.403265
H	1.134508	3.330743	-2.444575
C	-2.056503	3.195388	-1.306327
H	-2.083996	3.622093	-0.296998
H	-1.429611	3.839927	-1.932616
H	-3.075876	3.235219	-1.712565
C	-1.190865	0.919798	-3.098920
H	-2.128010	0.987939	-3.666454
H	-0.468487	1.599627	-3.569478
H	-0.800279	-0.098397	-3.201257
H	3.758667	1.166724	-0.982615
H	2.491609	0.659810	-2.123643

H	-0.800007	1.721364	1.263255
C	-2.655584	-2.289950	-1.641351
H	-2.257408	-3.303983	-1.539454
H	-3.745995	-2.336727	-1.730366
H	-2.239748	-1.844401	-2.549025
C	-3.176423	-2.037858	1.141466
H	-4.241319	-2.010327	0.887283
H	-2.867283	-3.078827	1.283611
H	-3.016728	-1.500186	2.079991
C	3.319288	-2.052311	-1.302612
H	4.367128	-1.789898	-1.482121
H	3.272716	-3.031485	-0.815462
H	2.791460	-2.115572	-2.258076
C	3.604657	-0.776491	1.222263
H	3.534911	-1.745936	1.725823
H	4.645729	-0.592680	0.936401
H	3.281968	-0.003510	1.923758
Ru	0.185648	-1.110179	0.101762
H	0.202158	-1.348614	-1.471654
H	-1.941313	0.407448	2.706040
C	-1.597164	1.385015	3.059549
H	-2.398866	1.878615	3.619862
O	-1.256566	2.222351	2.001114
O	-0.504720	1.113393	3.918672
H	0.592803	-0.613945	1.875941
H	-0.243262	1.937778	4.347580
H	-0.193714	-0.753894	1.924374

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	Coordinates (Angstroms)		
	X	Y	Z

N	0.178326	1.180527	-0.152745
C	-0.411327	-2.939423	0.244112
O	-0.605735	-4.087802	0.242010
C	-2.651304	1.066602	-0.584180
H	-3.526177	1.211588	-1.228358
H	-2.823731	1.616412	0.350048
C	2.763360	0.096133	-1.070032
P	2.208486	-1.409462	-0.209021
P	-2.431546	-0.693250	-0.165807
Si	1.882080	1.580370	-0.292273

Si	-1.026568	1.730748	-1.304335
C	2.588693	1.883917	1.425495
H	3.683689	1.817987	1.414434
H	2.315793	2.883357	1.783524
H	2.207807	1.161248	2.155212
C	2.257199	3.092043	-1.348962
H	1.805666	3.997976	-0.928874
H	3.343380	3.248211	-1.379175
H	1.909537	2.981284	-2.382469
C	-1.186806	3.606867	-1.388902
H	-1.139436	4.061895	-0.393351
H	-0.404762	4.057743	-2.009292
H	-2.153793	3.873756	-1.834614
C	-0.736311	1.121110	-3.060454
H	-1.583407	1.393386	-3.703229
H	0.160039	1.592996	-3.482159
H	-0.602147	0.036635	-3.115797
H	3.856528	0.183899	-1.075451
H	2.421605	0.010720	-2.110128
H	-0.213067	1.740282	0.935545
C	-3.107422	-1.589152	-1.608452
H	-2.983151	-2.665867	-1.457670
H	-4.170139	-1.363715	-1.745248
H	-2.558386	-1.299516	-2.508876
C	-3.646832	-1.092997	1.139732
H	-4.659295	-0.820276	0.823740
H	-3.610527	-2.168139	1.343586
H	-3.400973	-0.556899	2.060247
C	2.672010	-2.805743	-1.292626
H	3.743966	-2.774267	-1.514536
H	2.436945	-3.752886	-0.796935
H	2.106270	-2.749757	-2.226446
C	3.353172	-1.631876	1.199862
H	3.130581	-2.586861	1.686025
H	4.392541	-1.640759	0.854632
H	3.224287	-0.835045	1.935406
Ru	-0.118064	-1.125847	0.167218
H	-0.133242	-1.265214	-1.410779
H	-1.746298	0.848470	2.533796
C	-1.211881	1.739508	2.894058
H	-1.928931	2.393615	3.416761
O	-0.588535	2.421516	1.889239
O	-0.296531	1.215918	3.874432
H	0.336162	-0.926532	2.040576

H	0.166174	1.966288	4.267513
H	-0.457149	-0.892408	2.045545

B10

	Coordinates (Angstroms)		
	X	Y	Z

N	0.110519	1.198189	-0.189383
C	-0.134779	-2.958156	0.227445
O	-0.224659	-4.117496	0.243605
C	-2.692969	0.818955	-0.714161
H	-3.556430	0.908036	-1.383799
H	-2.948610	1.318696	0.229455
C	2.816122	0.335406	-0.961941
P	2.356152	-1.198719	-0.090199
P	-2.326100	-0.927578	-0.340089
Si	1.802931	1.768777	-0.271751
Si	-1.140098	1.671452	-1.371868
C	2.345788	2.194083	1.470208
H	3.438356	2.274518	1.520033
H	1.922993	3.157865	1.775511
H	2.021681	1.445082	2.199709
C	2.054435	3.263726	-1.374226
H	1.507397	4.137456	-1.004197
H	3.122522	3.517350	-1.372939
H	1.763192	3.082846	-2.414299
C	-1.454698	3.521877	-1.366310
H	-1.485439	3.911434	-0.342180
H	-0.692506	4.074821	-1.924672
H	-2.425354	3.732078	-1.832932
C	-0.676232	1.115703	-3.098491
H	-1.501876	1.328498	-3.788961
H	0.202710	1.661267	-3.460817
H	-0.456432	0.045335	-3.148517
H	3.896892	0.516544	-0.919898
H	2.536841	0.198460	-2.015126
H	-0.269833	1.542144	0.735981
C	-2.827575	-1.837711	-1.842266
H	-2.630069	-2.904612	-1.699845
H	-3.893935	-1.690773	-2.042179
H	-2.247575	-1.487703	-2.700127
C	-3.564900	-1.486725	0.880251

H	-4.579895	-1.312999	0.507908
H	-3.423414	-2.557576	1.059415
H	-3.428450	-0.955889	1.826004
C	2.994677	-2.566583	-1.115268
H	4.069340	-2.448603	-1.287751
H	2.815090	-3.519913	-0.608239
H	2.470232	-2.578896	-2.074352
C	3.429943	-1.280883	1.385088
H	3.273682	-2.245506	1.878164
H	4.484531	-1.188841	1.104791
H	3.173453	-0.488831	2.091834
Ru	-0.002310	-1.127296	0.138231
H	0.101491	-1.276002	-1.436753
H	-2.046407	0.614460	2.547299
C	-1.657642	1.551220	2.991179
H	-2.515152	2.086208	3.450853
O	-0.964452	2.317733	2.131055
O	-0.847187	1.050984	4.100420
H	0.327102	-0.929878	2.018895
H	-0.464082	1.825165	4.531979
H	-0.467091	-0.882536	1.998545

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	Coordinates (Angstroms)		
	X	Y	Z

N	0.338787	1.154518	-0.076636
C	-0.888595	-2.840603	-0.269467
O	-1.238290	-3.948331	-0.392108
C	-2.509333	1.486166	0.268826
H	-3.453219	1.973590	-0.002099
H	-2.345208	1.636822	1.344021
C	2.721191	-0.232626	-1.256188
P	1.938774	-1.644973	-0.406432
P	-2.571405	-0.315033	-0.020430
Si	2.021020	1.413571	-0.647524
Si	-1.008501	2.203752	-0.620087
C	3.015932	2.051302	0.804520
H	4.063071	2.195806	0.511723
H	2.626706	3.014015	1.155515
H	2.993455	1.352042	1.647467
C	2.147151	2.607400	-2.088678

H	1.727639	3.596876	-1.881733
H	3.213745	2.744429	-2.310097
H	1.674828	2.210288	-2.992902
C	-0.756372	3.969623	-0.041894
H	-0.611263	4.003657	1.043508
H	0.110160	4.444175	-0.515111
H	-1.638543	4.576059	-0.283215
C	-1.229681	2.146402	-2.480217
H	-2.267085	2.402182	-2.728554
H	-0.583688	2.873673	-2.981804
H	-1.019282	1.154516	-2.892812
H	3.814259	-0.269336	-1.166332
H	2.473292	-0.328638	-2.320848
H	0.351034	1.316236	0.951150
C	-3.597345	-0.522896	-1.518486
H	-3.733840	-1.591949	-1.709189
H	-4.578245	-0.053020	-1.390511
H	-3.094372	-0.082373	-2.382751
C	-3.655757	-0.988189	1.288380
H	-4.627407	-0.483407	1.286169
H	-3.805674	-2.059618	1.121347
H	-3.179040	-0.850945	2.262925
C	2.321725	-3.103542	-1.439495
H	3.399068	-3.182954	-1.618324
H	1.975779	-4.010456	-0.933608
H	1.799219	-3.018829	-2.396426
C	2.990575	-1.922743	1.064595
H	2.580918	-2.751035	1.650344
H	4.016648	-2.163569	0.766606
H	3.000919	-1.026825	1.690456
Ru	-0.345359	-1.105202	-0.118202
H	-0.374369	-0.968735	-1.749851
H	-0.902098	0.488458	3.711044
C	0.088647	0.968008	3.591993
H	0.545231	1.140833	4.583146
O	0.159755	1.947990	2.730837
O	0.968710	-0.227551	3.067149
H	0.313662	-0.760444	2.205101
H	1.082314	-0.890267	3.767481
H	-0.420355	-1.213095	1.654592

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	Coordinates (Angstroms)		
	X	Y	Z
N	-0.259456	1.207431	-0.077085
C	0.567749	-2.894672	-0.315970
O	0.780652	-4.045490	-0.380756
C	-2.930224	0.139924	0.160354
H	-3.973679	0.117811	-0.176773
H	-2.936772	0.317933	1.243626
C	2.478141	1.167299	-1.267961
P	2.484380	-0.495353	-0.511846
P	-2.104038	-1.464904	-0.131850
Si	1.139537	2.251550	-0.499193
Si	-1.931309	1.526820	-0.635496
C	1.723308	3.011724	1.110755
H	2.684989	3.520880	0.975748
H	0.999076	3.750292	1.474681
H	1.848819	2.255838	1.894730
C	0.727417	3.580877	-1.752899
H	-0.037864	4.283917	-1.409550
H	1.642306	4.157542	-1.941670
H	0.409560	3.154598	-2.710126
C	-2.566410	3.162046	0.030363
H	-2.421247	3.224405	1.114919
H	-2.065265	4.020612	-0.429223
H	-3.640735	3.259359	-0.170080
C	-2.028274	1.484556	-2.504580
H	-3.045559	1.219964	-2.817335
H	-1.798246	2.465072	-2.934440
H	-1.338747	0.748982	-2.931310
H	3.466463	1.640864	-1.213675
H	2.231873	1.029156	-2.328482
H	-0.326325	1.246701	0.947255
C	-2.891703	-2.108677	-1.651910
H	-2.447851	-3.078524	-1.897287
H	-3.971983	-2.228664	-1.518288
H	-2.701057	-1.424662	-2.483476
C	-2.767864	-2.587261	1.150031
H	-3.861462	-2.629973	1.108195
H	-2.360639	-3.592161	0.998091
H	-2.455520	-2.234839	2.137502
C	3.493774	-1.525226	-1.637370
H	4.475451	-1.070005	-1.805736
H	3.631276	-2.518329	-1.197342

H	2.974644	-1.637633	-2.593028
C	3.599966	-0.323642	0.928916
H	3.701902	-1.294353	1.423643
H	4.589742	0.022787	0.611922
H	3.186156	0.387962	1.647595
Ru	0.225644	-1.113160	-0.225588
H	0.120154	-0.978147	-1.905177
H	-1.390956	-0.244244	3.109057
C	-1.193258	0.736665	3.570403
H	-1.291564	0.814176	4.664884
O	-0.887879	1.702014	2.896071
O	1.436124	-0.394643	3.723548
H	1.115684	-0.646839	2.834267
H	2.050335	-1.095810	3.969874
H	0.297668	-1.087687	1.481853

B11'

	Coordinates (Angstroms)		
	X	Y	Z

N	0.434465	1.094297	-0.238518
C	-0.879196	-2.878343	-0.140175
O	-1.245647	-3.990672	-0.111740
C	-2.456120	1.493412	-0.184538
H	-3.337965	1.971534	-0.628437
H	-2.478074	1.701964	0.891931
C	2.901444	-0.420119	-0.982589
P	1.974248	-1.702327	-0.066349
P	-2.509497	-0.324504	-0.390295
Si	2.168032	1.294665	-0.687223
Si	-0.847105	2.161664	-0.901974
C	3.013192	2.140138	0.755330
H	4.063038	2.345262	0.513012
H	2.528264	3.096071	0.987747
H	2.993561	1.523134	1.660020
C	2.403672	2.305369	-2.244473
H	1.997527	3.318991	-2.160039
H	3.483528	2.397791	-2.418580
H	1.969928	1.822987	-3.125722
C	-0.568289	3.912011	-0.292045
H	-0.481776	3.929388	0.801349
H	0.345589	4.347846	-0.711881

H	-1.406642	4.562229	-0.570757
C	-0.901237	2.072032	-2.771440
H	-1.912756	2.323492	-3.112294
H	-0.209975	2.780988	-3.236106
H	-0.664547	1.066348	-3.134309
H	3.972906	-0.453931	-0.748331
H	2.786657	-0.653387	-2.048611
H	0.416151	1.233282	0.776532
C	-3.365072	-0.583939	-1.985375
H	-3.491481	-1.659537	-2.145284
H	-4.347538	-0.100518	-1.992922
H	-2.757795	-0.187116	-2.802699
C	-3.757869	-0.905726	0.812401
H	-4.717305	-0.400383	0.658807
H	-3.896784	-1.985422	0.695220
H	-3.401311	-0.711013	1.827670
C	2.516292	-3.289931	-0.791255
H	3.607862	-3.375581	-0.782725
H	2.087483	-4.116711	-0.216083
H	2.152364	-3.361223	-1.820126
C	2.767240	-1.734658	1.582783
H	2.299626	-2.519194	2.185590
H	3.841881	-1.931058	1.502886
H	2.613277	-0.778603	2.090973
Ru	-0.313453	-1.151449	-0.190243
H	-0.141727	-1.184991	-1.870719
H	-1.234150	1.645342	2.667791
C	-0.436820	1.602839	3.414850
H	-0.033414	2.602500	3.601839
O	0.633299	0.818318	2.961840
O	-1.036305	1.079928	4.579088
H	0.274070	0.028547	2.498166
H	-0.422400	1.180927	5.317365
H	-0.445822	-0.981519	1.513104

TSB11'-12'

	Coordinates (Angstroms)		
	X	Y	Z

N	0.285479	1.154616	-0.179347
C	-0.362081	-2.967416	-0.219448
O	-0.541435	-4.115589	-0.312020

C	-2.622629	1.101044	-0.374407
H	-3.526045	1.426657	-0.904371
H	-2.769963	1.317601	0.690891
C	3.006290	0.085784	-0.775568
P	2.268184	-1.358964	0.057037
P	-2.368473	-0.700196	-0.538966
Si	1.990776	1.646658	-0.458748
Si	-1.077733	2.007589	-0.965966
C	2.568643	2.533757	1.085338
H	3.594467	2.899760	0.957248
H	1.925266	3.397312	1.293791
H	2.549324	1.882771	1.965904
C	2.212666	2.760207	-1.949347
H	1.669624	3.707639	-1.868936
H	3.281734	2.999093	-2.022100
H	1.925209	2.267370	-2.883264
C	-1.150373	3.785017	-0.375804
H	-1.197467	3.826782	0.718978
H	-0.275290	4.358971	-0.700575
H	-2.043164	4.285852	-0.769801
C	-0.943497	1.901183	-2.831606
H	-1.942222	1.989650	-3.275883
H	-0.329346	2.709245	-3.240517
H	-0.514176	0.946122	-3.153381
H	4.061270	0.214844	-0.503711
H	2.965761	-0.121371	-1.852748
H	0.129529	1.254550	0.845546
C	-2.985490	-1.125527	-2.204135
H	-2.859189	-2.201324	-2.361374
H	-4.043390	-0.865980	-2.314135
H	-2.402225	-0.600012	-2.964297
C	-3.602299	-1.484472	0.555986
H	-4.612201	-1.130765	0.323761
H	-3.561396	-2.570315	0.422862
H	-3.367192	-1.253265	1.598682
C	3.090587	-2.817966	-0.666852
H	4.177322	-2.741490	-0.558425
H	2.741236	-3.722940	-0.160404
H	2.836279	-2.893021	-1.727862
C	2.935677	-1.314930	1.758062
H	2.597256	-2.207410	2.293162
H	4.030450	-1.288261	1.753019
H	2.552447	-0.436916	2.285112
Ru	-0.080675	-1.159976	-0.139548

H	0.128492	-1.189841	-1.730569
H	-2.089656	0.392304	2.742606
C	-1.368756	1.136306	3.132160
H	-1.751070	2.147477	2.899485
O	-0.111507	0.946825	2.654201
O	-1.461598	0.958990	4.563289
H	-0.170775	-0.399194	2.006178
H	-0.880700	1.612972	4.972043
H	-0.313215	-1.209996	1.743545

B12'

	Coordinates (Angstroms)		
	X	Y	Z

N	0.414312	1.141048	-0.148971
C	-0.729787	-2.876668	-0.434814
O	-1.049483	-3.998981	-0.537677
C	-2.474956	1.435247	-0.213729
H	-3.360334	1.904231	-0.659914
H	-2.536264	1.588177	0.870573
C	2.990213	-0.223749	-0.824848
P	2.064372	-1.599498	-0.055862
P	-2.451083	-0.369622	-0.522188
Si	2.159596	1.436202	-0.478710
Si	-0.866088	2.200301	-0.826583
C	2.882137	2.220068	1.062134
H	3.936566	2.474295	0.900587
H	2.346706	3.139136	1.329111
H	2.831102	1.537984	1.918111
C	2.429881	2.539258	-1.966786
H	1.982288	3.532119	-1.851697
H	3.511391	2.678279	-2.091258
H	2.049029	2.086646	-2.887849
C	-0.682168	3.927960	-0.121543
H	-0.661844	3.898733	0.974677
H	0.239847	4.410106	-0.466072
H	-1.523413	4.564378	-0.422465
C	-0.832132	2.207521	-2.698680
H	-1.834585	2.449782	-3.071815
H	-0.143071	2.958682	-3.095728
H	-0.550070	1.229604	-3.102512
H	4.042245	-0.225157	-0.512546

H	2.962408	-0.394566	-1.908312
H	0.320390	1.219370	0.869697
C	-3.250913	-0.573712	-2.154059
H	-3.296744	-1.642395	-2.387376
H	-4.264496	-0.159145	-2.155934
H	-2.654729	-0.081289	-2.926669
C	-3.710306	-1.060771	0.609138
H	-4.678983	-0.570373	0.465471
H	-3.818201	-2.133664	0.418587
H	-3.381782	-0.924557	1.643204
C	2.741527	-3.113501	-0.824361
H	3.829811	-3.154684	-0.710185
H	2.298409	-3.994412	-0.349398
H	2.487172	-3.126822	-1.887968
C	2.740813	-1.689742	1.642675
H	2.269597	-2.524599	2.170239
H	3.826288	-1.835898	1.629053
H	2.508274	-0.769858	2.186817
Ru	-0.234421	-1.133476	-0.293522
H	0.018854	-1.016070	-1.960000
H	-1.786839	0.879025	2.792658
C	-0.978004	1.118840	3.488573
H	-0.924960	2.198344	3.659226
O	0.262200	0.725998	2.965440
O	-1.295603	0.441367	4.684155
H	0.125376	-0.104148	2.455617
H	-0.697003	0.741084	5.379858
H	-0.461297	-1.132558	1.409306

TSB12'-13'

	Coordinates (Angstroms)		
	X	Y	Z

N	0.398264	1.170492	-0.101994
C	-0.754494	-2.835860	-0.552475
O	-1.075807	-3.947738	-0.723386
C	-2.483010	1.457201	-0.032437
H	-3.392291	1.945442	-0.403143
H	-2.475116	1.559924	1.060605
C	2.937528	-0.167466	-0.958121
P	2.050459	-1.579037	-0.211015
P	-2.480900	-0.331015	-0.422156

Si	2.133678	1.475062	-0.487437
Si	-0.909240	2.246298	-0.702114
C	2.897694	2.176384	1.072391
H	3.961954	2.391370	0.920899
H	2.399738	3.108780	1.364969
H	2.813283	1.473122	1.908764
C	2.355653	2.646516	-1.929783
H	1.908763	3.632240	-1.763908
H	3.433054	2.794618	-2.078405
H	1.951859	2.229842	-2.858128
C	-0.700446	3.955658	0.037691
H	-0.657384	3.905404	1.132234
H	0.215552	4.441669	-0.316859
H	-1.545291	4.600891	-0.233166
C	-0.937995	2.304887	-2.572545
H	-1.956819	2.533221	-2.907891
H	-0.279346	3.086183	-2.963609
H	-0.643893	1.348076	-3.015838
H	4.005802	-0.187509	-0.707858
H	2.849379	-0.283655	-2.045738
H	0.346464	1.238019	0.917522
C	-3.334598	-0.462851	-2.033402
H	-3.405157	-1.521233	-2.304048
H	-4.341182	-0.034361	-1.985008
H	-2.757473	0.049340	-2.807527
C	-3.702398	-1.068233	0.720493
H	-4.675605	-0.575838	0.622304
H	-3.813809	-2.133829	0.494719
H	-3.344087	-0.968293	1.748914
C	2.669503	-3.055732	-1.090514
H	3.763557	-3.094269	-1.070772
H	2.270157	-3.956655	-0.614195
H	2.323640	-3.029602	-2.127826
C	2.808436	-1.755064	1.444869
H	2.360778	-2.614306	1.953261
H	3.891350	-1.901459	1.371007
H	2.606409	-0.862426	2.043517
Ru	-0.256346	-1.103293	-0.310598
H	-0.073839	-0.897398	-1.960276
H	-1.788066	0.493719	3.009146
C	-0.938804	0.871670	3.594434
H	-0.870159	1.965250	3.553744
O	0.318911	0.332181	2.981628
O	-0.758709	0.302678	4.823972

H	0.087139	-0.380221	2.279138
H	0.296683	-0.096465	4.044183
H	-0.437734	-1.256050	1.409513

B13'

	Coordinates (Angstroms)		
	X	Y	Z

N	0.529994	-0.975484	-0.388343
C	-1.622462	2.545038	0.288401
O	-2.210814	3.539151	0.484050
C	2.700183	0.956017	-0.352148
H	3.579876	1.384195	-0.847650
H	2.996214	0.695806	0.671926
C	-2.264364	-1.797751	-1.054264
P	-2.619581	-0.358449	0.014843
P	1.339733	2.175226	-0.243304
Si	-0.490411	-2.395515	-0.822193
Si	2.090094	-0.612151	-1.199261
C	-0.338965	-3.581500	0.619315
H	-1.039528	-4.418301	0.514519
H	0.675730	-3.995376	0.668573
H	-0.548030	-3.087815	1.575314
C	0.032125	-3.222094	-2.418811
H	1.053801	-3.614284	-2.394406
H	-0.642970	-4.071536	-2.586314
H	-0.070124	-2.552420	-3.278671
C	3.312219	-1.993439	-0.864883
H	3.438645	-2.148752	0.213715
H	2.991584	-2.941973	-1.309432
H	4.295691	-1.746824	-1.283456
C	1.829261	-0.334383	-3.030831
H	2.620709	0.319565	-3.416093
H	1.877319	-1.273032	-3.591647
H	0.866397	0.145542	-3.234691
H	-2.992403	-2.604669	-0.901947
H	-2.363524	-1.452657	-2.091295
H	0.752389	-1.110332	0.599479
C	1.535549	3.214612	-1.735105
H	0.765260	3.992137	-1.725153
H	2.523625	3.685429	-1.766812
H	1.394365	2.604373	-2.631328

C	1.828355	3.319171	1.096468
H	2.810334	3.762325	0.899965
H	1.082711	4.116475	1.179905
H	1.858341	2.774056	2.044053
C	-4.162953	0.363579	-0.647614
H	-4.948178	-0.395864	-0.721931
H	-4.502631	1.164410	0.017163
H	-3.973117	0.791286	-1.635824
C	-3.200905	-1.110519	1.580017
H	-3.404195	-0.321534	2.310055
H	-4.115266	-1.689828	1.411804
H	-2.432798	-1.771236	1.990188
Ru	-0.696652	1.010751	-0.017842
H	-0.936973	1.114389	-1.685475
H	2.090828	-0.308950	2.483375
C	2.407248	-1.253060	2.955555
H	2.061974	-2.191322	2.491922
O	-0.347698	-1.045354	3.555981
O	3.123945	-1.259008	3.938691
H	-0.433545	-0.386730	2.838028
H	-0.093161	-0.533275	4.332152
H	-0.349678	0.765375	1.644315

C1

	Coordinates (Angstroms)		
	X	Y	Z

N	0.578806	1.056126	0.103005
C	-1.291398	-2.635205	-0.410596
O	-1.805050	-3.679866	-0.549670
C	-2.169872	1.806793	0.573954
H	-3.007974	2.495188	0.412423
H	-2.006829	1.724028	1.656757
C	2.792057	-0.623841	-0.978767
P	1.705154	-1.871074	-0.201215
P	-2.544321	0.126056	-0.048056
Si	2.291514	1.118207	-0.449584
Si	-0.564917	2.403337	-0.210265
C	3.317004	1.676752	1.016011
H	4.365989	1.810649	0.725833
H	2.951215	2.630209	1.415003
H	3.285873	0.937629	1.824547

C	2.530130	2.270163	-1.903382
H	2.295273	3.313531	-1.666981
H	3.589132	2.229171	-2.189671
H	1.942269	1.964824	-2.774954
C	0.038881	3.956053	0.646680
H	0.209591	3.775834	1.714376
H	0.975216	4.316396	0.205186
H	-0.702560	4.759451	0.555739
C	-0.790920	2.697646	-2.045629
H	-1.778785	3.141602	-2.218995
H	-0.043735	3.394713	-2.437081
H	-0.731812	1.767924	-2.620411
H	3.849702	-0.826305	-0.767565
H	2.643522	-0.705957	-2.062557
H	0.634636	1.000770	1.126251
H	-0.537470	-1.107366	1.497828
C	-3.535852	0.393190	-1.562167
H	-3.876012	-0.579794	-1.931435
H	-4.407402	1.024898	-1.360156
H	-2.922304	0.854415	-2.339382
C	-3.795282	-0.544696	1.104607
H	-4.661200	0.121978	1.176180
H	-4.126407	-1.526338	0.750202
H	-3.347644	-0.668265	2.094773
C	2.063527	-3.434574	-1.075360
H	3.139626	-3.636921	-1.088767
H	1.549076	-4.260093	-0.573271
H	1.691251	-3.367500	-2.101633
C	2.470524	-2.141377	1.439592
H	1.950252	-2.957950	1.949295
H	3.533137	-2.390430	1.346976
H	2.364615	-1.236773	2.045720
Ru	-0.490971	-1.017080	-0.202529
H	-0.375625	-0.779579	-1.880342
C	-0.153391	-0.079508	3.349195
H	-1.251846	-0.048110	3.403882
H	0.331693	-1.034678	3.597932
O	0.503715	0.935715	3.144249

TSC1-2

Coordinates (Angstroms)		
X	Y	Z

N	0.521827	1.093921	0.127545
C	-1.157601	-2.677617	-0.404740
O	-1.623977	-3.743261	-0.546889
C	-2.262506	1.723908	0.551883
H	-3.130869	2.367634	0.367996
H	-2.113912	1.660903	1.638162
C	2.822792	-0.464330	-0.960930
P	1.793835	-1.786725	-0.231379
P	-2.543690	0.021203	-0.058502
Si	2.241777	1.236108	-0.381998
Si	-0.672372	2.391018	-0.206634
C	3.208172	1.779859	1.127581
H	4.264536	1.936277	0.878270
H	2.813700	2.719081	1.532872
H	3.159941	1.024429	1.920137
C	2.472389	2.441117	-1.793853
H	2.191601	3.467118	-1.533451
H	3.538949	2.448780	-2.053754
H	1.918135	2.139978	-2.688653
C	-0.157042	3.966546	0.667909
H	0.008504	3.784300	1.736245
H	0.765548	4.380643	0.244820
H	-0.936657	4.732986	0.576716
C	-0.874655	2.676810	-2.046046
H	-1.874808	3.082567	-2.240615
H	-0.145846	3.400347	-2.424210
H	-0.767566	1.748604	-2.616409
H	3.888532	-0.624351	-0.754060
H	2.680149	-0.517236	-2.047535
H	0.555939	1.039276	1.154338
H	-0.466501	-1.107605	1.522074
C	-3.525758	0.223815	-1.588067
H	-3.805733	-0.768312	-1.956588
H	-4.434174	0.806655	-1.402279
H	-2.927993	0.715747	-2.358885
C	-3.773638	-0.702953	1.084543
H	-4.672925	-0.080294	1.140338
H	-4.050858	-1.702298	0.733668
H	-3.333542	-0.797514	2.081197
C	2.198629	-3.291621	-1.185016
H	3.280300	-3.459901	-1.211578
H	1.711616	-4.156837	-0.723994
H	1.819878	-3.185359	-2.205504

C	2.585411	-2.112862	1.386214
H	2.088020	-2.961163	1.866086
H	3.650608	-2.337660	1.266136
H	2.473447	-1.238911	2.034443
Ru	-0.434521	-1.022052	-0.191941
H	-0.342370	-0.775753	-1.857047
C	-0.217120	-0.238518	3.223004
H	-1.313212	-0.278212	3.298166
H	0.325903	-1.156526	3.488626
O	0.375166	0.838712	3.092021

C2

	Coordinates (Angstroms)		
	X	Y	Z

N	0.553753	1.053270	0.160624
C	-1.258382	-2.626963	-0.393305
O	-1.763186	-3.664843	-0.570656
C	-2.210854	1.820491	0.547370
H	-3.043693	2.503388	0.342257
H	-2.087224	1.752777	1.636282
C	2.801094	-0.547342	-0.967276
P	1.738129	-1.847931	-0.260579
P	-2.552552	0.133739	-0.064710
Si	2.267235	1.158862	-0.343320
Si	-0.569930	2.398076	-0.181975
C	3.297700	1.660520	1.139945
H	4.340685	1.824806	0.842964
H	2.921155	2.590223	1.582899
H	3.284912	0.889459	1.917306
C	2.553486	2.370283	-1.745064
H	2.301301	3.403215	-1.482516
H	3.624211	2.347496	-1.986832
H	2.005699	2.095045	-2.652094
C	-0.007438	3.962047	0.685157
H	0.145743	3.778066	1.754953
H	0.930627	4.343576	0.265828
H	-0.761644	4.752499	0.584682
C	-0.767048	2.689836	-2.025456
H	-1.758428	3.115499	-2.222745
H	-0.024817	3.397437	-2.407413
H	-0.678406	1.759087	-2.596059

H	3.862756	-0.748108	-0.776819
H	2.645800	-0.569504	-2.053670
H	0.551149	0.960207	1.240918
H	-0.454646	-1.015482	2.185403
C	-3.485573	0.340401	-1.620312
H	-3.785998	-0.648816	-1.980002
H	-4.379634	0.951788	-1.460702
H	-2.857008	0.805009	-2.383212
C	-3.807115	-0.561330	1.067865
H	-4.672445	0.105333	1.144831
H	-4.134832	-1.537170	0.695668
H	-3.366627	-0.697391	2.060030
C	2.092890	-3.363112	-1.212520
H	3.169768	-3.558494	-1.242351
H	1.584741	-4.213421	-0.747081
H	1.714771	-3.248815	-2.232373
C	2.463616	-2.198330	1.381268
H	1.919754	-3.025479	1.847324
H	3.522130	-2.464416	1.291746
H	2.366509	-1.319350	2.025501
Ru	-0.464998	-0.994132	-0.168280
H	-0.469930	-0.886406	-1.732681
C	-0.301780	-0.352285	3.083203
H	-1.327698	-0.126256	3.436906
H	0.144104	-1.034836	3.833800
O	0.460855	0.769647	2.837581

TSC2-3

	Coordinates (Angstroms)		
	X	Y	Z

N	0.539812	1.031871	0.160589
C	-1.247606	-2.633219	-0.368002
O	-1.751458	-3.674430	-0.534899
C	-2.223030	1.816052	0.532325
H	-3.053790	2.494185	0.304646
H	-2.111854	1.768316	1.623321
C	2.804636	-0.541039	-0.959721
P	1.746696	-1.842025	-0.251756
P	-2.551304	0.119580	-0.055146
Si	2.240579	1.156963	-0.331609
Si	-0.568257	2.368921	-0.192826

C	3.289456	1.663809	1.142154
H	4.331738	1.815685	0.835556
H	2.925702	2.601882	1.578548
H	3.274817	0.901453	1.928167
C	2.550585	2.370833	-1.732419
H	2.297062	3.404676	-1.474047
H	3.623699	2.346605	-1.963796
H	2.010877	2.097367	-2.645135
C	-0.018906	3.947351	0.664738
H	0.133741	3.772951	1.736246
H	0.917207	4.334883	0.246221
H	-0.778619	4.731848	0.557119
C	-0.785069	2.682495	-2.034917
H	-1.772319	3.124142	-2.219043
H	-0.036475	3.382464	-2.419500
H	-0.715249	1.756202	-2.615620
H	3.867596	-0.733469	-0.768206
H	2.648948	-0.564087	-2.046074
H	0.517825	0.945950	1.356433
H	-0.440239	-1.008016	2.206351
C	-3.489403	0.297335	-1.611698
H	-3.769493	-0.700154	-1.964990
H	-4.395569	0.892044	-1.456945
H	-2.869520	0.769697	-2.377099
C	-3.799473	-0.574976	1.086144
H	-4.669244	0.086428	1.159363
H	-4.121916	-1.556243	0.723626
H	-3.357199	-0.699762	2.078967
C	2.103922	-3.363228	-1.194295
H	3.181011	-3.557879	-1.223231
H	1.596599	-4.211812	-0.724664
H	1.725953	-3.255188	-2.214957
C	2.471994	-2.184091	1.392694
H	1.929779	-3.009988	1.863007
H	3.531146	-2.448726	1.305361
H	2.373593	-1.301955	2.032427
Ru	-0.456758	-0.993921	-0.160188
H	-0.467659	-0.896224	-1.724335
C	-0.295406	-0.272098	3.041073
H	-1.314161	-0.019737	3.387074
H	0.181312	-0.862293	3.843066
O	0.452683	0.840323	2.684079

C3

	Coordinates (Angstroms)		
	X	Y	Z
N	0.447070	1.021756	0.016400
C	-1.068491	-2.717011	-0.325295
O	-1.503889	-3.798222	-0.443547
C	-2.324771	1.666119	0.543506
H	-3.194773	2.299968	0.335002
H	-2.216228	1.584873	1.633000
C	2.847715	-0.363651	-0.967605
P	1.860386	-1.727273	-0.277948
P	-2.542328	-0.022386	-0.107546
Si	2.127550	1.281483	-0.346866
Si	-0.686466	2.328491	-0.146564
C	3.110200	1.823961	1.170980
H	4.154616	2.031816	0.904615
H	2.689424	2.738726	1.606845
H	3.111469	1.053708	1.950129
C	2.466382	2.563148	-1.691866
H	2.171379	3.575056	-1.389544
H	3.544071	2.586723	-1.901461
H	1.950338	2.321293	-2.627873
C	-0.199346	3.846685	0.863254
H	-0.048187	3.593756	1.919439
H	0.725405	4.303151	0.489198
H	-0.984894	4.611821	0.811730
C	-0.968879	2.902903	-1.925230
H	-1.937756	3.409892	-2.020742
H	-0.194332	3.613858	-2.234662
H	-0.953539	2.066358	-2.633376
H	3.917514	-0.483866	-0.756934
H	2.711170	-0.397974	-2.056554
H	0.450167	0.886162	1.810202
H	-0.367412	-1.105075	2.191230
C	-3.449976	0.179807	-1.680951
H	-3.642876	-0.808275	-2.109790
H	-4.401755	0.697138	-1.520686
H	-2.845792	0.748669	-2.391698
C	-3.785352	-0.836270	0.960375
H	-4.699442	-0.236648	1.026969
H	-4.028805	-1.819496	0.544776
H	-3.370780	-0.976948	1.963103

C	2.312041	-3.224741	-1.220144
H	3.396266	-3.378246	-1.216819
H	1.823369	-4.097756	-0.775832
H	1.963404	-3.121317	-2.251816
C	2.578572	-2.044966	1.375845
H	2.094121	-2.922939	1.814341
H	3.657183	-2.224048	1.310606
H	2.394785	-1.190247	2.033330
Ru	-0.388037	-1.017288	-0.201159
H	-0.415385	-0.994424	-1.766228
C	-0.399347	-0.387664	3.032170
H	-1.447523	-0.106136	3.198075
H	-0.033652	-0.915780	3.918433
O	0.418143	0.738212	2.794726

D1

	Coordinates (Angstroms)		
	X	Y	Z

N	0.643554	1.095599	0.152281
C	-1.393537	-2.443162	-0.667874
O	-1.966184	-3.409124	-0.990266
C	-2.080618	1.991517	0.517925
H	-2.873098	2.724089	0.323840
H	-1.970183	1.892911	1.606107
C	2.780612	-0.618400	-1.020097
P	1.645480	-1.893918	-0.375507
P	-2.512451	0.337047	-0.125530
Si	2.382725	1.077060	-0.286468
Si	-0.407003	2.503519	-0.183705
C	3.350036	1.369944	1.290832
H	4.426810	1.406965	1.086707
H	3.058720	2.321811	1.750907
H	3.174398	0.575901	2.025189
C	2.819274	2.364812	-1.574160
H	2.600190	3.389175	-1.255569
H	3.899541	2.302319	-1.758856
H	2.313712	2.179476	-2.527468
C	0.208244	4.018354	0.731755
H	0.313266	3.810002	1.803073
H	1.178745	4.360164	0.355030
H	-0.502660	4.846363	0.619409

C	-0.528053	2.821482	-2.025634
H	-1.473713	3.330114	-2.248573
H	0.283739	3.465544	-2.377834
H	-0.501614	1.889585	-2.600445
H	3.830023	-0.900971	-0.870277
H	2.602097	-0.561172	-2.101691
H	0.602835	0.960715	1.180314
C	-3.422406	0.631921	-1.680054
H	-3.775697	-0.329152	-2.067061
H	-4.281518	1.289451	-1.511541
H	-2.761460	1.079411	-2.426261
C	-3.808200	-0.301615	0.992098
H	-4.645829	0.400518	1.058328
H	-4.170929	-1.263793	0.616316
H	-3.383799	-0.454446	1.988543
C	1.889313	-3.348411	-1.451935
H	2.948036	-3.623048	-1.499904
H	1.316039	-4.194151	-1.060018
H	1.527834	-3.119174	-2.458407
C	2.390481	-2.425470	1.207905
H	1.826049	-3.275902	1.602082
H	3.435084	-2.721512	1.065586
H	2.343655	-1.615155	1.940787
Ru	-0.505210	-0.913379	-0.229481
H	-0.389970	-0.619104	-1.789304
C	-0.287553	-0.589673	3.040394
O	0.285990	0.523650	2.955001
O	-0.684335	-1.319295	2.089904
H	-0.470826	-0.992123	4.056113

D2

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.166168	1.194397	-0.111883
C	0.713259	-2.896046	0.192089
O	0.939573	-4.036331	0.164297
C	-2.725068	0.090328	-0.804397
H	-3.542896	-0.042679	-1.522520
H	-3.162411	0.474576	0.126541
C	2.708736	1.146569	-0.699901
P	2.643391	-0.493005	0.098580

P	-1.920186	-1.504807	-0.429523
Si	1.303080	2.216925	-0.046072
Si	-1.435563	1.350374	-1.364274
C	1.554143	2.675697	1.752675
H	2.585282	3.003003	1.930172
H	0.888697	3.502366	2.027236
H	1.338256	1.839311	2.425885
C	1.188991	3.773494	-1.080090
H	0.411395	4.448606	-0.706970
H	2.147710	4.303978	-1.013650
H	0.997827	3.571464	-2.139448
C	-2.232129	3.047936	-1.348276
H	-2.442622	3.371544	-0.322271
H	-1.603978	3.805990	-1.826639
H	-3.184816	3.014201	-1.891503
C	-0.719122	0.992092	-3.054650
H	-1.517655	0.999105	-3.806517
H	0.005677	1.763773	-3.339386
H	-0.216543	0.021634	-3.099462
H	3.692374	1.617003	-0.581534
H	2.536453	0.985903	-1.772594
H	-0.660599	1.350676	0.784796
C	-2.101566	-2.471568	-1.968471
H	-1.608040	-3.440938	-1.850079
H	-3.159746	-2.631337	-2.199190
H	-1.626157	-1.938668	-2.796538
C	-3.017409	-2.381683	0.735269
H	-4.028714	-2.468147	0.324341
H	-2.613764	-3.382502	0.919179
H	-3.051681	-1.835318	1.681697
C	3.727150	-1.571772	-0.897942
H	4.719347	-1.121933	-1.007222
H	3.826300	-2.545514	-0.408266
H	3.284313	-1.720826	-1.886330
C	3.580511	-0.324429	1.657112
H	3.667410	-1.311591	2.121442
H	4.583086	0.072898	1.467569
H	3.056358	0.335271	2.351761
Ru	0.349916	-1.095312	0.158138
H	0.565375	-1.169031	-1.409597
C	-2.593780	1.313359	2.864791
O	-1.763570	2.007255	2.216380
O	-2.469029	0.107896	3.195162
H	-3.529953	1.825816	3.174107

H	-0.263569	-0.953336	2.010653
H	0.522742	-0.881771	2.072449

TSD2-3

	Coordinates (Angstroms)		
	X	Y	Z

N	0.499947	1.097521	-0.030324
C	-0.914163	-2.819745	-0.291547
O	-1.306777	-3.910993	-0.428102
C	-2.365058	1.593512	-0.077409
H	-3.218577	2.126717	-0.513354
H	-2.395816	1.751333	1.008111
C	2.936148	-0.425805	-0.835033
P	1.970335	-1.751613	-0.036293
P	-2.475920	-0.206201	-0.376633
Si	2.256132	1.275933	-0.379999
Si	-0.709607	2.231191	-0.715760
C	3.061641	1.938295	1.175242
H	4.144106	2.037838	1.031413
H	2.660933	2.928912	1.421324
H	2.893486	1.283299	2.036917
C	2.607215	2.414633	-1.824605
H	2.217751	3.428223	-1.685826
H	3.697183	2.492326	-1.928995
H	2.216676	2.013838	-2.765417
C	-0.426735	3.959865	-0.047692
H	-0.388574	3.947569	1.047924
H	0.507488	4.398606	-0.415503
H	-1.246331	4.625357	-0.346064
C	-0.675206	2.201917	-2.588305
H	-1.660802	2.491027	-2.972641
H	0.055290	2.909325	-2.992487
H	-0.441567	1.204628	-2.975494
H	4.007579	-0.518058	-0.617857
H	2.804389	-0.554353	-1.916946
H	0.413707	1.211386	0.992810
C	-3.236477	-0.372306	-2.030409
H	-3.393858	-1.436020	-2.235791
H	-4.197821	0.149883	-2.077084
H	-2.566913	0.028241	-2.795345
C	-3.804547	-0.818922	0.718114

H	-4.737312	-0.272668	0.542454
H	-3.968901	-1.883201	0.520407
H	-3.505263	-0.699391	1.762257
C	2.468847	-3.294085	-0.877881
H	3.556395	-3.418283	-0.856857
H	2.000228	-4.149117	-0.380721
H	2.125500	-3.265819	-1.915979
C	2.715121	-1.929822	1.623864
H	2.242409	-2.772533	2.137407
H	3.794224	-2.105000	1.558350
H	2.529214	-1.026755	2.211819
Ru	-0.299412	-1.109178	-0.124135
H	-0.115320	-1.037456	-1.745930
C	-0.868325	1.222814	3.398205
O	0.124467	1.726128	2.852031
O	-1.433403	0.118093	3.069120
H	-1.343146	1.739273	4.249109
H	-0.832237	-0.533104	2.168092
H	-0.312235	-1.195287	1.658950

D3

	Coordinates (Angstroms)		
	X	Y	Z

N	0.474250	1.086637	-0.086199
C	-0.835712	-2.877631	-0.253592
O	-1.200558	-3.988447	-0.322446
C	-2.395851	1.494394	-0.062236
H	-3.279138	2.005051	-0.464433
H	-2.393728	1.642238	1.025335
C	2.972031	-0.390343	-0.798361
P	2.012639	-1.703816	0.033213
P	-2.462200	-0.307519	-0.376559
Si	2.218549	1.309540	-0.465900
Si	-0.781963	2.179119	-0.754656
C	3.011407	2.107417	1.032326
H	4.086479	2.245617	0.865862
H	2.571789	3.093436	1.224275
H	2.885402	1.498878	1.934418
C	2.496729	2.368120	-1.984579
H	2.089603	3.379503	-1.881939
H	3.579950	2.463061	-2.133915

H	2.080523	1.911109	-2.887924
C	-0.519964	3.926641	-0.127714
H	-0.460578	3.944896	0.966627
H	0.400814	4.368145	-0.525802
H	-1.354596	4.572141	-0.428467
C	-0.803355	2.134116	-2.627177
H	-1.807054	2.399456	-2.980822
H	-0.101782	2.854753	-3.058037
H	-0.560853	1.139727	-3.015396
H	4.034331	-0.431454	-0.526875
H	2.896525	-0.582923	-1.875974
H	0.403446	1.199267	0.933279
C	-3.285863	-0.471387	-2.001759
H	-3.447409	-1.535132	-2.204093
H	-4.250452	0.046984	-2.011984
H	-2.646650	-0.067442	-2.790402
C	-3.741169	-0.955117	0.758632
H	-4.694873	-0.436729	0.613319
H	-3.880969	-2.024499	0.569129
H	-3.411355	-0.826799	1.792897
C	2.610444	-3.269680	-0.694806
H	3.696386	-3.361127	-0.588552
H	2.128605	-4.113384	-0.190779
H	2.345488	-3.301879	-1.755423
C	2.710360	-1.764426	1.724096
H	2.241305	-2.588128	2.270975
H	3.794804	-1.916662	1.701687
H	2.484493	-0.834139	2.253527
Ru	-0.269936	-1.151175	-0.166100
H	-0.050638	-1.089308	-1.831454
C	-0.815120	1.448380	3.475305
O	0.131158	1.873193	2.831038
O	-1.425989	0.305544	3.259901
H	-1.255518	1.995919	4.317142
H	-1.003297	-0.201882	2.496783
H	-0.392952	-1.099907	1.548026

D4

	Coordinates (Angstroms)		
	X	Y	Z

N	0.168487	1.105637	-0.035839

C	-0.302756	-2.905522	-0.133019
O	-0.442263	-4.068970	-0.119598
C	-2.724410	1.040574	0.307143
H	-3.690114	1.416747	-0.052064
H	-2.753037	1.045040	1.403408
C	2.872122	0.396489	-0.918942
P	2.268076	-1.203943	-0.290869
P	-2.430337	-0.676387	-0.233730
Si	1.753573	1.779149	-0.248630
Si	-1.242006	2.089912	-0.246955
C	2.469754	2.421126	1.376920
H	3.450435	2.889810	1.223760
H	1.801985	3.175385	1.812787
H	2.590843	1.621576	2.116588
C	1.857078	3.202508	-1.487105
H	1.298812	4.087019	-1.157674
H	2.905640	3.504612	-1.608887
H	1.479163	2.908326	-2.473071
C	-1.216181	3.643033	0.824801
H	-1.075303	3.392106	1.883249
H	-0.412598	4.329597	0.531917
H	-2.163928	4.189845	0.734246
C	-1.547543	2.628179	-2.034111
H	-2.606218	2.868609	-2.195146
H	-0.963531	3.519921	-2.289484
H	-1.272592	1.837031	-2.741752
H	3.939487	0.539821	-0.711068
H	2.740787	0.374217	-2.009007
H	0.173506	0.566580	1.762898
H	-1.776131	-0.247987	2.976703
C	-3.205996	-0.774391	-1.885902
H	-3.075994	-1.783808	-2.287572
H	-4.274967	-0.543111	-1.828778
H	-2.722043	-0.069198	-2.567001
C	-3.531420	-1.731082	0.777496
H	-4.563176	-1.365668	0.737835
H	-3.497483	-2.758031	0.399659
H	-3.187791	-1.731916	1.816091
C	3.009909	-2.487024	-1.359922
H	4.099186	-2.382390	-1.399096
H	2.756090	-3.478490	-0.971225
H	2.601131	-2.396700	-2.370493
C	3.143231	-1.455041	1.296631
H	2.846145	-2.419287	1.720377

H	4.228447	-1.443581	1.149022
H	2.868638	-0.670691	2.006472
Ru	-0.087960	-1.083232	-0.174188
C	-0.891025	0.233773	3.410398
H	-1.103911	1.298088	3.571302
H	-0.693409	-0.228967	4.381451
O	0.258680	0.048686	2.600460
H	-0.113161	-1.197121	-1.736364

D5

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.248043	-1.136794	-0.060069
C	0.632473	2.874505	0.194253
O	0.905193	4.008821	0.179071
C	2.618116	-1.342671	-0.338176
H	3.467327	-1.555805	-0.998053
H	2.798049	-1.855637	0.614183
C	-2.774055	-0.007372	-1.024007
P	-2.078628	1.511474	-0.302686
P	2.496082	0.446008	-0.002138
Si	-1.937102	-1.476892	-0.150930
Si	0.945247	-1.941261	-1.013765
C	-2.712873	-1.653314	1.560331
H	-3.807028	-1.587086	1.503076
H	-2.462967	-2.628884	1.994607
H	-2.364794	-0.882949	2.256656
C	-2.413799	-3.031955	-1.110505
H	-2.044396	-3.939744	-0.620142
H	-3.507999	-3.106555	-1.160373
H	-2.034580	-3.021337	-2.139313
C	0.941034	-3.822959	-0.836398
H	0.795799	-4.122118	0.208775
H	0.156237	-4.295507	-1.437151
H	1.902655	-4.234128	-1.170511
C	0.866634	-1.560437	-2.861736
H	1.682355	-2.058648	-3.402009
H	-0.080081	-1.913224	-3.290782
H	0.939038	-0.484192	-3.056056
H	-3.870352	-0.008104	-0.989740
H	-2.462278	-0.036956	-2.076692

H	0.373039	-1.575457	1.625043
H	-0.706019	-2.539160	3.584231
C	3.388428	1.240593	-1.384630
H	3.353910	2.327760	-1.263698
H	4.432712	0.912705	-1.414591
H	2.901174	0.982032	-2.328930
C	3.585613	0.782057	1.426919
H	4.600939	0.417015	1.239133
H	3.616109	1.860359	1.614655
H	3.181321	0.284755	2.313338
C	-2.416824	2.856773	-1.492361
H	-3.488732	2.918176	-1.708266
H	-2.080208	3.811356	-1.075304
H	-1.870222	2.670307	-2.420879
C	-3.188430	1.945370	1.084516
H	-2.843841	2.881827	1.534136
H	-4.218656	2.071846	0.734908
H	-3.161703	1.167043	1.850554
Ru	0.212226	1.078758	0.141442
H	0.314357	1.158446	-1.440475
C	0.084537	-1.778462	3.595110
H	-0.379832	-0.791760	3.725034
H	0.730647	-1.969183	4.457410
O	0.890181	-1.835301	2.433461
H	-0.325254	0.921346	1.996600
H	0.457684	0.804638	2.035601

TSD5-6

	Coordinates (Angstroms)		
	X	Y	Z

N	0.172758	1.179787	0.061406
C	-0.515065	-2.902018	0.160955
O	-0.718892	-4.046909	0.111992
C	-2.574030	1.116408	-0.928906
H	-3.104571	0.995396	-1.880894
H	-3.169314	1.801757	-0.314219
C	2.795411	0.194046	-0.800882
P	2.124892	-1.410484	-0.254868
P	-2.475169	-0.508383	-0.082453
Si	1.890687	1.560350	0.145578
Si	-0.846603	1.845991	-1.213879

C	2.431971	1.564995	1.943487
H	3.525378	1.615650	2.016345
H	2.020469	2.439399	2.461132
H	2.095614	0.670670	2.477775
C	2.371392	3.216502	-0.603647
H	1.867510	4.047240	-0.096637
H	3.452347	3.361168	-0.479220
H	2.150818	3.280172	-1.674836
C	-1.014343	3.718488	-1.100194
H	-1.164765	4.038576	-0.062470
H	-0.138016	4.240849	-1.497654
H	-1.886818	4.047451	-1.679480
C	-0.222514	1.425874	-2.936844
H	-0.890672	1.863135	-3.689960
H	0.777913	1.842405	-3.106131
H	-0.177650	0.346040	-3.111672
H	3.887037	0.230674	-0.704468
H	2.545215	0.305006	-1.864386
H	-0.360594	1.566310	1.095428
H	-1.229584	2.227207	4.130940
C	-3.429140	-1.655490	-1.138051
H	-3.487164	-2.636250	-0.656160
H	-4.442808	-1.274262	-1.299161
H	-2.926205	-1.768678	-2.102415
C	-3.537420	-0.346329	1.394953
H	-4.566230	-0.101900	1.109730
H	-3.530621	-1.287941	1.952323
H	-3.144403	0.447029	2.035312
C	2.522412	-2.597041	-1.584769
H	3.596155	-2.580677	-1.799430
H	2.232965	-3.607928	-1.280909
H	1.966939	-2.332031	-2.488515
C	3.212612	-1.968139	1.103826
H	2.841440	-2.925194	1.483307
H	4.241535	-2.095020	0.751021
H	3.199474	-1.242882	1.921051
Ru	-0.186073	-1.085881	0.172057
H	-0.264897	-1.127043	-1.415990
C	-0.877403	1.532497	3.349363
H	0.167721	1.280230	3.598977
H	-1.460967	0.600501	3.471401
O	-1.011498	2.097390	2.078608
H	0.324013	-0.958773	1.997407
H	-0.472570	-0.896412	2.037592

D6

	Coordinates (Angstroms)		
	X	Y	Z
N	-0.504080	-1.108796	-0.004307
C	1.293982	2.659494	0.150949
O	1.821340	3.695276	0.103245
C	2.247978	-1.890773	-0.337176
H	3.040030	-2.297081	-0.976767
H	2.277418	-2.434583	0.615299
C	-2.646709	0.618598	-1.043281
P	-1.666637	1.948390	-0.271011
P	2.547034	-0.123520	0.016176
Si	-2.275064	-1.015508	-0.175704
Si	0.518681	-2.119323	-1.058472
C	-3.008777	-1.050538	1.547254
H	-4.065761	-0.759480	1.525085
H	-2.947560	-2.062603	1.963560
H	-2.480529	-0.378406	2.230904
C	-3.020521	-2.406062	-1.189779
H	-2.897184	-3.375704	-0.695420
H	-4.097187	-2.223096	-1.298790
H	-2.596042	-2.474067	-2.197300
C	0.077559	-3.939733	-0.933341
H	-0.118577	-4.222484	0.107614
H	-0.801070	-4.199328	-1.532794
H	0.916539	-4.548754	-1.292888
C	0.417896	-1.567377	-2.845674
H	1.058813	-2.208944	-3.463746
H	-0.603845	-1.656853	-3.233635
H	0.742252	-0.531304	-2.981963
H	-3.716235	0.860289	-1.065665
H	-2.298695	0.532121	-2.081304
H	-0.293717	-1.450210	0.987048
H	-1.276630	-2.256626	3.865152
C	3.606401	0.451419	-1.354416
H	3.828100	1.514477	-1.220700
H	4.544095	-0.113003	-1.383882
H	3.077025	0.321783	-2.302788
C	3.661921	-0.079087	1.461201
H	4.576644	-0.650187	1.271270

H	3.920467	0.961183	1.683239
H	3.142589	-0.502452	2.325980
C	-1.703954	3.341250	-1.451184
H	-2.737835	3.609305	-1.691938
H	-1.201194	4.209370	-1.013675
H	-1.178551	3.057970	-2.367108
C	-2.685415	2.579665	1.108816
H	-2.159759	3.414473	1.582523
H	-3.657637	2.929027	0.745265
H	-2.840201	1.801802	1.860133
Ru	0.467943	1.016584	0.165229
H	0.552583	1.035029	-1.416350
C	-0.303350	-1.763702	3.661822
H	-0.490945	-0.674475	3.774307
H	0.356389	-2.040853	4.510024
O	0.238119	-2.103367	2.428414
H	-0.026314	1.133673	2.043172
H	0.677259	0.772269	2.082762

TSD6-7

	Coordinates (Angstroms)		
	X	Y	Z

N	0.443256	1.171131	0.056845
C	-1.122545	-2.689605	-0.127878
O	-1.593682	-3.750829	-0.229940
C	-2.354478	1.810259	0.005765
H	-3.210983	2.299969	-0.471768
H	-2.320339	2.144558	1.050692
C	2.716960	-0.322429	-1.087902
P	1.804985	-1.762866	-0.433869
P	-2.546708	-0.007033	0.004263
Si	2.221039	1.231893	-0.142845
Si	-0.698117	2.267229	-0.773342
C	2.958069	1.250222	1.578356
H	4.039483	1.072951	1.536498
H	2.795098	2.225405	2.052403
H	2.513488	0.486519	2.223843
C	2.826130	2.729398	-1.092845
H	2.664260	3.656546	-0.532884
H	3.906745	2.623666	-1.253122
H	2.359177	2.832843	-2.078144

C	-0.344856	4.070382	-0.393056
H	-0.117489	4.212013	0.670243
H	0.493250	4.460986	-0.978964
H	-1.227362	4.678731	-0.628314
C	-0.665812	1.972377	-2.620775
H	-1.433088	2.585631	-3.109072
H	0.302944	2.253263	-3.049416
H	-0.855528	0.923470	-2.866736
H	3.800777	-0.491401	-1.087209
H	2.399106	-0.192175	-2.130884
H	0.256468	1.278214	1.080187
H	1.091722	1.447381	4.122678
C	-3.577618	-0.357979	-1.461147
H	-3.725401	-1.438380	-1.552128
H	-4.551864	0.134514	-1.377887
H	-3.067755	-0.000875	-2.360254
C	-3.654864	-0.406922	1.399268
H	-4.592028	0.155578	1.335058
H	-3.874314	-1.479593	1.384403
H	-3.148898	-0.167830	2.339013
C	2.004451	-3.075559	-1.687724
H	3.065018	-3.260227	-1.887786
H	1.540789	-3.998804	-1.326473
H	1.506013	-2.774260	-2.612951
C	2.811275	-2.394941	0.956357
H	2.355437	-3.319046	1.325118
H	3.838405	-2.602106	0.638331
H	2.824693	-1.671785	1.774886
Ru	-0.399382	-1.010178	-0.015978
H	-0.479239	-0.945365	-1.615143
C	0.294003	0.711883	3.909619
H	0.795699	-0.278963	3.852412
H	-0.347264	0.677548	4.810987
O	-0.422887	1.006422	2.753886
H	-0.163359	-1.180328	1.832514
H	-0.370450	-0.365206	2.005920

D7

	Coordinates (Angstroms)		
	X	Y	Z

N	0.350785	1.196883	-0.024149

C	-0.830814	-2.821407	0.016577
O	-1.183089	-3.938868	0.035273
C	-2.496849	1.547254	-0.195254
H	-3.374684	1.910688	-0.742851
H	-2.561068	1.947662	0.824933
C	2.798745	-0.155590	-0.994693
P	1.977264	-1.638367	-0.303898
P	-2.512862	-0.282381	-0.079968
Si	2.125435	1.398851	-0.170542
Si	-0.866730	2.146402	-0.930165
C	2.760966	1.579973	1.581853
H	3.857390	1.577265	1.601746
H	2.418355	2.526341	2.017789
H	2.410763	0.768070	2.226635
C	2.631350	2.897516	-1.176263
H	2.373203	3.830546	-0.664013
H	3.721028	2.880483	-1.305875
H	2.184433	2.914622	-2.175705
C	-0.692895	3.979611	-0.566317
H	-0.526679	4.154666	0.503466
H	0.135132	4.434685	-1.119721
H	-1.612015	4.506270	-0.852052
C	-0.734969	1.837018	-2.768986
H	-1.429639	2.498637	-3.301006
H	0.273949	2.051113	-3.139915
H	-0.976894	0.802704	-3.028508
H	3.891050	-0.226363	-0.921502
H	2.538183	-0.112329	-2.060350
H	0.142275	1.380119	0.964588
H	0.164292	2.324136	4.291266
C	-3.493396	-0.804926	-1.533117
H	-3.543037	-1.897898	-1.561192
H	-4.508921	-0.397234	-1.489230
H	-3.002354	-0.457664	-2.446508
C	-3.643866	-0.656688	1.307579
H	-4.615816	-0.171732	1.166976
H	-3.786628	-1.740170	1.375475
H	-3.195420	-0.306256	2.241655
C	2.341011	-2.984753	-1.486330
H	3.419647	-3.100528	-1.635351
H	1.930526	-3.922945	-1.098450
H	1.861196	-2.768161	-2.444503
C	3.005122	-2.124009	1.130534
H	2.597914	-3.046302	1.556709

H	4.045837	-2.294190	0.834708
H	2.972295	-1.351510	1.902270
Ru	-0.292961	-1.085101	-0.013178
H	-0.308193	-1.031279	-1.689338
C	-0.038425	1.278594	4.045700
H	0.916720	0.750290	3.947105
H	-0.608056	0.824992	4.866460
O	-0.776963	1.253411	2.831301
H	-0.182659	-1.013442	1.708764
H	-0.730718	0.346762	2.462017

D8

	Coordinates (Angstroms)		
	X	Y	Z

N	0.079794	1.128185	0.073396
C	-0.188678	-2.891894	0.017850
O	-0.271992	-4.061339	-0.003878
C	-2.757079	0.922315	0.680631
H	-3.772216	1.251870	0.427950
H	-2.674094	0.899501	1.775584
C	2.819862	0.574993	-0.752077
P	2.286063	-1.070129	-0.182992
P	-2.424238	-0.768982	0.087692
Si	1.629746	1.868949	-0.026830
Si	-1.370397	2.052658	0.038173
C	2.285584	2.433499	1.654847
H	3.317376	2.802122	1.585794
H	1.667055	3.250155	2.049033
H	2.265910	1.622468	2.392896
C	1.720545	3.372648	-1.171664
H	1.102407	4.205960	-0.816574
H	2.754214	3.737896	-1.235856
H	1.394218	3.118412	-2.187468
C	-1.339727	3.577648	1.156795
H	-1.143109	3.307500	2.201399
H	-0.573767	4.298535	0.846441
H	-2.307220	4.095817	1.121498
C	-1.837948	2.665975	-1.688993
H	-2.861120	3.063411	-1.713006
H	-1.163089	3.471077	-2.005352
H	-1.768348	1.865792	-2.435551

H	3.880112	0.755674	-0.537512
H	2.688206	0.592470	-1.842253
H	0.160107	-0.620508	2.586870
H	0.102047	-1.368567	2.594874
C	-3.315573	-0.889179	-1.504012
H	-3.180623	-1.891319	-1.922044
H	-4.384620	-0.696579	-1.365345
H	-2.909197	-0.163644	-2.213922
C	-3.393410	-1.883309	1.169449
H	-4.449264	-1.592696	1.187383
H	-3.309244	-2.913103	0.807434
H	-2.990418	-1.839770	2.185805
C	3.058461	-2.281631	-1.312903
H	4.138849	-2.115892	-1.380804
H	2.872046	-3.296906	-0.948897
H	2.615462	-2.182676	-2.308061
C	3.197123	-1.348805	1.380337
H	2.944655	-2.339186	1.771492
H	4.279055	-1.288839	1.220647
H	2.902597	-0.601369	2.121769
Ru	-0.065484	-1.057893	0.013438
H	-0.152552	-1.116299	-1.549117

TSD1-2'

	Coordinates (Angstroms)		
	X	Y	Z

N	0.687623	1.086058	0.171628
C	-1.461762	-2.375952	-0.717905
O	-2.066740	-3.311594	-1.068259
C	-2.019700	2.072759	0.488683
H	-2.782847	2.826991	0.262594
H	-1.937519	1.992008	1.580539
C	2.774977	-0.694245	-0.999512
P	1.594108	-1.937362	-0.376316
P	-2.493545	0.422897	-0.137315
Si	2.431214	1.007532	-0.255720
Si	-0.318481	2.523966	-0.188298
C	3.386417	1.256538	1.335578
H	4.466535	1.199636	1.155798
H	3.166590	2.239710	1.768756
H	3.127592	0.496734	2.081485

C	2.925915	2.282498	-1.533907
H	2.744919	3.313964	-1.214790
H	4.004400	2.176363	-1.709063
H	2.422609	2.118301	-2.492177
C	0.331543	4.024055	0.727029
H	0.410214	3.821792	1.801748
H	1.319719	4.329277	0.365118
H	-0.348040	4.874977	0.594809
C	-0.399118	2.828926	-2.033847
H	-1.313230	3.385455	-2.273212
H	0.449850	3.424867	-2.382388
H	-0.416962	1.890895	-2.598952
H	3.813397	-1.012780	-0.844954
H	2.607111	-0.620787	-2.081829
H	0.639672	0.965440	1.194795
C	-3.388982	0.725437	-1.698838
H	-3.760638	-0.230752	-2.080713
H	-4.234205	1.403213	-1.540764
H	-2.713709	1.153048	-2.444088
C	-3.811589	-0.166888	0.981014
H	-4.629999	0.558732	1.031915
H	-4.197744	-1.124188	0.616673
H	-3.397291	-0.316954	1.981828
C	1.797185	-3.389147	-1.464862
H	2.843794	-3.708686	-1.497632
H	1.181394	-4.213711	-1.092850
H	1.464167	-3.134278	-2.475093
C	2.306961	-2.506397	1.208753
H	1.710230	-3.340018	1.590926
H	3.342027	-2.837716	1.073962
H	2.279002	-1.700935	1.947928
Ru	-0.525338	-0.888230	-0.237252
H	-0.387196	-0.563240	-1.784986
C	-0.461684	-0.761787	3.100039
O	0.163826	0.432977	2.997132
O	-0.777167	-1.415946	2.094421
H	-0.099358	-0.029912	4.083335

D2'

Coordinates (Angstroms)		
X	Y	Z

N	0.699745	1.074338	0.167073
C	-1.492263	-2.359490	-0.721946
O	-2.106148	-3.291100	-1.067922
C	-1.987239	2.076526	0.544279
H	-2.747062	2.846803	0.365154
H	-1.880089	1.953978	1.630347
C	2.763076	-0.729590	-1.010776
P	1.567025	-1.953103	-0.376667
P	-2.492548	0.453068	-0.124737
Si	2.436262	0.983482	-0.284960
Si	-0.294985	2.528473	-0.154196
C	3.418050	1.245413	1.288545
H	4.494900	1.178002	1.093314
H	3.213254	2.235345	1.713661
H	3.165694	0.496214	2.047348
C	2.915296	2.246668	-1.580411
H	2.753748	3.280825	-1.259090
H	3.988506	2.127467	-1.778255
H	2.389204	2.086347	-2.527020
C	0.386181	4.009332	0.770136
H	0.481686	3.795553	1.841244
H	1.371301	4.305948	0.392751
H	-0.285078	4.869689	0.657872
C	-0.402026	2.866355	-1.992657
H	-1.321440	3.424166	-2.207821
H	0.440127	3.471777	-2.341482
H	-0.425073	1.939740	-2.575861
H	3.797380	-1.057951	-0.849197
H	2.599429	-0.667137	-2.094411
H	0.667385	0.933773	1.187136
C	-3.388647	0.812468	-1.673920
H	-3.793604	-0.124101	-2.070012
H	-4.211220	1.513043	-1.496771
H	-2.706863	1.231766	-2.417561
C	-3.819732	-0.140504	0.980719
H	-4.629912	0.593664	1.040566
H	-4.216371	-1.087009	0.599925
H	-3.410497	-0.310923	1.980047
C	1.751836	-3.416500	-1.452739
H	2.795192	-3.746318	-1.487519
H	1.130249	-4.231766	-1.069976
H	1.416244	-3.168128	-2.463721
C	2.275607	-2.516259	1.212117
H	1.647883	-3.312444	1.623217

H	3.293789	-2.895055	1.073508
H	2.292259	-1.691705	1.930077
Ru	-0.540675	-0.880823	-0.244722
H	-0.396090	-0.559391	-1.795646
C	-0.480332	-0.864965	3.155960
O	0.263705	0.304831	2.947653
O	-0.814826	-1.375857	2.069667
H	0.500819	0.657125	3.814661

D3'

	Coordinates (Angstroms)		
	X	Y	Z

N	1.159719	0.660111	0.299931
C	-2.352215	-1.333271	-0.780612
O	-3.328077	-1.882476	-1.111356
C	-0.748257	2.822882	0.561125
H	-1.042622	3.854462	0.333767
H	-0.778894	2.699891	1.651593
C	2.189460	-1.848816	-0.947862
P	0.522979	-2.402098	-0.450218
P	-1.924236	1.617876	-0.148111
Si	2.669301	-0.247101	-0.073186
Si	1.001283	2.419367	-0.012958
C	3.484741	-0.589410	1.577293
H	4.419529	-1.146788	1.445800
H	3.721222	0.351073	2.090068
H	2.832171	-1.175470	2.234289
C	3.831366	0.686940	-1.205342
H	4.157262	1.647921	-0.794309
H	4.727226	0.068127	-1.344192
H	3.394396	0.856853	-2.194410
C	2.221582	3.370359	1.046048
H	2.079308	3.138889	2.108366
H	3.261148	3.142030	0.785207
H	2.076297	4.450084	0.917493
C	1.231389	2.806806	-1.829164
H	0.698197	3.733439	-2.073466
H	2.287240	2.963805	-2.070888
H	0.841547	2.012259	-2.473425
H	2.938066	-2.638210	-0.804968
H	2.135097	-1.634671	-2.022765

H	1.030945	0.550698	1.312099
C	-2.483706	2.355898	-1.721832
H	-3.227416	1.690160	-2.171705
H	-2.930463	3.343110	-1.564193
H	-1.641263	2.441561	-2.412815
C	-3.418239	1.728308	0.898018
H	-3.815094	2.748791	0.903889
H	-4.182919	1.044846	0.515552
H	-3.170317	1.431662	1.921155
C	0.052129	-3.678076	-1.669397
H	0.817069	-4.458933	-1.728665
H	-0.900050	-4.128802	-1.372603
H	-0.073894	-3.213610	-2.651301
C	0.796706	-3.384687	1.067880
H	-0.152197	-3.829636	1.382290
H	1.526305	-4.182590	0.893634
H	1.154466	-2.738963	1.874422
Ru	-0.827007	-0.469904	-0.275443
H	-0.451591	-0.177407	-1.900551
C	-1.169433	-0.776839	1.789010
O	-0.225117	-0.235287	2.644977
O	-2.092659	-1.375829	2.358933
H	-0.476118	-0.449779	3.560148

TSD3'-4'

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.977450	-0.841650	0.232197
C	2.098973	1.807465	-0.654906
O	2.952560	2.528089	-0.975180
C	1.280085	-2.630294	0.492321
H	1.766668	-3.581205	0.245222
H	1.262258	-2.536437	1.585928
C	-2.454435	1.436404	-0.995005
P	-0.939783	2.293359	-0.459081
P	2.218714	-1.207498	-0.154851
Si	-2.623233	-0.235675	-0.129598
Si	-0.502689	-2.526140	-0.119665
C	-3.526840	-0.056904	1.501381
H	-4.528406	0.362102	1.347259
H	-3.637515	-1.033631	1.988172

H	-2.987284	0.599514	2.192598
C	-3.587604	-1.350375	-1.286889
H	-3.753980	-2.353809	-0.881668
H	-4.572801	-0.893870	-1.448429
H	-3.105581	-1.442715	-2.265465
C	-1.548758	-3.723667	0.874292
H	-1.527492	-3.462394	1.939127
H	-2.593988	-3.729408	0.546380
H	-1.161618	-4.745159	0.772320
C	-0.590921	-2.893373	-1.954897
H	0.126038	-3.684451	-2.205607
H	-1.585044	-3.243988	-2.249951
H	-0.345148	-2.011172	-2.555741
H	-3.340034	2.068287	-0.855508
H	-2.344962	1.243894	-2.069872
H	-0.830886	-0.728013	1.271855
C	2.904533	-1.749669	-1.756418
H	3.507422	-0.936647	-2.172487
H	3.531391	-2.638114	-1.629194
H	2.095540	-1.971678	-2.456403
C	3.705518	-1.063231	0.893963
H	4.276756	-1.997280	0.884830
H	4.336067	-0.249576	0.521883
H	3.409342	-0.832279	1.921122
C	-0.640338	3.609419	-1.686367
H	-1.519252	4.254932	-1.783114
H	0.216649	4.213139	-1.371400
H	-0.411440	3.156218	-2.654755
C	-1.423031	3.224280	1.035014
H	-0.574159	3.828296	1.369731
H	-2.273327	3.881926	0.826603
H	-1.688358	2.531269	1.837942
Ru	0.742602	0.649697	-0.200420
H	0.529102	0.391049	-1.820806
C	0.971074	0.974310	1.816303
O	-0.330488	-0.254371	2.808307
O	1.506210	1.541536	2.681890
H	0.314842	-0.804640	3.268327

D4'

	Coordinates (Angstroms)		
	X	Y	Z

N	-1.009170	-0.738542	0.234143
C	2.237880	1.691755	-0.709672
O	3.111099	2.340410	-1.100043
C	1.134758	-2.658333	0.547366
H	1.569004	-3.644600	0.346544
H	1.084108	-2.521447	1.635552
C	-2.282943	1.641250	-1.056283
P	-0.778928	2.380498	-0.357119
P	2.177489	-1.316300	-0.103937
Si	-2.586906	-0.075032	-0.324074
Si	-0.608338	-2.446979	-0.142609
C	-3.735451	0.039737	1.149985
H	-4.724047	0.385114	0.823106
H	-3.859778	-0.937630	1.630460
H	-3.364437	0.743149	1.902734
C	-3.404713	-1.090350	-1.670702
H	-3.623916	-2.121025	-1.373834
H	-4.363274	-0.605621	-1.897911
H	-2.819627	-1.107756	-2.595425
C	-1.786287	-3.600526	0.746928
H	-1.798409	-3.390790	1.822392
H	-2.810035	-3.505777	0.367287
H	-1.477392	-4.643692	0.606090
C	-0.598784	-2.792596	-1.986176
H	0.134950	-3.579796	-2.198594
H	-1.573344	-3.149520	-2.332779
H	-0.326567	-1.909938	-2.574193
H	-3.147341	2.304241	-0.928701
H	-2.103260	1.522121	-2.131936
H	-1.036635	-0.707953	1.298657
C	2.847569	-1.882609	-1.701637
H	3.569281	-1.139379	-2.055206
H	3.350132	-2.848774	-1.590768
H	2.051120	-1.965212	-2.443568
C	3.659512	-1.252002	0.957536
H	4.186668	-2.211273	0.935492
H	4.329516	-0.463420	0.600786
H	3.367697	-1.024178	1.986676
C	-0.355925	3.798821	-1.419655
H	-1.201015	4.491462	-1.486816
H	0.508365	4.323824	-1.001672
H	-0.098510	3.439149	-2.419723
C	-1.304734	3.147570	1.212773

H	-0.460250	3.690892	1.647240
H	-2.136259	3.840596	1.049982
H	-1.610886	2.369709	1.918730
Ru	0.816215	0.634290	-0.143659
H	0.543545	0.376851	-1.753175
C	1.151014	0.983879	1.760877
O	-1.111192	-0.722273	3.013728
O	1.450725	1.276050	2.830614
H	-0.230092	-0.716202	3.401525

TSD4'-5'

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.993998	-0.740732	0.246334
C	2.237912	1.705925	-0.663959
O	3.116504	2.360746	-1.034573
C	1.140080	-2.673802	0.502543
H	1.572155	-3.650941	0.258097
H	1.095314	-2.583254	1.595499
C	-2.296840	1.619579	-1.033465
P	-0.785110	2.377132	-0.376294
P	2.176155	-1.308190	-0.102949
Si	-2.565583	-0.086821	-0.255409
Si	-0.608981	-2.417392	-0.170235
C	-3.686602	0.074018	1.241266
H	-4.669975	0.451260	0.934045
H	-3.834183	-0.899824	1.723258
H	-3.280302	0.762280	1.990157
C	-3.475045	-1.093627	-1.558759
H	-3.687048	-2.123659	-1.254146
H	-4.440189	-0.603195	-1.741846
H	-2.934218	-1.118225	-2.510286
C	-1.761735	-3.622287	0.697047
H	-1.737713	-3.472834	1.782141
H	-2.799809	-3.510102	0.363877
H	-1.460949	-4.656829	0.488619
C	-0.605296	-2.772086	-2.018411
H	0.106678	-3.578400	-2.234913
H	-1.590062	-3.101898	-2.365093
H	-0.311986	-1.896296	-2.607185
H	-3.161528	2.283323	-0.912120

H	-2.130857	1.471681	-2.107900
H	-0.999802	-0.763450	1.473986
C	2.861309	-1.841296	-1.706716
H	3.569663	-1.082324	-2.053400
H	3.380666	-2.799765	-1.605709
H	2.065737	-1.932486	-2.449014
C	3.651965	-1.252446	0.968860
H	4.181447	-2.210445	0.942742
H	4.323309	-0.459239	0.624785
H	3.351728	-1.033357	1.997649
C	-0.368229	3.756799	-1.493376
H	-1.217102	4.441819	-1.586523
H	0.494735	4.302154	-1.099666
H	-0.111206	3.357065	-2.478233
C	-1.291972	3.207964	1.167625
H	-0.437060	3.749212	1.583742
H	-2.110602	3.910813	0.982408
H	-1.614695	2.460575	1.898211
Ru	0.810281	0.638165	-0.127179
H	0.555888	0.384773	-1.741550
C	1.110934	0.983225	1.780806
O	-1.031909	-0.818981	2.770942
O	1.386651	1.277015	2.857651
H	-0.153046	-1.069725	3.074630

D5'

	Coordinates (Angstroms)		
	X	Y	Z

N	0.113201	1.255830	0.120762
C	-0.373294	-2.809334	-0.386432
O	-0.537494	-3.930482	-0.627364
C	-2.745522	1.238622	-0.062574
H	-3.647208	1.471921	-0.640322
H	-2.915266	1.579728	0.966052
C	2.738958	0.592583	-0.980258
P	2.186707	-1.100441	-0.620127
P	-2.455168	-0.559991	-0.021918
Si	1.762949	1.761924	0.159099
Si	-1.164785	2.090764	-0.685455
C	2.478296	1.641760	1.900764
H	3.569547	1.757558	1.884351

H	2.070356	2.438443	2.535152
H	2.246560	0.687093	2.385218
C	2.090926	3.516859	-0.449984
H	1.648506	4.270087	0.211768
H	3.174207	3.694128	-0.474715
H	1.705452	3.682479	-1.462934
C	-1.311986	3.911651	-0.206696
H	-1.192971	4.057168	0.873565
H	-0.569340	4.534685	-0.716884
H	-2.303957	4.289628	-0.487593
C	-1.120967	2.030881	-2.570907
H	-1.969750	2.583516	-2.994335
H	-0.201459	2.497732	-2.947306
H	-1.156627	1.006648	-2.956935
H	3.829926	0.680790	-0.916211
H	2.436877	0.819054	-2.011543
H	-0.449646	1.459341	1.831916
C	-3.350896	-1.211981	-1.472702
H	-3.192612	-2.291648	-1.552006
H	-4.423202	-1.007502	-1.388677
H	-2.961833	-0.736747	-2.377631
C	-3.407844	-1.212904	1.392999
H	-4.465201	-0.939918	1.312656
H	-3.313531	-2.303056	1.422418
H	-2.998804	-0.804472	2.322284
C	2.598413	-2.121061	-2.077163
H	3.664653	-2.037612	-2.311745
H	2.356442	-3.168775	-1.871881
H	2.009179	-1.786780	-2.935099
C	3.335554	-1.743704	0.646229
H	3.055067	-2.773498	0.888702
H	4.365872	-1.729085	0.275585
H	3.274222	-1.144692	1.557971
Ru	-0.116080	-0.991630	-0.048350
H	-0.282283	-0.760468	-1.674036
C	0.126145	-1.255841	1.875209
O	-0.764314	1.599620	2.768370
O	0.278220	-1.510967	2.987694
H	-1.553467	1.053450	2.853448

D6'

Coordinates (Angstroms)

	X	Y	Z
N	-0.438593	1.128088	-0.159742
C	0.981027	-2.724075	-0.150690
O	1.366325	-3.815561	-0.218508
C	-2.898807	-0.242670	0.550936
H	-3.966033	-0.342995	0.319680
H	-2.783551	-0.306181	1.641564
C	2.279033	1.669585	-0.997573
P	2.509966	-0.030230	-0.396919
P	-1.933297	-1.614838	-0.148336
Si	0.729232	2.380476	-0.156026
Si	-2.122109	1.402629	-0.008157
C	1.198482	2.963755	1.583288
H	2.161910	3.489327	1.598543
H	0.439883	3.657230	1.969001
H	1.257108	2.124011	2.286007
C	0.221290	3.919961	-1.126539
H	-0.671191	4.395407	-0.701405
H	1.026560	4.666153	-1.108868
H	0.009709	3.681098	-2.175679
C	-2.577278	2.694447	1.296686
H	-2.121032	2.454911	2.264940
H	-2.245111	3.699026	1.006598
H	-3.664915	2.739182	1.440278
C	-2.952686	1.950496	-1.615869
H	-4.043732	2.007778	-1.508022
H	-2.595601	2.946078	-1.909094
H	-2.729031	1.265391	-2.442268
H	3.191095	2.263756	-0.866952
H	2.063319	1.602722	-2.071927
C	-2.647498	-1.922258	-1.799002
H	-2.152133	-2.786848	-2.250503
H	-3.722571	-2.116697	-1.724100
H	-2.479235	-1.055334	-2.442583
C	-2.393936	-3.112484	0.788850
H	-3.478922	-3.260043	0.780314
H	-1.908914	-3.986975	0.343454
H	-2.048583	-3.012474	1.822115
C	3.605152	-0.873379	-1.588935
H	4.535812	-0.310862	-1.716685
H	3.839762	-1.878904	-1.225656
H	3.096206	-0.960521	-2.552520
C	3.571757	0.117241	1.083211

H	3.770825	-0.881660	1.483068
H	4.521638	0.601385	0.833672
H	3.063772	0.701978	1.854777
Ru	0.351425	-0.967945	-0.075942
H	0.318652	-0.974420	-1.732993
C	0.338251	-0.797334	1.869777
O	0.311580	-0.668901	3.013183

E1

	Coordinates (Angstroms)		
	X	Y	Z

N	0.208137	1.143623	-0.318203
C	-0.037324	-3.026614	-0.236600
O	-0.110606	-4.196591	-0.193921
C	-2.664703	0.780932	-0.412379
H	-3.635822	1.032787	-0.855266
H	-2.735844	0.947432	0.669624
C	3.051870	0.339429	-0.780688
P	2.395045	-1.140604	0.068958
P	-2.244766	-0.982098	-0.666292
Si	1.854170	1.793949	-0.643324
Si	-1.258206	1.849520	-1.071635
C	2.308688	2.879605	0.813715
H	3.292576	3.339333	0.660412
H	1.576559	3.684568	0.948580
H	2.350499	2.301725	1.744194
C	1.933045	2.767131	-2.239706
H	1.276393	3.643788	-2.236516
H	2.962228	3.128105	-2.363705
H	1.692258	2.150700	-3.111617
C	-1.483559	3.622837	-0.508452
H	-1.544210	3.683950	0.584145
H	-0.653999	4.257974	-0.840432
H	-2.408612	4.044335	-0.921008
C	-1.175975	1.751905	-2.940639
H	-2.195368	1.705701	-3.342719
H	-0.692848	2.634688	-3.370056
H	-0.638721	0.861122	-3.281766
H	4.050380	0.600456	-0.407659
H	3.150165	0.079173	-1.841921
H	0.068474	1.255649	0.691721

H	-0.244718	-1.041729	1.359284
C	-2.905426	-1.385471	-2.323841
H	-2.743998	-2.451985	-2.511323
H	-3.976456	-1.167069	-2.392021
H	-2.369197	-0.823008	-3.091655
C	-3.378506	-1.925646	0.414448
H	-4.423866	-1.675804	0.204435
H	-3.225397	-2.996197	0.242825
H	-3.154366	-1.710320	1.462434
C	3.426234	-2.528423	-0.524563
H	4.490903	-2.316274	-0.381543
H	3.165982	-3.437445	0.027200
H	3.227276	-2.699156	-1.586351
C	2.970770	-0.928395	1.793267
H	2.647075	-1.785288	2.391743
H	4.061673	-0.842181	1.840902
H	2.521957	-0.025110	2.216049
Ru	0.069213	-1.214672	-0.302269
H	0.396168	-1.197636	-1.974950
C	-0.954460	1.067168	3.364744
O	-0.460739	1.897509	2.605401
C	-0.098496	0.179614	4.218370
H	-0.162325	0.539412	5.253099
H	-0.478401	-0.846359	4.208827
H	0.941569	0.204347	3.890490
C	-2.441059	0.912442	3.489823
H	-2.730407	-0.017913	2.986334
H	-2.730444	0.811689	4.540498
H	-2.963000	1.752287	3.027537

TSE1-2

	Coordinates (Angstroms)		
	X	Y	Z

N	0.439894	1.216854	0.161119
C	-0.906710	-2.586230	-0.832847
O	-1.302716	-3.663775	-1.065562
C	-2.436562	1.620339	0.267582
H	-3.310338	2.232557	0.012151
H	-2.448773	1.450023	1.351795
C	2.828554	0.059800	-1.193165
P	1.969727	-1.492413	-0.749063

P	-2.486906	-0.015044	-0.543038
Si	2.189869	1.492547	-0.144001
Si	-0.802878	2.468603	-0.146867
C	3.014170	1.535794	1.536969
H	4.104456	1.589905	1.434733
H	2.681128	2.416103	2.100082
H	2.770946	0.650347	2.134205
C	2.553423	3.078233	-1.074084
H	2.160552	3.971296	-0.577295
H	3.644205	3.188634	-1.130647
H	2.173608	3.051740	-2.100424
C	-0.561339	3.908679	1.028534
H	-0.583276	3.559631	2.067960
H	0.394928	4.417533	0.863590
H	-1.360181	4.650633	0.906980
C	-0.752265	3.024116	-1.935189
H	-1.744190	3.376456	-2.242510
H	-0.050955	3.852929	-2.074014
H	-0.458816	2.210838	-2.607534
H	3.918585	-0.048658	-1.130474
H	2.575448	0.275340	-2.238990
H	0.366181	1.027810	1.175837
H	-0.386392	-1.115381	1.279459
C	-3.154213	0.318123	-2.214154
H	-3.274462	-0.635816	-2.737207
H	-4.125768	0.819779	-2.151584
H	-2.462208	0.936528	-2.789757
C	-3.885983	-0.929280	0.198799
H	-4.808883	-0.343421	0.133669
H	-4.019844	-1.869227	-0.346508
H	-3.681337	-1.165575	1.244215
C	2.295017	-2.642974	-2.134515
H	3.369846	-2.748580	-2.314480
H	1.874563	-3.625284	-1.895779
H	1.806638	-2.269229	-3.038317
C	3.031010	-2.204441	0.563527
H	2.577466	-3.117898	0.958518
H	4.019075	-2.440795	0.154286
H	3.155338	-1.491314	1.381061
Ru	-0.304293	-0.909663	-0.461361
H	-0.165242	-0.524619	-2.072995
C	-0.333810	-0.669997	2.907725
O	-0.047866	0.560460	2.939733
C	0.737435	-1.674470	3.278623

H	0.780937	-1.711956	4.376039
H	0.513280	-2.676501	2.906735
H	1.710334	-1.349141	2.909401
C	-1.754951	-1.088623	3.220468
H	-1.990476	-2.080488	2.828856
H	-1.851308	-1.116668	4.314796
H	-2.463604	-0.352490	2.836872

E2

	Coordinates (Angstroms)		
	X	Y	Z

N	0.495310	1.140030	0.098521
C	-0.803744	-2.640235	-0.939277
O	-1.165754	-3.712914	-1.225566
C	-2.374053	1.628782	-0.015908
H	-3.203532	2.256224	-0.363822
H	-2.489056	1.491145	1.066264
C	3.024864	-0.118730	-0.831408
P	2.052395	-1.592722	-0.379159
P	-2.410485	-0.028841	-0.781156
Si	2.250302	1.440474	-0.090935
Si	-0.684735	2.406565	-0.332477
C	2.979885	1.812935	1.594921
H	4.053180	2.020672	1.504611
H	2.501138	2.694055	2.038688
H	2.852459	0.978139	2.292048
C	2.651076	2.853231	-1.256884
H	2.231687	3.812092	-0.934259
H	3.743166	2.964464	-1.276129
H	2.323801	2.654265	-2.282259
C	-0.473494	3.900749	0.779948
H	-0.523319	3.602575	1.834022
H	0.488672	4.399058	0.614296
H	-1.265595	4.637994	0.599643
C	-0.555735	2.883706	-2.143228
H	-1.534105	3.227726	-2.500410
H	0.156334	3.699443	-2.299870
H	-0.249223	2.037074	-2.767355
H	4.082280	-0.234662	-0.563430
H	2.966013	-0.026146	-1.923622
H	0.339662	0.919578	1.148928

H	-1.406174	-0.569972	1.760450
C	-3.005677	0.222387	-2.488927
H	-3.123982	-0.756266	-2.964611
H	-3.967630	0.745172	-2.492580
H	-2.279337	0.798113	-3.067055
C	-3.811554	-0.907345	-0.003152
H	-4.734745	-0.327793	-0.107314
H	-3.942741	-1.881909	-0.483972
H	-3.604401	-1.067991	1.058629
C	2.636542	-2.935273	-1.469787
H	3.719537	-3.067927	-1.380229
H	2.136426	-3.869912	-1.197453
H	2.385918	-2.697130	-2.507500
C	2.703498	-2.085237	1.257665
H	2.262820	-3.043162	1.549581
H	3.792939	-2.189951	1.218458
H	2.436850	-1.337943	2.009797
Ru	-0.229475	-0.953899	-0.529304
H	0.012042	-0.776289	-2.065012
C	-0.952032	-0.413786	2.770063
O	0.089768	0.502919	2.695632
C	-0.478623	-1.801928	3.223159
H	-0.009112	-1.741959	4.214366
H	-1.309380	-2.517661	3.276622
H	0.258698	-2.199082	2.517775
C	-2.089872	0.079200	3.674938
H	-2.933873	-0.621905	3.696007
H	-1.721551	0.202532	4.702586
H	-2.461295	1.052806	3.333044

TSE2-3

	Coordinates (Angstroms)		
	X	Y	Z

N	0.394527	1.150874	0.061189
C	-0.604015	-2.749034	-0.775208
O	-0.879925	-3.866884	-0.976409
C	-2.508024	1.426603	-0.063657
H	-3.373560	1.973269	-0.456342
H	-2.638238	1.327646	1.020812
C	2.993104	0.073930	-0.891487
P	2.159807	-1.453503	-0.354857

P	-2.406660	-0.258084	-0.759282
Si	2.102864	1.581097	-0.166364
Si	-0.867610	2.307562	-0.391068
C	2.863516	2.052270	1.484107
H	3.906458	2.362650	1.344700
H	2.319501	2.892214	1.933213
H	2.849942	1.225528	2.201404
C	2.407965	2.997764	-1.363653
H	1.943045	3.938545	-1.050005
H	3.492052	3.166327	-1.406504
H	2.072514	2.764587	-2.379297
C	-0.781182	3.852649	0.673768
H	-0.820377	3.595080	1.738823
H	0.142877	4.415444	0.496222
H	-1.622906	4.521873	0.455283
C	-0.810659	2.780311	-2.211370
H	-1.811813	3.082666	-2.543155
H	-0.136948	3.623852	-2.391041
H	-0.486053	1.945563	-2.842527
H	4.066291	0.056844	-0.664478
H	2.882451	0.125443	-1.982483
H	0.253303	0.937039	1.225208
H	-1.386636	-0.549794	1.783544
C	-3.024678	-0.129012	-2.473375
H	-3.046026	-1.131191	-2.912669
H	-4.034423	0.293984	-2.493014
H	-2.358870	0.494252	-3.075005
C	-3.730153	-1.219091	0.059135
H	-4.698080	-0.721349	-0.061898
H	-3.781920	-2.218917	-0.383563
H	-3.509558	-1.321859	1.125475
C	2.817471	-2.792916	-1.406641
H	3.911347	-2.819798	-1.366081
H	2.419609	-3.753272	-1.063526
H	2.496860	-2.633608	-2.439983
C	2.895197	-1.824008	1.279291
H	2.554467	-2.805980	1.621264
H	3.988539	-1.829283	1.212785
H	2.582474	-1.076511	2.012928
Ru	-0.163016	-0.999093	-0.479033
H	0.042991	-0.882073	-2.026307
C	-0.888909	-0.301868	2.747199
O	0.093091	0.670992	2.540390
C	-0.297969	-1.619361	3.260637

H	0.221008	-1.463958	4.215951
H	-1.077775	-2.376752	3.411265
H	0.423359	-2.018295	2.539341
C	-1.982657	0.207476	3.689909
H	-2.789472	-0.525322	3.815116
H	-1.555619	0.417685	4.679376
H	-2.419903	1.136867	3.306628

E3

	Coordinates (Angstroms)		
	X	Y	Z

N	0.421888	1.126877	-0.028531
C	-0.625549	-2.668673	-0.859915
O	-0.927945	-3.788221	-1.029111
C	-2.461565	1.504857	-0.048590
H	-3.310144	2.100210	-0.406245
H	-2.616882	1.306406	1.019568
C	3.069671	0.108614	-0.770541
P	2.162666	-1.436526	-0.448169
P	-2.361343	-0.110755	-0.887090
Si	2.108627	1.546998	0.011253
Si	-0.779330	2.361452	-0.242112
C	2.735113	1.815605	1.771650
H	3.802637	2.071194	1.767388
H	2.195383	2.639372	2.256180
H	2.607739	0.923702	2.394579
C	2.579052	3.094877	-0.963861
H	2.122872	4.004293	-0.555598
H	3.668163	3.228769	-0.921339
H	2.295954	3.014236	-2.019420
C	-0.662023	3.716658	1.065559
H	-0.745890	3.297270	2.075437
H	0.291082	4.255640	1.000262
H	-1.465341	4.454312	0.940264
C	-0.741429	3.193141	-1.940599
H	-1.716892	3.636026	-2.178431
H	0.003440	3.996124	-1.972053
H	-0.493287	2.476944	-2.732605
H	4.116761	0.041703	-0.451282
H	3.056769	0.261570	-1.857867
H	0.127669	0.622617	1.756353

H	-1.465212	-0.747730	1.654779
C	-2.882504	0.209944	-2.609651
H	-2.882100	-0.733290	-3.164239
H	-3.886640	0.645705	-2.639111
H	-2.178927	0.893147	-3.091912
C	-3.752909	-1.105364	-0.235934
H	-4.701450	-0.572390	-0.360977
H	-3.804297	-2.059227	-0.770514
H	-3.594649	-1.309288	0.827404
C	2.830611	-2.672831	-1.617552
H	3.918778	-2.749809	-1.521745
H	2.381557	-3.650711	-1.416442
H	2.577821	-2.381725	-2.641103
C	2.812257	-2.030282	1.158142
H	2.401095	-3.021982	1.369746
H	3.905368	-2.095391	1.131053
H	2.513677	-1.351808	1.961708
Ru	-0.143420	-0.918102	-0.589402
H	0.073269	-0.812111	-2.136928
C	-1.071210	-0.660650	2.678422
O	-0.066506	0.353714	2.688595
C	-0.471858	-2.005708	3.067018
H	-0.020574	-1.952746	4.065210
H	-1.244192	-2.782763	3.077011
H	0.299588	-2.303752	2.350798
C	-2.204795	-0.243283	3.603307
H	-3.000679	-0.995371	3.610133
H	-1.832993	-0.127821	4.628853
H	-2.633756	0.712569	3.284806

Table S14. Atomic cartesian coordinates of intermediates and transition states (presented in Å) of $RuH_2(Ph_2PCH_2SiMe_2)_2NH(CO)$.

Ph-A2

	Coordinates (Angstroms)		
	X	Y	Z

N	0.065528	1.920152	0.038766
C	-0.024747	-2.095714	-0.264145
O	-0.062857	-3.259328	-0.383820
C	-2.564748	1.496469	1.158691
H	-3.616041	1.788084	1.250807
H	-2.176214	1.350655	2.175624

C	2.661865	1.552158	-1.230913
P	2.327110	-0.074739	-0.508017
P	-2.318415	-0.105645	0.326980
Si	1.518795	2.776129	-0.318765
Si	-1.414405	2.756901	0.319001
C	2.408143	3.409654	1.223319
H	3.418413	3.767326	0.986281
H	1.855163	4.249231	1.663269
H	2.494564	2.630756	1.989906
C	1.305625	4.259497	-1.467419
H	0.689767	5.045775	-1.014354
H	2.284136	4.702402	-1.695192
H	0.840449	3.968631	-2.416566
C	-1.243869	4.226372	1.491772
H	-0.812186	3.918982	2.451763
H	-0.603513	5.010042	1.068791
H	-2.224282	4.678147	1.691165
C	-2.233061	3.390127	-1.260731
H	-3.257893	3.736818	-1.078033
H	-1.665333	4.235514	-1.668277
H	-2.268011	2.610441	-2.030328
H	3.723244	1.822034	-1.203818
H	2.332423	1.524230	-2.276954
Ru	0.006886	-0.258072	-0.142951
H	-0.269514	-0.259749	-1.678090
C	3.190771	-0.048799	1.106464
C	4.545892	0.282117	1.217155
C	2.455124	-0.328270	2.261087
C	5.150963	0.343241	2.469793
H	5.129527	0.497882	0.325414
C	3.059869	-0.268769	3.516511
H	1.399987	-0.582108	2.172888
C	4.407783	0.070092	3.620812
H	6.202509	0.603014	2.550932
H	2.479604	-0.484131	4.409104
H	4.881935	0.122041	4.596621
C	3.255714	-1.343058	-1.443444
C	3.840297	-1.081322	-2.685037
C	3.350380	-2.631356	-0.899192
C	4.512869	-2.094142	-3.372068
H	3.779223	-0.090101	-3.124651
C	4.024712	-3.638385	-1.582833
H	2.899005	-2.848045	0.066477
C	4.607737	-3.371287	-2.823410

H	4.966558	-1.880353	-4.335550
H	4.096502	-4.630930	-1.147673
H	5.133191	-4.157320	-3.358088
C	-3.040595	-1.358637	1.458616
C	-4.414405	-1.625082	1.496040
C	-2.193386	-2.024435	2.351379
C	-4.929133	-2.543425	2.409636
H	-5.089362	-1.118992	0.810994
C	-2.708611	-2.939247	3.268649
H	-1.123653	-1.830276	2.329174
C	-4.077710	-3.202084	3.297390
H	-5.996477	-2.744516	2.427141
H	-2.039431	-3.450889	3.954349
H	-4.479586	-3.919517	4.007106
C	-3.443784	-0.145334	-1.117013
C	-4.500385	0.754169	-1.285594
C	-3.231761	-1.134837	-2.086284
C	-5.325344	0.673379	-2.407778
H	-4.689378	1.528275	-0.549688
C	-4.063319	-1.224067	-3.199686
H	-2.411134	-1.838512	-1.971921
C	-5.109491	-0.314949	-3.365853
H	-6.135649	1.386268	-2.530214
H	-3.888339	-1.996722	-3.942671
H	-5.751284	-0.376793	-4.239962

Ph-B1

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.125935	-1.371056	-1.520035
C	0.212931	1.648875	1.368526
O	0.348151	2.478252	2.182990
C	2.646431	-1.564948	-0.884869
H	3.695718	-1.683375	-1.172379
H	2.366982	-2.431636	-0.273290
C	-2.576925	0.221651	-1.968332
P	-2.272574	0.650315	-0.222096
P	2.355820	-0.053757	0.100473
Si	-1.712948	-1.409680	-2.356148
Si	1.452278	-1.561591	-2.344402
C	-2.649191	-2.865732	-1.644663

H	-3.653804	-2.929084	-2.079800
H	-2.127983	-3.805017	-1.864974
H	-2.762116	-2.783878	-0.558258
C	-1.565236	-1.551914	-4.215822
H	-1.149049	-2.514982	-4.529052
H	-2.568593	-1.467112	-4.651938
H	-0.954248	-0.750940	-4.645068
C	1.570940	-3.224371	-3.200365
H	1.206942	-4.024847	-2.545274
H	0.994971	-3.254297	-4.131256
H	2.616319	-3.445411	-3.449341
C	1.775494	-0.151085	-3.528988
H	2.854705	-0.047163	-3.695661
H	1.306894	-0.328989	-4.502916
H	1.402234	0.799460	-3.134814
H	-3.637426	0.204232	-2.240732
H	-2.081276	0.989302	-2.573626
H	-0.154793	-2.147280	-0.850871
H	-1.472356	-3.192116	1.365602
Ru	0.043728	0.358971	0.097197
H	0.126085	1.475139	-1.169722
C	-0.443137	-3.563472	1.392338
O	0.208903	-3.840933	0.402532
O	-0.013112	-3.697402	2.637584
H	0.901852	-4.027048	2.641256
H	-0.066914	-0.888444	1.238584
C	-3.491565	-0.360566	0.716459
C	-4.818524	-0.479351	0.281345
C	-3.102062	-1.011616	1.888588
C	-5.727298	-1.258017	0.993000
H	-5.153077	0.033848	-0.616053
C	-4.013705	-1.786403	2.607323
H	-2.075721	-0.920575	2.233285
C	-5.325171	-1.917610	2.156348
H	-6.750191	-1.351054	0.639469
H	-3.693772	-2.290249	3.514942
H	-6.033706	-2.527173	2.709833
C	-2.946096	2.336862	0.039147
C	-3.340852	3.162083	-1.016666
C	-3.033102	2.818813	1.352448
C	-3.817968	4.449476	-0.763888
H	-3.283730	2.811921	-2.042695
C	-3.511465	4.101674	1.603360
H	-2.729928	2.188650	2.185544

C	-3.904676	4.921734	0.543898
H	-4.123095	5.081063	-1.593368
H	-3.576836	4.462310	2.625885
H	-4.277854	5.922997	0.738614
C	3.111447	-0.345519	1.748790
C	3.727631	0.703516	2.440016
C	2.981738	-1.589130	2.377159
C	4.220943	0.507321	3.729676
H	3.829272	1.680611	1.975563
C	3.480006	-1.786310	3.663328
H	2.486017	-2.412683	1.871015
C	4.102276	-0.738766	4.343094
H	4.699043	1.331052	4.251977
H	3.378008	-2.758902	4.136351
H	4.490909	-0.892889	5.345586
C	3.505234	1.178309	-0.631157
C	4.857398	0.860996	-0.821333
C	3.051387	2.451208	-0.981149
C	5.732685	1.796400	-1.365775
H	5.236986	-0.116974	-0.536180
C	3.928991	3.391797	-1.522864
H	2.005664	2.704410	-0.835970
C	5.268585	3.065355	-1.719706
H	6.777608	1.538306	-1.511877
H	3.561479	4.378263	-1.790840
H	5.952578	3.795785	-2.142374

Ph-TSB1-2

	Coordinates (Angstroms)		
	X	Y	Z

N	0.077838	-1.214838	1.754783
C	0.002781	1.292430	-1.573590
O	0.010564	2.003957	-2.500664
C	-2.738492	-0.980880	1.515269
H	-3.728008	-0.754296	1.923514
H	-2.736320	-2.034164	1.206439
C	2.694458	0.101354	1.904854
P	2.345474	0.448616	0.150916
P	-2.334622	0.031607	0.046448
Si	1.735985	-1.448348	2.391843
Si	-1.344114	-0.852136	2.777736

C	2.431162	-2.982522	1.578195
H	3.483973	-3.115910	1.854601
H	1.882366	-3.872834	1.907505
H	2.376528	-2.934197	0.485761
C	1.792599	-1.618453	4.255296
H	1.325167	-2.550681	4.589556
H	2.841622	-1.638418	4.576792
H	1.306541	-0.780957	4.768628
C	-1.631965	-2.179250	4.072132
H	-1.493249	-3.181561	3.649669
H	-0.961864	-2.070598	4.930710
H	-2.661669	-2.111727	4.445383
C	-1.172834	0.829255	3.579882
H	-1.535487	1.628902	2.926353
H	-1.747185	0.860852	4.513703
H	-0.126126	1.046487	3.822759
H	3.762675	0.044945	2.137796
H	2.262904	0.923667	2.487492
H	-0.155918	-2.073982	1.231684
H	0.955395	-2.965621	-1.356824
Ru	0.021896	0.207020	-0.107284
H	0.002204	1.519392	0.895336
C	-0.122359	-2.918015	-1.170518
O	-0.643257	-3.371236	-0.129384
O	-0.791284	-2.949165	-2.357950
H	-1.740898	-3.031968	-2.177318
H	0.012208	-1.301935	-0.993228
C	3.461111	-0.644908	-0.810796
C	4.785078	-0.882012	-0.421106
C	2.979819	-1.232984	-1.983535
C	5.603923	-1.711801	-1.183552
H	5.187127	-0.421699	0.477249
C	3.801654	-2.057576	-2.751713
H	1.954427	-1.046758	-2.292285
C	5.112859	-2.303210	-2.349107
H	6.627536	-1.894908	-0.869674
H	3.413219	-2.509689	-3.659713
H	5.753095	-2.949910	-2.942165
C	3.034040	2.108336	-0.225391
C	3.185716	3.085848	0.762568
C	3.336508	2.431766	-1.554536
C	3.639867	4.362101	0.428900
H	2.953286	2.866420	1.800110
C	3.787427	3.707084	-1.886670

H	3.221053	1.687994	-2.338908
C	3.941046	4.676381	-0.895225
H	3.756024	5.110623	1.207538
H	4.017041	3.942170	-2.921965
H	4.293070	5.670893	-1.153688
C	-3.218533	-0.759189	-1.357770
C	-2.924056	-0.327444	-2.657562
C	-4.163125	-1.775045	-1.179830
C	-3.555824	-0.902985	-3.756462
H	-2.191666	0.457740	-2.818900
C	-4.789538	-2.358922	-2.282179
H	-4.418945	-2.124059	-0.184432
C	-4.486822	-1.926188	-3.571623
H	-3.313521	-0.559491	-4.757977
H	-5.516529	-3.151343	-2.129083
H	-4.971499	-2.383982	-4.429040
C	-3.314354	1.571365	0.268388
C	-4.701184	1.496388	0.459773
C	-2.701748	2.825082	0.220178
C	-5.456786	2.655522	0.611250
H	-5.198051	0.529538	0.487780
C	-3.459931	3.988292	0.367068
H	-1.628588	2.895302	0.074401
C	-4.836202	3.905865	0.564374
H	-6.529873	2.583336	0.763189
H	-2.970384	4.956974	0.325840
H	-5.424905	4.811342	0.680084

Ph-C1

	Coordinates (Angstroms)		
	X	Y	Z

N	0.162384	1.949997	-0.531996
C	-0.120506	-2.110498	0.447186
O	-0.173634	-3.247535	0.715401
C	-2.604595	1.818785	0.214713
H	-3.653628	2.084743	0.049278
H	-2.301753	2.219012	1.189104
C	2.596654	0.763905	-1.751167
P	2.305689	-0.409030	-0.387167
P	-2.337786	0.012699	0.221702
Si	1.693464	2.378017	-1.373707

Si	-1.431672	2.594297	-1.040288
C	2.671665	3.442481	-0.185522
H	3.670509	3.648930	-0.588123
H	2.167463	4.402681	-0.022409
H	2.795459	2.955514	0.788351
C	1.424660	3.248763	-3.007810
H	0.923907	4.216898	-2.906449
H	2.409867	3.430446	-3.456363
H	0.856313	2.629858	-3.709468
C	-1.481764	4.453826	-0.824118
H	-1.231966	4.727319	0.207784
H	-0.777425	4.962786	-1.491078
H	-2.485497	4.839588	-1.040858
C	-1.835574	2.078028	-2.792047
H	-2.923563	2.015329	-2.915636
H	-1.462086	2.806621	-3.518981
H	-1.413942	1.096518	-3.031688
H	3.658771	0.925868	-1.964004
H	2.127119	0.343343	-2.647302
H	0.285602	2.285349	0.428695
H	0.057599	0.160764	1.640830
Ru	-0.018367	-0.344069	0.013341
H	-0.083156	-0.674680	-1.637030
C	-0.098192	2.026078	3.042185
H	-1.126610	1.647950	3.145378
H	0.683389	1.506752	3.617025
O	0.155075	3.025697	2.386223
C	3.510780	0.126603	0.896137
C	4.850782	0.366371	0.561103
C	3.099774	0.305479	2.217208
C	5.752716	0.798508	1.529195
H	5.199810	0.215198	-0.457147
C	4.003345	0.735359	3.190221
H	2.063818	0.113153	2.477871
C	5.329102	0.988563	2.846759
H	6.787687	0.986135	1.258127
H	3.667880	0.873438	4.214272
H	6.033596	1.328803	3.600257
C	3.015044	-2.020624	-0.897560
C	3.343919	-2.312940	-2.223490
C	3.183038	-3.008444	0.082121
C	3.837432	-3.573598	-2.564400
H	3.223068	-1.565270	-3.001207
C	3.676923	-4.264479	-0.258737

H	2.928413	-2.797289	1.118325
C	4.004837	-4.550499	-1.585344
H	4.090115	-3.788106	-3.598862
H	3.802474	-5.021103	0.510472
H	4.389670	-5.530444	-1.852526
C	-3.154626	-0.632067	1.734898
C	-3.292277	-2.019909	1.874514
C	-3.622650	0.201148	2.754106
C	-3.880963	-2.561529	3.013627
H	-2.948315	-2.685496	1.086644
C	-4.211029	-0.342590	3.897564
H	-3.540259	1.279884	2.666992
C	-4.339912	-1.722828	4.031362
H	-3.983793	-3.638719	3.107211
H	-4.571327	0.319087	4.680138
H	-4.798252	-2.145386	4.920730
C	-3.497469	-0.594977	-1.071891
C	-4.865296	-0.302767	-0.974508
C	-3.040280	-1.354143	-2.149463
C	-5.754322	-0.751890	-1.946544
H	-5.242017	0.273816	-0.132722
C	-3.931376	-1.807502	-3.124169
H	-1.981665	-1.583129	-2.230636
C	-5.287425	-1.505429	-3.026258
H	-6.811712	-0.518809	-1.860068
H	-3.561804	-2.396631	-3.958641
H	-5.981968	-1.857508	-3.783633

Ph-TSC1-2

	Coordinates (Angstroms)		
	X	Y	Z

N	0.140439	2.000673	-0.554039
C	-0.093612	-2.014417	0.581977
O	-0.137507	-3.138484	0.899235
C	-2.640308	1.844687	0.086058
H	-3.687771	2.088791	-0.116228
H	-2.363158	2.305456	1.042160
C	2.596911	0.826721	-1.717124
P	2.306505	-0.364925	-0.371300
P	-2.341924	0.051140	0.212840
Si	1.711378	2.441296	-1.306670

Si	-1.441807	2.562920	-1.179727
C	2.656262	3.429562	-0.029581
H	3.678714	3.624604	-0.374401
H	2.170393	4.395786	0.151618
H	2.718864	2.897831	0.926449
C	1.537546	3.388798	-2.910717
H	1.066972	4.368730	-2.783610
H	2.544488	3.555292	-3.314814
H	0.976381	2.824127	-3.662560
C	-1.570316	4.429243	-1.093161
H	-1.292816	4.787912	-0.094625
H	-0.924047	4.924464	-1.825273
H	-2.601123	4.748762	-1.289813
C	-1.742143	1.915674	-2.909202
H	-2.818496	1.800283	-3.084906
H	-1.356839	2.609709	-3.663717
H	-1.270905	0.939140	-3.060792
H	3.657206	0.979154	-1.944369
H	2.110376	0.424759	-2.613231
H	0.188345	2.376636	0.402862
H	0.081723	0.346737	1.678779
Ru	-0.008170	-0.267317	0.067350
H	-0.083236	-0.678757	-1.544856
C	-0.152686	1.809787	2.858742
H	-1.174647	1.430675	2.999754
H	0.634148	1.326328	3.454420
O	0.058516	2.885026	2.281525
C	3.527875	0.092330	0.923011
C	4.856839	0.390046	0.593293
C	3.136276	0.122786	2.262540
C	5.767706	0.737038	1.587382
H	5.190509	0.349127	-0.440051
C	4.049295	0.465401	3.260618
H	2.110071	-0.120585	2.519598
C	5.363970	0.780086	2.923869
H	6.794451	0.971376	1.321385
H	3.730152	0.488211	4.298745
H	6.075218	1.054064	3.697699
C	2.968248	-1.981145	-0.931885
C	3.248149	-2.253520	-2.273209
C	3.149580	-2.990587	0.022864
C	3.707713	-3.515589	-2.653874
H	3.114675	-1.489586	-3.032961
C	3.608583	-4.248551	-0.357886

H	2.933497	-2.794996	1.070778
C	3.888994	-4.514166	-1.699365
H	3.923783	-3.714126	-3.699756
H	3.745355	-5.021708	0.392741
H	4.247323	-5.495186	-1.997815
C	-3.187218	-0.518634	1.740176
C	-3.290650	-1.898696	1.963228
C	-3.709071	0.363228	2.690261
C	-3.898286	-2.385193	3.117047
H	-2.907333	-2.601504	1.227509
C	-4.316112	-0.125681	3.849017
H	-3.654576	1.436620	2.537817
C	-4.410028	-1.498086	4.066383
H	-3.974615	-3.457052	3.275183
H	-4.716377	0.572278	4.578875
H	-4.882263	-1.877923	4.967673
C	-3.439959	-0.677212	-1.070392
C	-4.799256	-0.335431	-1.104136
C	-2.946511	-1.594750	-1.999400
C	-5.642077	-0.886074	-2.065114
H	-5.207803	0.361295	-0.375904
C	-3.792420	-2.151837	-2.960316
H	-1.895604	-1.867496	-1.976588
C	-5.138345	-1.795390	-2.998006
H	-6.692492	-0.610194	-2.084727
H	-3.396029	-2.863764	-3.678725
H	-5.796628	-2.225176	-3.747652

Ph-D1

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.116442	-2.064000	0.165446
C	0.089351	2.024952	-0.599190
O	0.142598	3.149187	-0.902661
C	2.559825	-1.549963	1.045454
H	3.613865	-1.829368	1.140054
H	2.124177	-1.507626	2.051275
C	-2.692571	-1.556108	-1.233560
P	-2.330028	0.100229	-0.561570
P	2.323550	0.083448	0.270379
Si	-1.543600	-2.888988	-0.533500

Si	1.515643	-2.790516	0.078860
C	-2.358072	-3.877716	0.831623
H	-3.295830	-4.327539	0.484370
H	-1.694907	-4.689903	1.153700
H	-2.578880	-3.259669	1.708327
C	-1.076191	-4.008858	-1.956633
H	-0.437376	-4.843244	-1.647796
H	-1.998640	-4.435300	-2.371460
H	-0.575002	-3.462191	-2.762143
C	1.536448	-4.449985	0.945592
H	1.139932	-4.363645	1.964026
H	0.931810	-5.187478	0.404835
H	2.558217	-4.842903	1.012467
C	2.112162	-2.934413	-1.689901
H	3.209101	-2.933458	-1.705316
H	1.775370	-3.866410	-2.154042
H	1.769462	-2.096646	-2.305495
H	-3.756215	-1.811929	-1.169061
H	-2.454751	-1.473222	-2.302136
H	-0.329328	-1.936108	1.173478
Ru	0.000456	0.247010	-0.184694
H	0.180937	-0.064955	-1.729846
C	-0.517886	-0.137608	3.026042
O	-0.762468	-1.361751	2.893388
O	-0.151969	0.667518	2.125746
H	-0.628058	0.298610	4.038189
C	-3.117406	1.257904	-1.744573
C	-4.442888	1.681390	-1.595034
C	-2.383809	1.687913	-2.856373
C	-5.021098	2.528618	-2.539527
H	-5.029485	1.356560	-0.740164
C	-2.965660	2.528065	-3.803778
H	-1.353122	1.367565	-2.982909
C	-4.284292	2.953627	-3.644692
H	-6.048596	2.855927	-2.409358
H	-2.385437	2.856241	-4.661337
H	-4.734693	3.617209	-4.377208
C	-3.308764	0.298961	0.966613
C	-4.129332	-0.700177	1.495053
C	-3.162330	1.504021	1.667888
C	-4.785898	-0.502370	2.711329
H	-4.267205	-1.641108	0.972712
C	-3.823406	1.704442	2.874569
H	-2.514890	2.283938	1.274263

C	-4.633369	0.696724	3.402961
H	-5.417075	-1.289345	3.113837
H	-3.699014	2.642428	3.407738
H	-5.141744	0.847538	4.350924
C	2.984391	1.338691	1.430747
C	3.212071	2.633065	0.944147
C	3.206828	1.070218	2.783578
C	3.661825	3.638089	1.795803
H	3.043008	2.858433	-0.106154
C	3.658444	2.078735	3.636280
H	3.031340	0.078617	3.188735
C	3.886297	3.362731	3.145773
H	3.835846	4.636286	1.404627
H	3.830572	1.857334	4.685616
H	4.236863	4.145904	3.811669
C	3.539657	0.154075	-1.096245
C	4.888357	-0.137246	-0.853536
C	3.140138	0.521483	-2.382875
C	5.818358	-0.076519	-1.887203
H	5.218741	-0.408226	0.146192
C	4.073202	0.586088	-3.418664
H	2.096259	0.749301	-2.577173
C	5.410960	0.284323	-3.173470
H	6.861462	-0.305920	-1.689779
H	3.751650	0.871275	-4.416249
H	6.137878	0.331926	-3.979182

Ph-TSD2-3

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.214745	-1.761600	-0.830971
C	0.197244	2.138368	0.611819
O	0.299646	3.256525	0.920781
C	2.559107	-1.808799	-0.046449
H	3.597332	-2.100777	-0.233840
H	2.226312	-2.294776	0.877824
C	-2.587387	-0.330756	-1.895723
P	-2.299104	0.561721	-0.335852
P	2.356685	-0.011207	0.169580
Si	-1.703721	-1.998073	-1.811756
Si	1.371427	-2.373416	-1.398558

C	-2.752611	-3.280342	-0.941844
H	-3.701058	-3.419030	-1.474570
H	-2.232573	-4.245506	-0.916935
H	-2.983452	-2.994367	0.089636
C	-1.363527	-2.528660	-3.573929
H	-0.814540	-3.473426	-3.643600
H	-2.333596	-2.674807	-4.066767
H	-0.821251	-1.764072	-4.138585
C	1.360375	-4.245242	-1.449143
H	1.056348	-4.655378	-0.479032
H	0.671050	-4.627933	-2.210444
H	2.360832	-4.630525	-1.680844
C	1.839611	-1.631914	-3.053437
H	2.931002	-1.544945	-3.118382
H	1.509049	-2.264505	-3.883179
H	1.417623	-0.630761	-3.189023
H	-3.651631	-0.443975	-2.129917
H	-2.111907	0.245546	-2.697458
H	-0.389448	-2.255353	0.061067
Ru	0.028767	0.398990	0.065143
H	0.131085	0.909802	-1.470584
C	0.082676	-3.069656	2.614417
O	-0.573348	-3.372229	1.605994
O	0.577277	-1.915825	2.877369
H	0.284541	-3.837362	3.380186
H	0.203781	-0.969189	2.099638
H	-0.181738	-0.162818	1.745525
C	-3.497391	-0.230209	0.813322
C	-4.859939	-0.256005	0.482964
C	-3.071804	-0.849563	1.988922
C	-5.773729	-0.901952	1.310239
H	-5.212950	0.229901	-0.423593
C	-3.987510	-1.497902	2.819290
H	-2.021045	-0.833977	2.254341
C	-5.337545	-1.528745	2.480159
H	-6.826679	-0.917274	1.043960
H	-3.639436	-1.979983	3.728230
H	-6.050599	-2.035915	3.123736
C	-3.016772	2.234088	-0.531226
C	-3.494908	2.710293	-1.754093
C	-3.067363	3.064004	0.596737
C	-4.020873	4.000223	-1.847906
H	-3.467886	2.082803	-2.639936
C	-3.595451	4.348036	0.502393

H	-2.693847	2.704236	1.553090
C	-4.073182	4.819369	-0.722175
H	-4.393062	4.360964	-2.802515
H	-3.631984	4.982121	1.383509
H	-4.485758	5.821316	-0.796857
C	3.208170	0.446964	1.728933
C	3.389043	1.809369	2.005429
C	3.653842	-0.499927	2.654157
C	4.002007	2.215386	3.187071
H	3.060528	2.560163	1.290896
C	4.266633	-0.091217	3.840218
H	3.532436	-1.561283	2.463221
C	4.440488	1.264147	4.110276
H	4.139402	3.274217	3.386328
H	4.609252	-0.837422	4.551259
H	4.917848	1.580287	5.033204
C	3.472707	0.738936	-1.078143
C	4.816632	0.344903	-1.131815
C	3.010507	1.712930	-1.964750
C	5.676744	0.901396	-2.073718
H	5.198369	-0.396719	-0.434169
C	3.874230	2.274604	-2.906698
H	1.971777	2.026612	-1.925733
C	5.204728	1.866452	-2.966297
H	6.715146	0.585116	-2.110953
H	3.503357	3.028798	-3.594774
H	5.876109	2.299723	-3.702151

Ph-D5

	Coordinates (Angstroms)		
	X	Y	Z

N	0.090624	-1.563900	1.325549
C	-0.132287	1.450084	-1.457371
O	-0.238465	2.326479	-2.215771
C	-2.765326	-1.442565	1.107733
H	-3.744535	-1.299101	1.574224
H	-2.786103	-2.389906	0.558071
C	2.629581	-0.244760	1.834833
P	2.292982	0.475874	0.205783
P	-2.364574	-0.105274	-0.062012
Si	1.688294	-1.900561	1.874777

Si	-1.310777	-1.550538	2.329413
C	2.577752	-3.120080	0.745062
H	3.652722	-3.147806	0.964896
H	2.181474	-4.132176	0.894703
H	2.459490	-2.866352	-0.314512
C	1.843000	-2.567623	3.631034
H	1.375263	-3.553209	3.734676
H	2.906156	-2.679848	3.880461
H	1.397141	-1.896714	4.374829
C	-1.572386	-3.124667	3.335675
H	-1.379639	-4.021451	2.734782
H	-0.926978	-3.161124	4.220345
H	-2.611267	-3.174447	3.687204
C	-1.424489	-0.092786	3.523674
H	-2.381819	-0.099674	4.061048
H	-0.623606	-0.137449	4.272812
H	-1.338483	0.867171	3.001762
H	3.693983	-0.290289	2.085205
H	2.125205	0.385915	2.577085
H	-0.352877	-3.010238	0.205853
H	0.871471	-4.782057	-0.977061
Ru	-0.002259	0.077293	-0.222295
H	-0.117290	1.137361	0.949397
C	-0.048308	-4.289489	-1.316064
H	0.218662	-3.511640	-2.042295
H	-0.667845	-5.034181	-1.824834
O	-0.803162	-3.774611	-0.235282
H	0.551407	-1.272801	-1.448614
H	-0.238656	-1.319480	-1.504668
C	3.551395	-0.219995	-0.934070
C	4.873675	-0.423056	-0.520852
C	3.198310	-0.519552	-2.252921
C	5.817359	-0.938792	-1.406053
H	5.176177	-0.180615	0.493818
C	4.144649	-1.027529	-3.142614
H	2.179559	-0.353754	-2.592296
C	5.454373	-1.244306	-2.718634
H	6.837935	-1.100073	-1.070978
H	3.856843	-1.254140	-4.165130
H	6.191345	-1.645420	-3.408412
C	2.774233	2.247298	0.248663
C	2.942729	2.938120	1.451573
C	2.915723	2.940272	-0.960980
C	3.250368	4.299832	1.445511

H	2.837155	2.426431	2.403214
C	3.222846	4.298381	-0.965725
H	2.787413	2.421541	-1.907938
C	3.390074	4.982788	0.239267
H	3.381508	4.823021	2.388406
H	3.331528	4.821437	-1.911464
H	3.627455	6.042706	0.236096
C	-3.209899	-0.466069	-1.652910
C	-3.869319	0.537004	-2.370943
C	-3.087816	-1.741567	-2.220543
C	-4.416715	0.264914	-3.625102
H	-3.963210	1.536870	-1.957071
C	-3.639231	-2.012504	-3.470623
H	-2.551237	-2.528695	-1.695128
C	-4.306986	-1.010170	-4.176211
H	-4.928787	1.053683	-4.168818
H	-3.541341	-3.006929	-3.896793
H	-4.736334	-1.221899	-5.151120
C	-3.281580	1.350261	0.573042
C	-4.651598	1.233746	0.849462
C	-2.654469	2.582836	0.767793
C	-5.374205	2.326678	1.318701
H	-5.163571	0.288443	0.688476
C	-3.378974	3.679878	1.236857
H	-1.594527	2.691269	0.564093
C	-4.737918	3.554087	1.514010
H	-6.434607	2.220666	1.528346
H	-2.876523	4.631352	1.384816
H	-5.301322	4.407446	1.880224

Ph-TSD5-6

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.111064	-1.709998	-1.203059
C	0.198188	1.517640	1.417676
O	0.318073	2.438079	2.115476
C	2.745442	-1.455519	-1.144467
H	3.700872	-1.297677	-1.653592
H	2.804672	-2.404563	-0.600423
C	-2.554272	-0.218510	-1.795399
P	-2.258945	0.490254	-0.149725

P	2.385794	-0.124515	0.046273
Si	-1.749612	-1.934464	-1.813369
Si	1.262197	-1.617685	-2.308563
C	-2.708601	-3.111611	-0.711854
H	-3.739711	-3.199174	-1.077140
H	-2.258459	-4.111080	-0.732150
H	-2.750567	-2.779296	0.329629
C	-1.864665	-2.584343	-3.572878
H	-1.472101	-3.604125	-3.653268
H	-2.922427	-2.612648	-3.864421
H	-1.339620	-1.954360	-4.299086
C	1.518057	-3.199893	-3.290611
H	1.348466	-4.082218	-2.662363
H	0.856500	-3.265208	-4.160400
H	2.551064	-3.244197	-3.658583
C	1.175678	-0.162293	-3.491415
H	2.083728	-0.132873	-4.107567
H	0.320028	-0.249457	-4.171376
H	1.095337	0.794103	-2.964695
H	-3.606737	-0.209648	-2.094999
H	-1.985166	0.385204	-2.512885
H	0.166838	-2.649575	-0.483284
H	-0.221118	-5.021608	1.565206
Ru	0.032567	0.066168	0.287443
H	0.105271	1.045222	-0.954684
C	-0.025402	-3.945115	1.414193
H	-0.996707	-3.433485	1.527225
H	0.599961	-3.616818	2.266784
O	0.578820	-3.698532	0.179574
H	-0.429862	-1.096847	1.731287
H	0.352315	-1.212311	1.670557
C	-3.574878	-0.185951	0.933372
C	-4.897312	-0.279873	0.481298
C	-3.269279	-0.590395	2.234671
C	-5.889000	-0.795731	1.311625
H	-5.162001	0.049276	-0.519777
C	-4.263875	-1.098855	3.070308
H	-2.251004	-0.508307	2.603602
C	-5.573315	-1.209214	2.607082
H	-6.909202	-0.873973	0.947192
H	-4.012966	-1.409227	4.080397
H	-6.347594	-1.611483	3.253961
C	-2.706254	2.267553	-0.211162
C	-2.843012	2.958849	-1.417534

C	-2.857025	2.962048	0.996349
C	-3.129814	4.325163	-1.416348
H	-2.730490	2.444429	-2.367007
C	-3.142668	4.324632	0.995691
H	-2.749663	2.440361	1.944682
C	-3.279213	5.010364	-0.212485
H	-3.237784	4.850232	-2.361074
H	-3.258182	4.850112	1.939230
H	-3.500440	6.073763	-0.213641
C	3.278694	-0.513351	1.601667
C	3.900805	0.492938	2.348239
C	3.224624	-1.813648	2.120107
C	4.479383	0.199089	3.582929
H	3.940682	1.511385	1.972339
C	3.804997	-2.105140	3.352478
H	2.718981	-2.605160	1.571955
C	4.436011	-1.099883	4.086475
H	4.963868	0.989159	4.149382
H	3.759220	-3.118491	3.740931
H	4.888858	-1.327662	5.046992
C	3.286170	1.328732	-0.611955
C	4.660757	1.220969	-0.869410
C	2.643449	2.544409	-0.853896
C	5.374455	2.308864	-1.362196
H	5.180653	0.285679	-0.677153
C	3.359641	3.636379	-1.347332
H	1.579457	2.644140	-0.668361
C	4.723854	3.521085	-1.601633
H	6.438480	2.211160	-1.556676
H	2.846768	4.576025	-1.530512
H	5.280538	4.371070	-1.985417

Ph-D6

	Coordinates (Angstroms)		
	X	Y	Z

N	0.083316	-1.652078	1.272906
C	-0.085452	1.300976	-1.667747
O	-0.117937	2.102617	-2.505946
C	-2.739813	-1.392915	1.130590
H	-3.742962	-1.318973	1.559760
H	-2.696009	-2.340064	0.576780

C	2.519820	-0.161265	1.803765
P	2.256873	0.481837	0.124560
P	-2.389116	-0.093928	-0.095534
Si	1.745991	-1.882367	1.875132
Si	-1.315818	-1.489889	2.367524
C	2.607375	-3.089534	0.734076
H	3.686153	-3.100290	0.931329
H	2.222973	-4.101989	0.903954
H	2.458691	-2.844077	-0.322366
C	1.853773	-2.505441	3.637882
H	1.422413	-3.507438	3.737169
H	2.912019	-2.569778	3.921156
H	1.360140	-1.842046	4.356019
C	-1.581260	-3.008985	3.432022
H	-1.427571	-3.929510	2.857363
H	-0.912881	-3.026136	4.298805
H	-2.612027	-3.017968	3.808141
C	-1.134375	0.028201	3.446514
H	-1.974198	0.091803	4.149004
H	-0.216384	-0.035388	4.043583
H	-1.099800	0.955708	2.866988
H	3.563529	-0.125784	2.129933
H	1.925354	0.460403	2.484852
H	-0.140072	-2.498154	0.661223
H	0.838226	-5.079968	-0.971963
Ru	-0.015251	0.009548	-0.350726
H	-0.158650	1.148064	0.746111
C	-0.009515	-4.424332	-1.262091
H	0.423724	-3.669136	-1.952220
H	-0.671556	-5.055247	-1.891280
O	-0.671422	-3.865774	-0.177295
H	0.569053	-1.366403	-1.514236
H	-0.223043	-1.442721	-1.560050
C	-3.438496	-0.499367	-1.546128
C	-4.573262	0.239925	-1.892672
C	-3.090349	-1.617174	-2.316007
C	-5.344304	-0.129952	-2.995723
H	-4.866739	1.106302	-1.307888
C	-3.865622	-1.989887	-3.410321
H	-2.216141	-2.209769	-2.054974
C	-4.993115	-1.243031	-3.756229
H	-6.222336	0.454340	-3.255918
H	-3.587131	-2.862268	-3.994524
H	-5.594487	-1.529445	-4.614255

C	-3.111642	1.454266	0.568060
C	-3.888304	1.477491	1.729932
C	-2.864396	2.660042	-0.102837
C	-4.399822	2.681304	2.216964
H	-4.100503	0.565334	2.276220
C	-3.384871	3.858530	0.375538
H	-2.268666	2.671786	-1.010483
C	-4.151144	3.873322	1.542214
H	-4.992177	2.681225	3.127381
H	-3.186316	4.782622	-0.159383
H	-4.550067	4.809323	1.922117
C	3.586685	-0.232360	-0.912643
C	4.898533	-0.336932	-0.434153
C	3.298467	-0.649907	-2.214262
C	5.897661	-0.879205	-1.238656
H	5.150278	0.004588	0.566006
C	4.301059	-1.184025	-3.023461
H	2.288206	-0.556324	-2.602644
C	5.599781	-1.307026	-2.533445
H	6.909570	-0.967163	-0.854032
H	4.064814	-1.504756	-4.033804
H	6.379975	-1.730243	-3.159448
C	2.690406	2.262844	0.130173
C	2.745485	3.005814	1.312474
C	2.915410	2.906484	-1.093591
C	3.024015	4.372689	1.271759
H	2.576735	2.530707	2.273818
C	3.190174	4.270945	-1.132155
H	2.878096	2.345528	-2.024178
C	3.244705	5.008121	0.051600
H	3.068373	4.937406	2.198557
H	3.360999	4.758326	-2.087629
H	3.458654	6.072524	0.021322

Ph-TSD6-7

	Coordinates (Angstroms)		
	X	Y	Z

N	0.086522	-1.624025	1.378477
C	-0.161920	1.416701	-1.475574
O	-0.246988	2.282341	-2.246856
C	-2.758218	-1.241018	1.378823

H	-3.689966	-0.996036	1.898361
H	-2.902887	-2.222325	0.908979
C	2.614709	-0.241304	1.785688
P	2.281551	0.432671	0.128001
P	-2.384318	-0.079813	0.019990
Si	1.770715	-1.925336	1.893349
Si	-1.267674	-1.437593	2.524212
C	2.499936	-3.169652	0.703794
H	3.581815	-3.259757	0.858554
H	2.053922	-4.155877	0.878646
H	2.327038	-2.898812	-0.342074
C	1.938095	-2.564040	3.645690
H	1.443149	-3.533182	3.770197
H	3.004765	-2.708022	3.860067
H	1.542416	-1.868848	4.393827
C	-1.551471	-2.983183	3.545122
H	-1.482962	-3.884738	2.924924
H	-0.832077	-3.075193	4.364987
H	-2.556221	-2.955594	3.984883
C	-0.965305	0.034251	3.637309
H	-1.773340	0.122042	4.373701
H	-0.029686	-0.091714	4.194813
H	-0.903148	0.972129	3.077073
H	3.679230	-0.259865	2.040168
H	2.099429	0.399681	2.511884
H	-0.174004	-2.385142	0.706168
H	0.594707	-4.776777	-1.062095
Ru	-0.031953	0.070851	-0.230374
H	-0.113958	1.194425	0.904495
C	-0.047043	-4.057388	-1.603667
H	0.630486	-3.480863	-2.270564
H	-0.696310	-4.656800	-2.269151
O	-0.775760	-3.230392	-0.753019
H	0.168788	-1.203252	-1.598544
H	-0.261868	-1.815485	-1.187686
C	-3.401071	-0.633584	-1.399337
C	-4.764375	-0.907331	-1.227795
C	-2.827481	-0.770570	-2.664770
C	-5.538963	-1.316831	-2.309505
H	-5.224378	-0.799046	-0.248442
C	-3.605042	-1.179195	-3.749552
H	-1.770445	-0.566771	-2.805921
C	-4.959343	-1.453147	-3.573140
H	-6.594819	-1.528112	-2.167490

H	-3.148193	-1.286090	-4.729097
H	-5.564661	-1.773086	-4.416452
C	-3.179505	1.512848	0.458665
C	-3.542462	1.836093	1.768829
C	-3.367041	2.463699	-0.553768
C	-4.084805	3.088393	2.061890
H	-3.411193	1.121955	2.574857
C	-3.910375	3.711205	-0.260707
H	-3.093448	2.231586	-1.580182
C	-4.269387	4.028185	1.050595
H	-4.362532	3.324283	3.085153
H	-4.051784	4.437088	-1.056270
H	-4.694097	5.001278	1.279155
C	3.531032	-0.334485	-0.973011
C	4.880754	-0.390881	-0.602078
C	3.141312	-0.848136	-2.211793
C	5.818817	-0.972176	-1.451322
H	5.208496	0.021436	0.348705
C	4.081466	-1.426336	-3.064968
H	2.098012	-0.803832	-2.509632
C	5.419770	-1.494023	-2.683565
H	6.862180	-1.017156	-1.152722
H	3.764542	-1.826022	-4.023890
H	6.152501	-1.947684	-3.344730
C	2.806447	2.188469	0.124240
C	2.983419	2.916383	1.303514
C	2.970467	2.832750	-1.109006
C	3.325188	4.268727	1.250596
H	2.859008	2.441358	2.271735
C	3.310516	4.181880	-1.159929
H	2.831847	2.282430	-2.036790
C	3.488484	4.903908	0.021420
H	3.463873	4.821825	2.175094
H	3.435525	4.669679	-2.122292
H	3.751808	5.956900	-0.018127

Table S15. Atomic cartesian coordinates of intermediates and transition states (presented in Å) of $RuH_2(Me_2PCH_2CMe_2)_2NH(CO)$.

C-A2

Coordinates (Angstroms)		
X	Y	Z

N	-0.011780	1.186854	-0.106217
C	-0.011268	-2.723185	-0.282086
O	-0.013294	-3.867259	-0.551311
C	2.384343	1.002392	-0.704114
H	3.373515	1.462446	-0.600513
H	2.210523	0.827164	-1.773703
C	-2.391010	1.095589	0.634599
P	-2.310992	-0.658590	0.152163
P	2.321442	-0.660804	0.038726
C	-1.782159	2.402606	-1.417199
H	-2.803812	2.798412	-1.365395
H	-1.151642	3.183522	-1.845924
H	-1.776024	1.555828	-2.109860
C	-1.261702	3.224403	0.891000
H	-0.633198	4.032040	0.514111
H	-2.279479	3.624662	0.967295
H	-0.933031	2.969278	1.902800
C	1.306101	3.127964	-1.161613
H	1.032211	2.797905	-2.168958
H	0.655553	3.956230	-0.879735
H	2.325895	3.527833	-1.209144
C	1.730337	2.461752	1.223471
H	2.807075	2.668544	1.231727
H	1.222540	3.385887	1.504185
H	1.518061	1.716911	1.995741
H	-3.383563	1.527523	0.464223
H	-2.226624	1.073831	1.719515
C	3.309573	-0.640458	1.578925
H	3.416910	-1.668643	1.939244
H	4.304172	-0.218355	1.400093
H	2.804112	-0.059988	2.353593
C	3.353358	-1.690133	-1.064814
H	4.350007	-1.253589	-1.192180
H	3.455868	-2.692070	-0.636749
H	2.870494	-1.779399	-2.041919
C	-3.330166	-1.527273	1.393907
H	-4.358355	-1.149710	1.394959
H	-3.341815	-2.598133	1.168453
H	-2.891833	-1.388265	2.386067
C	-3.286407	-0.884363	-1.380164
H	-3.395025	-1.957093	-1.570484
H	-4.281893	-0.438171	-1.282736
H	-2.770802	-0.437439	-2.233287
Ru	-0.003694	-0.916048	0.079199

H	0.006366	-1.331419	1.601184
C	1.278355	1.944969	-0.167223
C	-1.287958	1.970970	-0.015807

C-B1

	Coordinates (Angstroms)		
	X	Y	Z

N	0.233980	1.238686	-0.331454
C	-0.092632	-2.916246	-0.227975
O	-0.167100	-4.085023	-0.161935
C	-2.209267	1.184145	-0.146854
H	-3.152399	1.659642	-0.436339
H	-2.133034	1.249617	0.945677
C	2.666574	0.689819	-0.801902
P	2.311248	-0.887161	0.056687
P	-2.237888	-0.615046	-0.530040
C	2.040709	2.707909	0.562470
H	3.020637	3.155457	0.368896
H	1.327737	3.518367	0.730484
H	2.116527	2.124644	1.484980
C	1.715072	2.646937	-1.915647
H	1.153445	3.581682	-1.879919
H	2.768330	2.909042	-2.060188
H	1.402941	2.067974	-2.787358
C	-1.126265	3.389994	-0.257619
H	-1.052927	3.410891	0.834833
H	-0.358860	4.046930	-0.670334
H	-2.097761	3.809177	-0.539415
C	-1.196732	1.940155	-2.315436
H	-2.261012	2.018103	-2.558693
H	-0.698654	2.784263	-2.792509
H	-0.810320	1.016197	-2.753711
H	3.661926	1.067547	-0.541101
H	2.699501	0.397966	-1.857874
H	0.169209	1.294152	0.685254
H	0.102840	-0.169061	3.779278
C	-3.172557	-0.817072	-2.091893
H	-3.366278	-1.884690	-2.239464
H	-4.129025	-0.285087	-2.052180
H	-2.589382	-0.457859	-2.941509
C	-3.429861	-1.280720	0.686355

H	-4.405195	-0.791715	0.589963
H	-3.554190	-2.354693	0.516267
H	-3.041866	-1.132061	1.697199
C	3.528334	-2.044191	-0.661172
H	4.551121	-1.675194	-0.530979
H	3.431079	-3.014851	-0.165183
H	3.320892	-2.178826	-1.726254
C	2.911324	-0.701892	1.774823
H	2.800878	-1.661557	2.290211
H	3.963240	-0.398272	1.802398
H	2.303529	0.037976	2.301871
Ru	0.030496	-1.100235	-0.320621
H	0.316682	-1.111969	-2.007525
C	-0.543400	0.646703	3.441257
O	-0.137723	1.699449	2.986784
O	-1.823735	0.354030	3.623673
H	-2.378334	1.092696	3.319286
H	-0.235228	-0.927262	1.337254
C	1.621969	1.825538	-0.625005
C	-1.029545	1.949879	-0.788685

C-TSB1-2

	Coordinates (Angstroms)		
	X	Y	Z

N	0.337235	1.309305	-0.002132
C	-0.463959	-2.699764	-0.695738
O	-0.677884	-3.837923	-0.868164
C	-2.095159	1.465197	0.312884
H	-2.985863	2.091357	0.196644
H	-1.975690	1.258752	1.383895
C	2.651946	0.644498	-0.802336
P	2.194158	-1.043954	-0.263913
P	-2.332398	-0.177410	-0.475768
C	2.361977	2.329417	1.043508
H	3.378248	2.697725	0.871831
H	1.769466	3.152648	1.449385
H	2.412223	1.542345	1.800165
C	1.888874	2.901279	-1.339868
H	1.435748	3.848560	-1.043998
H	2.956505	3.088352	-1.494522
H	1.472076	2.584621	-2.297959

C	-0.763314	3.504145	0.657752
H	-0.638127	3.252446	1.716273
H	0.055185	4.160204	0.357438
H	-1.692610	4.073742	0.552840
C	-1.080649	2.604866	-1.675802
H	-2.140815	2.826085	-1.833231
H	-0.523222	3.494352	-1.969344
H	-0.800051	1.784854	-2.342308
H	3.704109	0.856006	-0.580018
H	2.557137	0.593126	-1.893262
H	0.334109	1.151881	1.012449
H	0.496731	-1.461806	2.996071
C	-3.273467	0.070711	-2.025162
H	-3.585187	-0.913334	-2.390971
H	-4.166092	0.680153	-1.848986
H	-2.655255	0.537961	-2.792842
C	-3.587567	-0.992663	0.570778
H	-4.499471	-0.389540	0.636317
H	-3.834917	-1.963934	0.131107
H	-3.183071	-1.159142	1.571544
C	3.155735	-2.118775	-1.383201
H	4.228498	-1.911919	-1.308564
H	2.973991	-3.165307	-1.119628
H	2.822984	-1.960628	-2.412647
C	3.008567	-1.328690	1.348210
H	2.835724	-2.364022	1.658014
H	4.086804	-1.152370	1.273053
H	2.589988	-0.664019	2.107742
Ru	-0.124039	-0.923320	-0.431472
H	0.088734	-0.676129	-2.062986
C	-0.182587	-0.615601	2.861535
O	0.202581	0.571512	2.910376
O	-1.430336	-0.954447	3.302116
H	-1.966293	-0.147403	3.335648
H	-0.330412	-1.010034	1.303817
C	1.767240	1.804720	-0.274109
C	-0.855204	2.232773	-0.202232

C-C1

Coordinates (Angstroms)		
X	Y	Z

N	0.216535	1.268529	-0.107112
C	-0.381859	-2.848137	-0.272462
O	-0.530710	-4.010577	-0.308754
C	-2.184974	1.348353	0.389873
H	-3.123174	1.896126	0.250708
H	-1.974538	1.331465	1.466405
C	2.519437	0.617616	-0.955967
P	2.183293	-0.998982	-0.167532
P	-2.377013	-0.414367	-0.099363
C	2.227002	2.544637	0.632853
H	3.210565	2.928889	0.345091
H	1.612961	3.392075	0.946998
H	2.363966	1.885513	1.495200
C	1.573881	2.716396	-1.773739
H	1.077876	3.671364	-1.595109
H	2.616065	2.936288	-2.027595
H	1.122216	2.229811	-2.640562
C	-0.967114	3.484338	0.293440
H	-0.757924	3.412838	1.366043
H	-0.210501	4.120951	-0.167639
H	-1.933112	3.985576	0.170685
C	-1.399450	2.203768	-1.834574
H	-2.477878	2.360832	-1.935323
H	-0.907917	3.050055	-2.314566
H	-1.133784	1.293668	-2.378954
H	3.565547	0.913453	-0.817794
H	2.382256	0.408947	-2.023040
H	0.290272	1.261634	0.910625
H	-0.172065	-0.990784	1.469703
C	-3.510211	-0.465054	-1.536482
H	-3.762365	-1.512612	-1.732039
H	-4.431943	0.092446	-1.338971
H	-3.022734	-0.061483	-2.425794
C	-3.435275	-1.108456	1.219530
H	-4.389158	-0.574408	1.285622
H	-3.630219	-2.163600	1.003446
H	-2.914478	-1.043669	2.178429
C	3.196036	-2.159615	-1.148002
H	4.249807	-1.861462	-1.151234
H	3.110736	-3.161393	-0.715517
H	2.820683	-2.192960	-2.174429
C	3.047884	-0.989452	1.444193
H	2.930349	-1.970111	1.916479
H	4.114928	-0.776654	1.318889

H	2.604020	-0.239552	2.103374
Ru	-0.139473	-1.040773	-0.226291
H	-0.077635	-0.935515	-1.923173
C	-0.066141	0.184994	3.399162
H	-1.124207	-0.113742	3.452980
H	0.684024	-0.587187	3.628356
O	0.256775	1.343508	3.181281
C	1.591709	1.793774	-0.548870
C	-1.043305	2.087558	-0.345206

C-TSC1-2

	Coordinates (Angstroms)		
	X	Y	Z

N	0.206040	1.288334	-0.031999
C	-0.367431	-2.814502	-0.335356
O	-0.514450	-3.974445	-0.411151
C	-2.201311	1.331007	0.455517
H	-3.141516	1.880205	0.337892
H	-1.995084	1.262124	1.530790
C	2.507050	0.691673	-0.925953
P	2.194369	-0.960735	-0.205245
P	-2.378095	-0.407043	-0.116645
C	2.215216	2.539432	0.757344
H	3.189675	2.952403	0.478758
H	1.591847	3.360258	1.120066
H	2.371612	1.840026	1.583572
C	1.551415	2.823083	-1.633734
H	1.048957	3.764667	-1.408657
H	2.591907	3.062586	-1.876535
H	1.103770	2.376230	-2.523600
C	-0.994027	3.474484	0.466553
H	-0.791991	3.352120	1.535922
H	-0.236557	4.135399	0.042536
H	-1.961068	3.977258	0.360213
C	-1.411393	2.293928	-1.721771
H	-2.490073	2.451291	-1.818596
H	-0.922845	3.163706	-2.160543
H	-1.140402	1.412201	-2.308620
H	3.553089	0.989877	-0.792184
H	2.353254	0.527768	-1.998534
H	0.279998	1.245495	0.987632

H	-0.162048	-1.005725	1.487499
C	-3.480870	-0.407581	-1.578032
H	-3.732457	-1.447866	-1.809972
H	-4.404693	0.146120	-1.379818
H	-2.976182	0.022054	-2.445090
C	-3.456750	-1.166754	1.148172
H	-4.415231	-0.641557	1.217552
H	-3.640381	-2.212347	0.882200
H	-2.959146	-1.141138	2.120714
C	3.178857	-2.073674	-1.266464
H	4.233955	-1.780526	-1.277751
H	3.097300	-3.096513	-0.885640
H	2.781075	-2.049952	-2.284724
C	3.101314	-1.028131	1.381132
H	2.994852	-2.028712	1.812005
H	4.164901	-0.814304	1.231256
H	2.684899	-0.304952	2.086379
Ru	-0.130943	-1.007177	-0.230395
H	-0.065021	-0.866244	-1.906743
C	-0.046799	-0.195960	3.168152
H	-1.086404	-0.525550	3.306213
H	0.730858	-0.945938	3.371853
O	0.232722	1.005328	3.066333
C	1.577206	1.841664	-0.455255
C	-1.059465	2.109097	-0.238266

C-D1

	Coordinates (Angstroms)		
	X	Y	Z

N	0.213602	1.348265	0.001598
C	-0.378955	-2.709746	-0.644915
O	-0.540064	-3.829484	-0.937462
C	-2.209392	1.387363	0.430907
H	-3.142224	1.946464	0.302075
H	-2.041432	1.276931	1.508929
C	2.510126	0.782148	-0.924931
P	2.209894	-0.909737	-0.299618
P	-2.380078	-0.328227	-0.202286
C	2.229664	2.491870	0.907500
H	3.219983	2.898948	0.680492
H	1.616555	3.299442	1.315666

H	2.348302	1.731271	1.684300
C	1.609930	2.979925	-1.459778
H	1.115965	3.908237	-1.171201
H	2.658554	3.222572	-1.660929
H	1.177127	2.614544	-2.392938
C	-0.986273	3.509130	0.586812
H	-0.809765	3.324208	1.651694
H	-0.215449	4.189293	0.222362
H	-1.948139	4.023289	0.487982
C	-1.355298	2.443016	-1.674835
H	-2.428982	2.621627	-1.790015
H	-0.843593	3.323697	-2.062242
H	-1.083658	1.583817	-2.295016
H	3.560484	1.069459	-0.801458
H	2.329415	0.683690	-2.001947
H	0.256426	1.230663	1.022694
C	-3.440331	-0.294520	-1.688994
H	-3.684406	-1.327993	-1.955451
H	-4.368844	0.252580	-1.496044
H	-2.915568	0.162103	-2.530132
C	-3.457831	-1.129126	1.035133
H	-4.410188	-0.597271	1.131588
H	-3.652314	-2.161693	0.729664
H	-2.951747	-1.144816	2.004052
C	3.160002	-1.963951	-1.445858
H	4.214531	-1.670602	-1.473121
H	3.087451	-3.005666	-1.119051
H	2.733230	-1.884453	-2.449523
C	3.117588	-1.089309	1.275757
H	3.032670	-2.125329	1.618110
H	4.176069	-0.842287	1.143175
H	2.687300	-0.439884	2.041848
Ru	-0.124869	-0.937840	-0.270851
H	-0.088745	-0.676763	-1.841326
C	-0.069809	-0.529633	2.987937
O	0.139786	0.701870	2.888510
O	-0.176680	-1.363837	2.044872
H	-0.173363	-0.952854	4.006870
C	-1.040063	2.183888	-0.194013
C	1.595941	1.904771	-0.364664

C-TSD2-3

	Coordinates (Angstroms)		
	X	Y	Z
N	0.215728	1.250616	-0.272195
C	-0.102962	-2.899919	-0.163748
O	-0.183265	-4.064419	-0.190209
C	-2.243494	1.186380	-0.176470
H	-3.174383	1.645239	-0.526418
H	-2.220991	1.290732	0.914651
C	2.638335	0.691565	-0.828825
P	2.338920	-0.891617	0.032045
P	-2.245023	-0.623001	-0.490982
C	2.052162	2.659065	0.635326
H	3.041259	3.091625	0.455863
H	1.352235	3.477519	0.824460
H	2.111891	2.047860	1.540488
C	1.711056	2.702828	-1.836556
H	1.145977	3.633148	-1.775460
H	2.765014	2.975396	-1.953820
H	1.419444	2.158723	-2.736575
C	-1.161226	3.388256	-0.288211
H	-1.148528	3.424426	0.805700
H	-0.370499	4.038929	-0.662962
H	-2.114235	3.805888	-0.629612
C	-1.152053	1.892641	-2.322049
H	-2.208055	1.928841	-2.607004
H	-0.665152	2.742919	-2.799372
H	-0.720986	0.972733	-2.726219
H	3.648766	1.064538	-0.626659
H	2.606979	0.411416	-1.888556
H	0.130155	1.368514	0.742387
C	-3.048484	-0.917175	-2.106547
H	-3.218511	-1.993540	-2.212528
H	-4.010561	-0.397847	-2.166260
H	-2.405544	-0.591258	-2.925567
C	-3.500700	-1.266793	0.668296
H	-4.471374	-0.789211	0.496663
H	-3.603841	-2.345796	0.518648
H	-3.182617	-1.083493	1.696967
C	3.459969	-2.058387	-0.810140
H	4.497950	-1.713485	-0.759949
H	3.383823	-3.037223	-0.327108
H	3.160160	-2.164586	-1.856128
C	3.065304	-0.759793	1.702727

H	2.987120	-1.734361	2.195305
H	4.118122	-0.462011	1.658106
H	2.503789	-0.034779	2.297084
Ru	0.026775	-1.071369	-0.169647
H	0.234568	-1.109108	-1.785845
C	-1.078024	1.115725	3.420492
O	-0.278827	1.845247	2.816550
O	-1.377951	-0.092363	3.104961
H	-1.602458	1.498536	4.312664
H	-0.649403	-0.547302	2.152035
H	0.017903	-0.979190	1.612457
C	-1.039899	1.938670	-0.790727
C	1.610966	1.827552	-0.579228

C-D5

	Coordinates (Angstroms)		
	X	Y	Z
N	-0.240763	1.223418	-0.136310
C	0.552271	-2.789612	0.404598
O	0.761860	-3.936639	0.450665
C	-2.486566	0.533855	-0.829725
H	-3.184415	0.462633	-1.671534
H	-3.025204	1.011217	-0.005043
C	2.193133	1.335286	-0.829204
P	2.446291	-0.337732	-0.133622
P	-2.052353	-1.141480	-0.236138
C	1.382010	2.316009	1.344199
H	2.391329	2.736172	1.426866
H	0.680578	3.029605	1.787703
H	1.343081	1.402098	1.940562
C	0.941365	3.454424	-0.776568
H	0.171008	4.078000	-0.317964
H	1.903012	3.954544	-0.613987
H	0.777793	3.416935	-1.856254
C	-1.889612	2.844147	-1.279896
H	-2.034623	3.266853	-0.280984
H	-1.300996	3.542380	-1.874560
H	-2.873167	2.779677	-1.759287
C	-0.801081	1.063936	-2.633896
H	-1.619531	1.207791	-3.350530
H	0.026686	1.706239	-2.949889

H	-0.465922	0.025815	-2.704199
H	3.117007	1.924437	-0.773349
H	1.957101	1.187852	-1.888931
H	-1.116390	1.619417	1.228221
H	-2.044299	1.989055	3.981952
C	-2.525423	-2.290516	-1.574789
H	-2.277132	-3.316985	-1.287619
H	-3.598827	-2.225688	-1.781365
H	-1.967199	-2.038837	-2.480927
C	-3.288613	-1.501868	1.060812
H	-4.306639	-1.399573	0.669688
H	-3.146052	-2.522013	1.430392
H	-3.150805	-0.804601	1.892585
C	3.385204	-1.247267	-1.409477
H	4.346037	-0.760154	-1.606486
H	3.569218	-2.270238	-1.066992
H	2.803462	-1.290308	-2.334116
C	3.693237	-0.205137	1.200497
H	3.970916	-1.216513	1.515007
H	4.589628	0.312767	0.843193
H	3.288904	0.324018	2.065292
Ru	0.222803	-0.971806	0.227505
H	0.321499	-1.185527	-1.341458
C	-1.451591	1.444567	3.238192
H	-0.390513	1.571492	3.493666
H	-1.698751	0.376692	3.329409
O	-1.757154	1.958882	1.961213
H	0.497617	-0.577806	2.053860
H	-0.291884	-0.713581	2.021425
C	1.008369	2.056276	-0.130304
C	-1.267244	1.419550	-1.207613

C-TSD5-6

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.220574	1.256480	-0.106498
C	0.473947	-2.807185	0.367224
O	0.651848	-3.959683	0.365945
C	-2.482957	0.601118	-0.799094
H	-3.181426	0.543611	-1.641338
H	-3.010605	1.091881	0.024822

C	2.200341	1.269969	-0.855142
P	2.422112	-0.406153	-0.151033
P	-2.093571	-1.085220	-0.200709
C	1.488779	2.263531	1.338367
H	2.520076	2.630287	1.390460
H	0.838975	3.005354	1.811124
H	1.422666	1.344067	1.924406
C	1.028948	3.440882	-0.762451
H	0.279109	4.078714	-0.289342
H	2.004724	3.915158	-0.607992
H	0.851645	3.415367	-1.840204
C	-1.836282	2.900290	-1.261885
H	-1.977942	3.328041	-0.265135
H	-1.226609	3.581597	-1.854896
H	-2.817705	2.855973	-1.747274
C	-0.782191	1.091116	-2.602650
H	-1.602227	1.238235	-3.316050
H	0.048151	1.725786	-2.926053
H	-0.457274	0.049873	-2.668528
H	3.142409	1.831203	-0.826093
H	1.936419	1.122464	-1.907765
H	-0.928438	1.632774	1.060144
H	-1.835058	2.120579	3.928249
C	-2.591302	-2.221961	-1.540734
H	-2.370477	-3.254307	-1.252293
H	-3.661944	-2.129108	-1.750558
H	-2.023751	-1.985282	-2.445099
C	-3.347297	-1.411639	1.088250
H	-4.359184	-1.285332	0.688275
H	-3.232098	-2.434803	1.459114
H	-3.200021	-0.717864	1.921153
C	3.293236	-1.352654	-1.447394
H	4.262658	-0.897866	-1.676578
H	3.453790	-2.378245	-1.100679
H	2.682907	-1.384153	-2.353862
C	3.709103	-0.307852	1.147711
H	3.979665	-1.328368	1.437962
H	4.602473	0.201611	0.771327
H	3.339253	0.213603	2.032220
Ru	0.190756	-0.980705	0.255489
H	0.261463	-1.158241	-1.315571
C	-1.343606	1.497832	3.166929
H	-0.270595	1.470494	3.412586
H	-1.733823	0.472872	3.286645

O	-1.593470	2.024202	1.890591
H	0.517726	-0.690671	2.104600
H	-0.273683	-0.801024	2.097113
C	1.066902	2.037989	-0.128003
C	-1.248557	1.462867	-1.183977

C-D6

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.133436	1.266079	-0.232205
C	0.293040	-2.815949	0.487906
O	0.396323	-3.970673	0.581888
C	-2.473710	0.727825	-0.745608
H	-3.246729	0.734785	-1.521273
H	-2.882286	1.252281	0.124939
C	2.264445	1.062195	-0.966545
P	2.394753	-0.572866	-0.146732
P	-2.168094	-0.994107	-0.191047
C	1.608872	2.283080	1.149001
H	2.660448	2.582720	1.194460
H	1.000062	3.103722	1.539154
H	1.464851	1.423480	1.808307
C	1.252099	3.316290	-1.055051
H	0.565861	4.045592	-0.621556
H	2.263889	3.723198	-0.955751
H	1.047925	3.213867	-2.123077
C	-1.701291	2.970428	-1.329291
H	-1.742314	3.423241	-0.333542
H	-1.076216	3.586266	-1.974856
H	-2.712297	2.994201	-1.748388
C	-0.830290	1.030800	-2.652182
H	-1.666175	1.200947	-3.339008
H	0.027527	1.590879	-3.033099
H	-0.579961	-0.032087	-2.673206
H	3.238757	1.563009	-0.984072
H	1.982036	0.858983	-2.005507
H	-0.563856	1.570016	0.667329
H	-0.466945	3.029682	3.607275
C	-2.718367	-2.077985	-1.551614
H	-2.536589	-3.122640	-1.280655
H	-3.785466	-1.936700	-1.751290

H	-2.146983	-1.848942	-2.455020
C	-3.423899	-1.285521	1.100766
H	-4.430049	-1.088695	0.716098
H	-3.363149	-2.326270	1.433343
H	-3.224423	-0.630083	1.953136
C	3.218591	-1.641515	-1.374664
H	4.202980	-1.241590	-1.639132
H	3.340996	-2.644870	-0.955055
H	2.600684	-1.712616	-2.273460
C	3.669380	-0.444521	1.157368
H	3.847970	-1.445447	1.562878
H	4.605740	-0.053325	0.745795
H	3.334707	0.201022	1.971121
Ru	0.126986	-0.992579	0.260229
H	0.208654	-1.268923	-1.297224
C	-0.964038	2.049724	3.439929
H	-0.178103	1.285118	3.628204
H	-1.688205	1.940089	4.275247
O	-1.555472	1.935608	2.191590
H	0.422112	-0.615799	2.102501
H	-0.375200	-0.669566	2.071718
C	1.212555	1.976242	-0.304623
C	-1.229102	1.500656	-1.252410

C-TSD6-7

	Coordinates (Angstroms)		
	X	Y	Z

N	0.088647	1.328001	-0.136452
C	-0.236559	-2.803645	0.239109
O	-0.350729	-3.961915	0.297891
C	-2.326093	1.292417	-0.541059
H	-3.126130	1.553066	-1.241908
H	-2.573936	1.759394	0.419726
C	2.398699	0.779580	-0.954842
P	2.239075	-0.930415	-0.301234
P	-2.328908	-0.518435	-0.234700
C	1.996766	1.887214	1.283544
H	3.080474	2.031459	1.330727
H	1.515353	2.738165	1.776896
H	1.740226	0.989017	1.849346
C	1.805138	3.176415	-0.805719

H	1.288847	3.974548	-0.270020
H	2.878979	3.373079	-0.723103
H	1.549404	3.225127	-1.866291
C	-1.174206	3.413741	-0.917574
H	-1.085522	3.733277	0.126287
H	-0.473516	3.984748	-1.525630
H	-2.180132	3.675126	-1.261183
C	-0.732403	1.520824	-2.506820
H	-1.554193	1.900982	-3.122661
H	0.193266	1.970653	-2.875380
H	-0.662753	0.440406	-2.650446
H	3.447803	1.095981	-0.954217
H	2.065853	0.736584	-1.998370
H	-0.240019	1.551588	0.815098
H	0.284472	2.199286	3.905184
C	-3.099140	-1.282695	-1.703606
H	-3.126910	-2.368294	-1.566666
H	-4.118499	-0.910154	-1.848069
H	-2.502427	-1.060418	-2.591912
C	-3.604253	-0.752195	1.050955
H	-4.556085	-0.308754	0.740199
H	-3.747894	-1.823069	1.224364
H	-3.270934	-0.286658	1.982054
C	2.883417	-1.980237	-1.648375
H	3.931526	-1.744665	-1.861289
H	2.808133	-3.032094	-1.356216
H	2.285502	-1.826693	-2.550175
C	3.519534	-1.157670	0.987525
H	3.596102	-2.228075	1.204746
H	4.492786	-0.796762	0.638519
H	3.249705	-0.641096	1.910205
Ru	-0.062279	-0.977713	0.100674
H	-0.055809	-1.173129	-1.485791
C	-0.310725	1.269389	3.817389
H	0.412457	0.433384	3.951587
H	-0.974530	1.239474	4.703014
O	-1.006865	1.179444	2.618516
H	0.116466	-0.829788	1.948448
H	-0.402677	-0.147497	2.005952
C	1.539087	1.798918	-0.181030
C	-0.985494	1.885891	-1.044460

Table S16. Atomic cartesian coordinates of intermediates and transition states (presented in Å) of

$RuH_2(Me_2PCH_2SiMe_2)_2NH(CO)$ in toluene.

A1

	Coordinates (Angstroms)		
	X	Y	Z
N	-0.479816	1.184956	-0.413508
C	1.066332	-2.682316	0.165684
O	1.507082	-3.751820	0.320503
C	2.357150	1.688949	-0.699769
H	3.242043	2.282447	-0.438026
H	2.264210	1.702123	-1.793732
C	-2.819942	-0.304819	0.722749
P	-1.833172	-1.708121	0.073817
P	2.528712	-0.067360	-0.190142
Si	-2.211118	1.336265	0.019003
Si	0.763274	2.393401	0.018571
C	-3.112449	1.762232	-1.570604
H	-4.193225	1.843040	-1.406628
H	-2.762648	2.722185	-1.969645
H	-2.951278	1.002381	-2.344122
C	-2.516706	2.657554	1.313319
H	-2.195116	3.656991	1.002768
H	-3.597094	2.707322	1.499309
H	-2.035619	2.414828	2.265786
C	0.389570	4.031406	-0.824598
H	0.270489	3.897771	-1.906390
H	-0.527537	4.492928	-0.441661
H	1.205802	4.747263	-0.668516
C	0.879838	2.593954	1.874763
H	1.876077	2.963984	2.145038
H	0.151340	3.315270	2.257767
H	0.723984	1.634157	2.378340
H	-3.896528	-0.446575	0.562582
H	-2.643230	-0.282143	1.805160
H	-0.441192	1.062890	-1.427077
H	0.377884	-1.114503	-1.767157
C	3.527170	0.008545	1.343584
H	3.693874	-1.012553	1.699951
H	4.494236	0.498089	1.183307
H	2.969623	0.539073	2.119440
C	3.729385	-0.771927	-1.380078
H	4.658720	-0.192538	-1.409762

H	3.958745	-1.803946	-1.096388
H	3.273333	-0.792348	-2.373006
C	-2.247079	-3.106118	1.181025
H	-3.329784	-3.245876	1.268472
H	-1.800682	-4.024643	0.787443
H	-1.818236	-2.916998	2.168530
C	-2.713552	-2.178044	-1.465052
H	-2.229441	-3.061787	-1.890999
H	-3.772056	-2.395231	-1.283354
H	-2.627888	-1.374131	-2.201010
Ru	0.391623	-1.003519	-0.062617
H	0.330258	-0.724353	1.611974

TSA2-1

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.224312	1.209499	-0.275413
C	0.490681	-2.875418	-0.149615
O	0.675240	-4.021893	-0.222265
C	2.633651	1.197715	-0.685624
H	3.610915	1.634273	-0.447639
H	2.542201	1.161729	-1.779243
C	-2.800556	0.282308	0.785565
P	-2.131629	-1.318949	0.219507
P	2.487146	-0.522780	-0.086528
Si	-1.867355	1.713959	-0.048375
Si	1.167430	2.209565	-0.026432
C	-2.671014	2.119494	-1.702858
H	-3.748880	2.299909	-1.609874
H	-2.216835	3.023393	-2.127704
H	-2.522500	1.313588	-2.431059
C	-2.059270	3.207691	1.083869
H	-1.615737	4.115985	0.661251
H	-3.125216	3.412756	1.245658
H	-1.604929	3.031236	2.065125
C	1.108538	3.823786	-0.997658
H	0.923509	3.634152	-2.061506
H	0.321586	4.495524	-0.635860
H	2.059939	4.364016	-0.913475
C	1.446788	2.607762	1.795916
H	2.494229	2.860641	2.002349

H	0.837612	3.463671	2.109219
H	1.169048	1.756300	2.427905
H	-3.889774	0.335123	0.664454
H	-2.578900	0.348739	1.859045
H	-0.098492	0.272802	-1.348415
H	0.015375	-0.579072	-1.836029
C	3.382328	-0.540410	1.508802
H	3.358186	-1.554407	1.918208
H	4.423486	-0.222252	1.388586
H	2.880916	0.119272	2.220603
C	3.592714	-1.508963	-1.162491
H	4.588367	-1.057527	-1.227111
H	3.686729	-2.524082	-0.764428
H	3.159236	-1.574014	-2.164206
C	-2.730597	-2.560942	1.421832
H	-3.817400	-2.503592	1.544033
H	-2.460695	-3.565176	1.080388
H	-2.245437	-2.388867	2.386135
C	-3.105689	-1.724718	-1.277427
H	-2.756175	-2.678820	-1.683312
H	-4.176355	-1.796913	-1.057660
H	-2.947341	-0.958282	-2.040575
Ru	0.189893	-1.063867	-0.044933
H	0.287054	-1.194553	1.568946

A2

	Coordinates (Angstroms)		
	X	Y	Z

N	0.107820	1.087524	-0.060114
C	-0.313743	-2.855812	-0.328007
O	-0.454841	-3.988290	-0.569713
C	2.865828	0.421278	-0.709193
H	3.922712	0.603063	-0.479812
H	2.765650	0.348096	-1.800240
C	-2.684825	1.009542	0.772619
P	-2.419289	-0.706679	0.221669
P	2.261057	-1.154174	-0.017133
Si	-1.305110	2.077142	0.012814
Si	1.681728	1.792481	-0.126791
C	-1.853336	2.682995	-1.691080
H	-2.850904	3.138946	-1.664115

H	-1.155120	3.439450	-2.069883
H	-1.869644	1.867072	-2.422760
C	-1.141229	3.608357	1.108467
H	-0.410410	4.325690	0.716811
H	-2.103487	4.132270	1.174947
H	-0.838056	3.341072	2.127401
C	1.826657	3.216255	-1.360715
H	1.509220	2.907975	-2.363704
H	1.218913	4.080463	-1.066911
H	2.865834	3.562720	-1.430303
C	2.284946	2.442817	1.543365
H	3.368019	2.619589	1.544222
H	1.798178	3.394044	1.789294
H	2.053063	1.742368	2.353415
H	-3.702866	1.362410	0.568957
H	-2.534227	1.024161	1.859821
C	3.064750	-1.281940	1.622337
H	2.811910	-2.247526	2.069501
H	4.153454	-1.194318	1.541635
H	2.687621	-0.497488	2.282451
C	3.105146	-2.477843	-0.963300
H	4.188216	-2.316722	-0.987447
H	2.899248	-3.450003	-0.504720
H	2.722237	-2.496462	-1.987684
C	-3.351738	-1.774521	1.378423
H	-4.403733	-1.476189	1.437633
H	-3.289867	-2.816492	1.049384
H	-2.900667	-1.704862	2.372002
C	-3.396098	-0.853319	-1.322995
H	-3.295025	-1.867470	-1.721709
H	-4.456405	-0.640251	-1.149901
H	-3.011449	-0.154847	-2.071340
Ru	-0.102557	-1.052893	0.012044
H	-0.083248	-1.494577	1.509754

A3

	Coordinates (Angstroms)		
	X	Y	Z

N	0.691320	1.076500	0.116519
C	-1.299848	-2.526607	-0.709822
O	-1.857185	-3.525797	-0.937852

C	-2.064562	1.972952	0.116046
H	-2.821441	2.693722	-0.216723
H	-2.096534	1.950280	1.213062
C	2.918864	-0.739499	-0.737222
P	1.665978	-1.962398	-0.193225
P	-2.418988	0.271837	-0.483093
Si	2.460435	0.996769	-0.157446
Si	-0.319282	2.452195	-0.412637
C	3.278903	1.381247	1.486409
H	4.371014	1.381900	1.390217
H	2.973584	2.367202	1.856683
H	3.014696	0.644088	2.252579
C	3.032091	2.207266	-1.468136
H	2.845224	3.254130	-1.207136
H	4.116026	2.089507	-1.590989
H	2.571289	2.002215	-2.439415
C	0.199309	4.019423	0.484367
H	0.163289	3.887162	1.571928
H	1.218455	4.320834	0.216697
H	-0.466309	4.852950	0.229206
C	-0.226137	2.686241	-2.267679
H	-1.148416	3.159286	-2.625585
H	0.603854	3.337444	-2.557812
H	-0.115018	1.724545	-2.778950
H	3.934002	-1.020633	-0.428458
H	2.890072	-0.738989	-1.833869
H	0.548607	0.980182	1.124136
H	-0.660028	-1.072328	1.318816
C	-3.195235	0.527051	-2.123136
H	-3.488893	-0.449875	-2.519770
H	-4.078567	1.172902	-2.067263
H	-2.467319	0.955075	-2.816037
C	-3.853809	-0.273424	0.516678
H	-4.665502	0.461363	0.486420
H	-4.222293	-1.230059	0.132910
H	-3.534972	-0.429643	1.550031
C	2.022619	-3.455491	-1.189878
H	3.075878	-3.745575	-1.113166
H	1.397833	-4.284358	-0.843148
H	1.772401	-3.253819	-2.234734
C	2.257711	-2.467356	1.467446
H	1.579049	-3.226775	1.866641
H	3.277248	-2.867884	1.436564
H	2.225553	-1.610307	2.146101

Ru	-0.435332	-0.955687	-0.364849
H	-0.115920	-0.689672	-2.010977
C	-0.935982	0.126267	3.509782
O	-0.101118	0.897159	3.234141
O	-1.774950	-0.593320	3.872032

TSA3-4

	Coordinates (Angstroms)		
	X	Y	Z

N	0.768217	1.040486	0.206649
C	-1.635919	-2.219838	-0.868782
O	-2.305908	-3.121384	-1.178944
C	-1.861942	2.197603	0.541917
H	-2.565657	3.019751	0.363071
H	-1.802242	2.043739	1.627041
C	2.741764	-0.855069	-1.012652
P	1.406952	-2.012246	-0.527183
P	-2.438350	0.620896	-0.198260
Si	2.500284	0.833378	-0.203853
Si	-0.121289	2.564018	-0.082978
C	3.461406	0.939826	1.402979
H	4.535094	0.806439	1.226114
H	3.318963	1.913911	1.885746
H	3.146487	0.170472	2.116549
C	3.108355	2.127593	-1.415055
H	3.024133	3.152177	-1.038169
H	4.171866	1.937902	-1.607846
H	2.587015	2.063713	-2.375177
C	0.625223	3.947564	0.943992
H	0.626350	3.687146	2.009042
H	1.659082	4.164464	0.652043
H	0.051817	4.875320	0.829775
C	-0.139155	2.996621	-1.903940
H	-1.009263	3.626052	-2.125949
H	0.751356	3.557492	-2.203077
H	-0.205436	2.092607	-2.518165
H	3.739005	-1.269912	-0.817743
H	2.644871	-0.714345	-2.096407
H	0.680661	0.848296	1.209786
H	-0.717057	-1.079339	1.291775
C	-3.333823	1.123679	-1.713736

H	-3.754663	0.227971	-2.180854
H	-4.141232	1.831468	-1.496731
H	-2.634090	1.568353	-2.425346
C	-3.805025	0.075333	0.890525
H	-4.577032	0.846466	0.985806
H	-4.256253	-0.835469	0.484941
H	-3.399028	-0.162933	1.877124
C	1.537309	-3.391430	-1.722329
H	2.558452	-3.783773	-1.774032
H	0.861087	-4.198894	-1.425440
H	1.230265	-3.036867	-2.709900
C	2.033726	-2.779556	1.016187
H	1.298448	-3.506603	1.372277
H	2.996735	-3.279797	0.865248
H	2.145530	-2.014547	1.790511
Ru	-0.587508	-0.795058	-0.403498
H	-0.382789	-0.389466	-2.015137
C	-0.384140	-0.803471	3.124061
O	0.158043	0.248907	3.096018
O	-0.856042	-1.791158	3.549022

A4

	Coordinates (Angstroms)		
	X	Y	Z

N	0.781553	0.984312	0.176456
C	-1.605463	-2.290925	-0.767774
O	-2.260739	-3.192410	-1.090481
C	-1.840477	2.208065	0.394617
H	-2.522315	3.032430	0.153609
H	-1.816099	2.102513	1.487178
C	2.781433	-0.948839	-0.890619
P	1.454180	-2.071257	-0.336397
P	-2.421505	0.613743	-0.286991
Si	2.528363	0.781152	-0.163943
Si	-0.073036	2.511297	-0.191024
C	3.442505	0.970180	1.457556
H	4.520117	0.821025	1.322256
H	3.289710	1.971628	1.876234
H	3.089600	0.253210	2.205996
C	3.175911	2.002723	-1.430392
H	3.080210	3.047399	-1.117213

H	4.245457	1.805300	-1.576521
H	2.688719	1.884291	-2.403396
C	0.667267	3.935331	0.776961
H	0.645855	3.723785	1.851970
H	1.707064	4.133190	0.493553
H	0.100320	4.858606	0.607312
C	-0.054918	2.851994	-2.035820
H	-0.904515	3.491019	-2.305038
H	0.853677	3.375030	-2.348415
H	-0.132129	1.924550	-2.613322
H	3.778252	-1.353435	-0.675507
H	2.684706	-0.865830	-1.980746
H	0.679140	0.848789	1.214192
H	-0.599543	-1.076793	1.655786
C	-3.221770	1.016851	-1.879607
H	-3.652519	0.101943	-2.297470
H	-4.014915	1.761050	-1.752070
H	-2.481910	1.394060	-2.589526
C	-3.823724	0.107581	0.768480
H	-4.573313	0.902823	0.836153
H	-4.290500	-0.790891	0.353034
H	-3.451077	-0.133797	1.768653
C	1.597078	-3.564616	-1.378035
H	2.609724	-3.978710	-1.340555
H	0.889174	-4.321674	-1.027532
H	1.345188	-3.313581	-2.412120
C	1.997408	-2.655897	1.310215
H	1.282424	-3.395990	1.681684
H	2.994212	-3.107140	1.267533
H	2.005702	-1.822750	2.018510
Ru	-0.555813	-0.840692	-0.328150
H	-0.385916	-0.624706	-1.882918
C	-0.674429	-0.494888	2.673211
O	0.185745	0.401764	2.821601
O	-1.573662	-0.909861	3.401346

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	Coordinates (Angstroms)		
	X	Y	Z

N	0.471829	1.132137	0.129693
C	-1.091493	-2.623323	-0.398811

O	-1.568238	-3.671443	-0.555171
C	-2.302646	1.879688	-0.023459
H	-3.103188	2.431817	-0.529178
H	-2.363609	2.109737	1.047409
C	2.847875	-0.222989	-0.955632
P	1.854158	-1.692868	-0.540786
P	-2.499406	0.077266	-0.223776
Si	2.216025	1.225707	0.100584
Si	-0.554822	2.337576	-0.605746
C	2.908006	1.063330	1.844812
H	3.993796	0.908246	1.824118
H	2.713699	1.976284	2.419709
H	2.462824	0.236419	2.407873
C	2.940521	2.799342	-0.640978
H	2.749303	3.674649	-0.011350
H	4.028954	2.687104	-0.723100
H	2.557148	3.008999	-1.645927
C	-0.226237	4.095241	-0.011905
H	-0.049843	4.123362	1.069803
H	0.634900	4.554032	-0.508388
H	-1.098086	4.728149	-0.220529
C	-0.486749	2.315273	-2.488051
H	-1.255276	2.965863	-2.923718
H	0.485216	2.672600	-2.849629
H	-0.628317	1.302719	-2.881822
H	3.924922	-0.410193	-0.867515
H	2.630616	0.021787	-2.003922
H	0.055901	1.121529	1.562224
H	-0.053883	-0.949476	2.013934
C	-3.409168	-0.119477	-1.797693
H	-3.557992	-1.183803	-2.002885
H	-4.383296	0.378184	-1.752012
H	-2.824671	0.309453	-2.615822
C	-3.725293	-0.460721	1.022868
H	-4.655255	0.110901	0.937468
H	-3.940916	-1.524803	0.882735
H	-3.313873	-0.327902	2.027577
C	2.101400	-2.886880	-1.904771
H	3.166564	-3.070602	-2.079871
H	1.610295	-3.834106	-1.661236
H	1.647400	-2.492543	-2.817666
C	2.743775	-2.505250	0.839376
H	2.218930	-3.426120	1.111130
H	3.773172	-2.750848	0.557277

H	2.766010	-1.858247	1.719342
Ru	-0.357496	-0.936857	-0.200895
H	-0.395332	-0.849908	-1.756487
C	-0.435885	-0.266339	2.826839
O	-0.315533	1.001800	2.571074
O	-0.882708	-0.756086	3.842488

A5

	Coordinates (Angstroms)		
	X	Y	Z

N	0.553930	1.004998	0.048695
C	-1.306880	-2.577217	-0.535882
O	-1.830976	-3.600791	-0.708342
C	-2.177041	1.897740	0.413765
H	-2.974105	2.609343	0.168831
H	-2.111845	1.833860	1.507829
C	2.810647	-0.549687	-1.057164
P	1.697616	-1.853438	-0.449060
P	-2.531069	0.224143	-0.220227
Si	2.260158	1.118171	-0.325155
Si	-0.466592	2.394320	-0.239438
C	3.266864	1.477898	1.225328
H	4.332041	1.585529	0.986154
H	2.935387	2.413629	1.691468
H	3.171580	0.692005	1.982015
C	2.730212	2.420049	-1.606732
H	2.503328	3.443120	-1.287764
H	3.813655	2.368606	-1.775397
H	2.239989	2.246107	-2.570611
C	0.090306	3.914912	0.721821
H	0.173940	3.696968	1.792692
H	1.060110	4.293535	0.379222
H	-0.635228	4.729799	0.605038
C	-0.641052	2.856103	-2.061070
H	-1.584175	3.388237	-2.237248
H	0.168604	3.517813	-2.386442
H	-0.624446	1.969075	-2.704249
H	3.865582	-0.784903	-0.870331
H	2.664319	-0.493177	-2.143482
H	0.504023	0.877513	1.630081
H	-0.469351	-0.975250	2.025868

C	-3.420414	0.475940	-1.797431
H	-3.679948	-0.499487	-2.219170
H	-4.335479	1.058642	-1.648897
H	-2.774689	0.991661	-2.511665
C	-3.834592	-0.459154	0.869933
H	-4.682283	0.229905	0.945671
H	-4.186002	-1.418137	0.476693
H	-3.424593	-0.629308	1.870067
C	2.005273	-3.323838	-1.490500
H	3.075771	-3.546324	-1.547665
H	1.480986	-4.189475	-1.074550
H	1.619380	-3.141858	-2.497228
C	2.405928	-2.351816	1.166707
H	1.795528	-3.149017	1.601633
H	3.434739	-2.710815	1.056140
H	2.402621	-1.507302	1.861436
Ru	-0.469311	-0.941702	-0.322422
H	-0.501114	-0.861639	-1.878096
C	-0.209143	-0.363036	2.925756
O	0.408710	0.758002	2.668762
O	-0.504599	-0.767409	4.028840

B1

	Coordinates (Angstroms)		
	X	Y	Z

N	0.522688	1.105452	-0.084699
C	-0.959043	-2.805655	-0.438616
O	-1.363665	-3.894114	-0.556464
C	-2.329715	1.596967	-0.006978
H	-3.202552	2.171994	-0.339873
H	-2.276428	1.672612	1.086800
C	2.953030	-0.488176	-0.815631
P	1.898664	-1.759461	-0.023615
P	-2.470020	-0.185405	-0.424406
Si	2.261729	1.239756	-0.488978
Si	-0.702100	2.249623	-0.700716
C	3.115476	2.019674	0.988964
H	4.190114	2.134915	0.804512
H	2.701759	3.013293	1.196741
H	2.992906	1.418982	1.896473
C	2.567121	2.277874	-2.018998

H	2.223174	3.312295	-1.915330
H	3.649743	2.310714	-2.195615
H	2.104467	1.841351	-2.909376
C	-0.377445	3.970352	-0.021129
H	-0.294816	3.949857	1.071510
H	0.549462	4.397676	-0.421043
H	-1.192647	4.655645	-0.283783
C	-0.747781	2.274582	-2.573235
H	-1.743318	2.587704	-2.910606
H	-0.027172	2.983365	-2.992080
H	-0.543317	1.282076	-2.987159
H	4.006405	-0.576938	-0.520204
H	2.889978	-0.668205	-1.895726
H	0.463414	1.163238	0.938224
H	0.218269	-0.399174	3.504261
C	-3.352116	-0.208963	-2.030629
H	-3.556371	-1.251518	-2.293837
H	-4.297804	0.342939	-1.990967
H	-2.712085	0.207248	-2.811443
C	-3.760107	-0.830695	0.705004
H	-4.696841	-0.269883	0.615186
H	-3.949831	-1.883442	0.472231
H	-3.392212	-0.777939	1.732766
C	2.457454	-3.344263	-0.748531
H	3.540374	-3.473354	-0.648270
H	1.951227	-4.174363	-0.245953
H	2.182799	-3.368726	-1.806542
C	2.580890	-1.858802	1.677483
H	2.039522	-2.629395	2.234017
H	3.651506	-2.092922	1.678354
H	2.426441	-0.902762	2.186721
Ru	-0.328419	-1.101418	-0.276838
H	-0.049623	-1.000036	-1.951809
C	-0.286110	0.570710	3.501944
O	0.101507	1.556176	2.909974
O	-1.379564	0.545118	4.259235
H	-1.793374	1.422570	4.228440
H	-0.562168	-1.052973	1.403342

TSB1-2

	Coordinates (Angstroms)		
	X	Y	Z

N	0.668502	1.068491	0.135714
C	-1.340802	-2.481333	-0.735741
O	-1.898479	-3.475219	-0.979363
C	-2.082456	1.951830	0.358118
H	-2.860084	2.691028	0.130768
H	-2.037223	1.843601	1.449131
C	2.855871	-0.666495	-0.924199
P	1.654485	-1.908597	-0.325162
P	-2.467111	0.300007	-0.342213
Si	2.415953	1.046949	-0.258525
Si	-0.368978	2.469785	-0.238593
C	3.346983	1.402638	1.327993
H	4.430578	1.336307	1.175005
H	3.119294	2.410569	1.694746
H	3.063736	0.700721	2.119144
C	2.881917	2.298569	-1.574860
H	2.670736	3.333524	-1.286237
H	3.963694	2.224197	-1.744287
H	2.388087	2.095471	-2.530193
C	0.197515	3.978517	0.724563
H	0.253712	3.760802	1.797415
H	1.186050	4.323639	0.400475
H	-0.500977	4.813125	0.588660
C	-0.405622	2.818974	-2.079689
H	-1.347629	3.314132	-2.343945
H	0.406726	3.483418	-2.388417
H	-0.333690	1.890920	-2.656184
H	3.891572	-0.948412	-0.696218
H	2.747627	-0.634469	-2.015319
H	0.622689	0.933910	1.163750
H	0.036312	-1.624353	3.070259
C	-3.328757	0.656728	-1.917405
H	-3.632309	-0.292242	-2.369805
H	-4.215958	1.280466	-1.763029
H	-2.647117	1.151517	-2.612712
C	-3.821762	-0.354370	0.698665
H	-4.643849	0.364149	0.786288
H	-4.203607	-1.281443	0.259700
H	-3.421894	-0.587342	1.689203
C	1.969029	-3.394597	-1.344647
H	3.028674	-3.670608	-1.328776
H	1.376076	-4.233743	-0.968605
H	1.659642	-3.192002	-2.373493

C	2.327705	-2.402892	1.306317
H	1.709150	-3.205136	1.720139
H	3.361590	-2.756388	1.227369
H	2.289903	-1.553858	1.995480
Ru	-0.468026	-0.914620	-0.367138
H	-0.231610	-0.634628	-1.987243
C	-0.306479	-0.597201	2.918246
O	0.462413	0.380075	2.884613
O	-1.570903	-0.457073	3.415227
H	-1.723849	0.494597	3.496698
H	-0.663797	-1.017506	1.366618

B2

	Coordinates (Angstroms)		
	X	Y	Z

N	0.624195	1.037486	0.110686
C	-1.275543	-2.564699	-0.622998
O	-1.800636	-3.575272	-0.853654
C	-2.136800	1.891277	0.335605
H	-2.928309	2.612134	0.098771
H	-2.087690	1.777131	1.426329
C	2.870921	-0.612848	-0.919414
P	1.726711	-1.878370	-0.275895
P	-2.488439	0.228649	-0.334863
Si	2.363740	1.097959	-0.281655
Si	-0.427776	2.422105	-0.259895
C	3.309603	1.528986	1.275670
H	4.392372	1.488017	1.107177
H	3.058235	2.542588	1.609946
H	3.048812	0.850765	2.093971
C	2.797108	2.326730	-1.634463
H	2.568721	3.363714	-1.366840
H	3.879935	2.269878	-1.805212
H	2.304110	2.096823	-2.584185
C	0.117503	3.949017	0.685422
H	0.197903	3.730688	1.756131
H	1.089487	4.321695	0.342374
H	-0.607042	4.763207	0.561774
C	-0.489674	2.772951	-2.106219
H	-1.446356	3.242302	-2.365105
H	0.301858	3.459745	-2.420352

H	-0.393377	1.852253	-2.691585
H	3.917483	-0.853800	-0.695200
H	2.753921	-0.608364	-2.010529
H	0.592909	0.916116	1.204198
H	0.042833	-1.379267	3.292118
C	-3.296683	0.499838	-1.953101
H	-3.583552	-0.471330	-2.367797
H	-4.191525	1.123042	-1.852288
H	-2.602406	0.970328	-2.652363
C	-3.846423	-0.433319	0.692544
H	-4.690428	0.264144	0.720524
H	-4.186108	-1.392370	0.289350
H	-3.462739	-0.585100	1.705649
C	2.081819	-3.394318	-1.232536
H	3.153767	-3.617776	-1.231141
H	1.541254	-4.241416	-0.799751
H	1.739477	-3.260984	-2.262360
C	2.378387	-2.270573	1.388105
H	1.805847	-3.100003	1.813796
H	3.436656	-2.549726	1.347266
H	2.253985	-1.401840	2.042037
Ru	-0.440031	-0.953249	-0.308135
H	-0.310307	-0.807191	-1.876479
C	-0.316604	-0.510066	2.706215
O	0.508615	0.510341	2.662832
O	-1.632713	-0.178684	3.192816
H	-1.479919	0.613105	3.722044
H	-0.559179	-0.991950	1.669009

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	Coordinates (Angstroms)		
	X	Y	Z

N	0.598242	1.027718	0.104142
C	-1.228525	-2.603366	-0.577397
O	-1.732999	-3.628823	-0.789611
C	-2.176281	1.851535	0.314054
H	-2.974955	2.557251	0.056915
H	-2.137167	1.752506	1.406479
C	2.880030	-0.576667	-0.913457
P	1.760812	-1.854990	-0.257086
P	-2.493642	0.175252	-0.334212

Si	2.322294	1.129498	-0.297221
Si	-0.464553	2.388775	-0.276013
C	3.292599	1.606370	1.235185
H	4.371127	1.611926	1.036290
H	3.007488	2.609093	1.575332
H	3.087399	0.920671	2.062839
C	2.741349	2.345387	-1.670005
H	2.505303	3.383985	-1.414937
H	3.823995	2.295762	-1.844885
H	2.245347	2.099958	-2.614405
C	0.050582	3.937488	0.655920
H	0.137075	3.731087	1.728521
H	1.015006	4.325975	0.308401
H	-0.689152	4.737036	0.525636
C	-0.549572	2.751182	-2.122965
H	-1.512626	3.214108	-2.370484
H	0.233229	3.446129	-2.441541
H	-0.449744	1.835503	-2.715794
H	3.930930	-0.791574	-0.683029
H	2.766083	-0.588252	-2.004888
H	0.572189	0.900820	1.296903
H	0.077746	-1.222466	3.386329
C	-3.301988	0.404222	-1.958912
H	-3.548898	-0.579642	-2.369270
H	-4.220064	0.994164	-1.867299
H	-2.621629	0.897321	-2.656255
C	-3.841932	-0.503844	0.696476
H	-4.701659	0.174701	0.711243
H	-4.158199	-1.475783	0.305175
H	-3.463395	-0.632576	1.714458
C	2.138196	-3.379098	-1.192744
H	3.213983	-3.583355	-1.194407
H	1.615108	-4.229479	-0.744972
H	1.788027	-3.267334	-2.222552
C	2.418177	-2.216186	1.412603
H	1.855195	-3.044255	1.853543
H	3.479387	-2.484488	1.374444
H	2.288316	-1.337437	2.051396
Ru	-0.421875	-0.969019	-0.294164
H	-0.310507	-0.856012	-1.858747
C	-0.305319	-0.433519	2.713215
O	0.528279	0.591942	2.577317
O	-1.616555	-0.060138	3.166885
H	-1.459978	0.657917	3.791216

H	-0.539784	-0.995070	1.738737

B3

	Coordinates (Angstroms)		
	X	Y	Z

N	0.524123	1.002259	-0.025752
C	-1.108908	-2.678742	-0.480670
O	-1.573818	-3.740622	-0.593920
C	-2.265225	1.740454	0.273180
H	-3.089095	2.412829	0.006066
H	-2.248800	1.626382	1.364728
C	2.917481	-0.449608	-0.931102
P	1.850576	-1.778874	-0.296465
P	-2.483079	0.065902	-0.411002
Si	2.225625	1.214998	-0.321675
Si	-0.552383	2.345607	-0.269061
C	3.168007	1.722407	1.231861
H	4.228476	1.893847	1.007513
H	2.762995	2.652874	1.648013
H	3.106648	0.964346	2.019377
C	2.671438	2.482856	-1.648864
H	2.414899	3.508253	-1.358628
H	3.756425	2.457551	-1.814776
H	2.185143	2.268115	-2.606520
C	-0.093460	3.842362	0.784419
H	-0.028113	3.578317	1.846177
H	0.870999	4.270131	0.484593
H	-0.845131	4.635500	0.682691
C	-0.680563	2.929803	-2.064301
H	-1.638985	3.433740	-2.242518
H	0.111603	3.644640	-2.311508
H	-0.601182	2.093165	-2.767456
H	3.974099	-0.607277	-0.682032
H	2.821753	-0.464867	-2.024427
H	0.527576	0.873095	1.811957
H	0.025535	-1.069645	3.749420
C	-3.239980	0.303173	-2.060862
H	-3.408008	-0.675927	-2.519202
H	-4.193888	0.836001	-1.986198
H	-2.563399	0.867332	-2.706749
C	-3.848159	-0.694414	0.542339

H	-4.735280	-0.051682	0.539399
H	-4.108955	-1.664970	0.109133
H	-3.516684	-0.844557	1.573449
C	2.296085	-3.288248	-1.227951
H	3.376345	-3.465882	-1.202095
H	1.780761	-4.154531	-0.801810
H	1.972548	-3.177635	-2.266564
C	2.503066	-2.128914	1.381026
H	1.963990	-2.978727	1.811136
H	3.573198	-2.360937	1.354129
H	2.342762	-1.261046	2.027245
Ru	-0.367281	-0.990435	-0.342560
H	-0.308533	-1.017136	-1.900705
C	-0.342564	-0.439915	2.929525
O	0.529045	0.615650	2.772988
O	-1.673038	-0.037690	3.186072
H	-1.664116	0.510027	3.978996
H	-0.412757	-1.067854	2.019662

B4

	Coordinates (Angstroms)		
	X	Y	Z

N	0.025953	1.146263	-0.010004
C	-0.040399	-2.836644	-0.418157
O	-0.039023	-4.001031	-0.420107
C	-2.807232	0.748797	0.468775
H	-3.837178	1.063031	0.262241
H	-2.712062	0.608562	1.553555
C	2.710598	0.834815	-1.146879
P	2.313190	-0.864761	-0.636904
P	-2.394352	-0.836044	-0.332361
Si	1.516658	2.015273	-0.253883
Si	-1.485278	2.006356	-0.058922
C	2.292590	2.576801	1.368127
H	3.263303	3.057605	1.193260
H	1.646675	3.309402	1.866923
H	2.440784	1.752902	2.073748
C	1.381013	3.546049	-1.351183
H	0.747702	4.326975	-0.915393
H	2.379699	3.981424	-1.486391
H	0.987656	3.304950	-2.344769

C	-1.556792	3.451265	1.148436
H	-1.318865	3.123909	2.166757
H	-0.854423	4.248368	0.878222
H	-2.559991	3.895466	1.163038
C	-1.933310	2.649722	-1.779642
H	-3.016611	2.787237	-1.885262
H	-1.464189	3.620233	-1.974884
H	-1.599743	1.960310	-2.563310
H	3.771016	1.074525	-1.003187
H	2.489994	0.903987	-2.219787
H	0.123606	0.787220	1.920514
C	-3.254381	-0.789601	-1.946737
H	-3.108947	-1.746837	-2.455932
H	-4.326765	-0.609837	-1.816823
H	-2.830851	-0.003384	-2.575377
C	-3.341512	-2.123644	0.563626
H	-4.404941	-1.867347	0.612973
H	-3.229697	-3.085991	0.054743
H	-2.953965	-2.232296	1.580605
C	3.120897	-1.974102	-1.844803
H	4.187831	-1.746579	-1.939302
H	3.003308	-3.015280	-1.528919
H	2.639802	-1.857251	-2.819628
C	3.310489	-1.135808	0.877014
H	3.204855	-2.172772	1.211252
H	4.370785	-0.937546	0.687223
H	2.967556	-0.479476	1.681245
Ru	-0.030330	-0.986222	-0.413578
H	-0.109020	-1.158432	-1.961106
H	-1.133495	-0.953755	2.399884
C	-0.350368	-0.677580	3.125562
H	-0.768382	-0.699260	4.134503
O	0.110088	0.609807	2.887293
O	0.661091	-1.661737	3.114437
H	0.888722	-1.857591	2.197271

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	Coordinates (Angstroms)		
	X	Y	Z

N	0.305117	1.186196	0.098958
C	-0.882793	-2.739066	-0.407289

O	-1.236380	-3.837323	-0.548023
C	-2.528519	1.578446	0.358879
H	-3.457891	2.069818	0.049290
H	-2.397447	1.721541	1.438792
C	2.679440	0.080653	-1.266003
P	1.908019	-1.479920	-0.718792
P	-2.566047	-0.218970	0.049973
Si	2.018654	1.504746	-0.205689
Si	-0.969121	2.281155	-0.447442
C	2.957821	1.565850	1.414727
H	4.024017	1.745493	1.228845
H	2.582672	2.373526	2.052743
H	2.857030	0.633836	1.977129
C	2.378531	3.104458	-1.130410
H	2.157876	3.986744	-0.520520
H	3.451334	3.131800	-1.360588
H	1.841374	3.195599	-2.080161
C	-0.747803	4.040759	0.179726
H	-0.383693	4.045942	1.213546
H	-0.052516	4.623458	-0.432786
H	-1.710586	4.566386	0.166753
C	-1.137558	2.295461	-2.319277
H	-2.059048	2.808492	-2.621281
H	-0.302886	2.821933	-2.795280
H	-1.161600	1.278324	-2.724034
H	3.774787	0.020503	-1.277909
H	2.341022	0.250726	-2.296619
H	0.152116	1.125145	1.272915
C	-3.646074	-0.420827	-1.412380
H	-3.750841	-1.485291	-1.642097
H	-4.638257	0.008587	-1.237899
H	-3.190268	0.069789	-2.276300
C	-3.573508	-0.940617	1.396006
H	-4.547315	-0.445187	1.469518
H	-3.725559	-2.008844	1.212514
H	-3.045355	-0.825462	2.346680
C	2.253759	-2.687274	-2.048505
H	3.328794	-2.763227	-2.242544
H	1.874075	-3.672434	-1.761338
H	1.741162	-2.377831	-2.963285
C	2.933539	-2.096086	0.664870
H	2.674550	-3.143724	0.849316
H	4.003297	-2.029265	0.439972
H	2.705358	-1.541515	1.579733

Ru	-0.339835	-0.986710	-0.220977
H	-0.536507	-0.851485	-1.774918
H	-0.039805	-1.051106	1.791709
C	-0.023418	-0.417124	2.752127
H	-0.832529	-0.846312	3.371403
O	-0.138250	0.891544	2.558371
O	1.229216	-0.805092	3.341965
H	1.499318	-0.024158	3.839769

B5

	Coordinates (Angstroms)		
	X	Y	Z

N	0.359724	1.166705	0.122042
C	-0.866895	-2.707254	-0.657398
O	-1.211275	-3.787819	-0.909707
C	-2.481314	1.464750	0.586996
H	-3.417372	2.017882	0.445467
H	-2.306058	1.353955	1.665299
C	2.774231	0.034000	-1.200164
P	1.963505	-1.475637	-0.573082
P	-2.551507	-0.215653	-0.120831
Si	2.026250	1.563671	-0.368349
Si	-0.959555	2.338357	-0.111357
C	2.988244	2.027088	1.170644
H	4.049088	2.192178	0.948390
H	2.586878	2.948284	1.609056
H	2.907622	1.253056	1.940226
C	2.138640	2.957400	-1.623210
H	1.736990	3.906658	-1.253908
H	3.199715	3.123289	-1.849757
H	1.637140	2.711570	-2.564680
C	-0.641733	3.902190	0.874370
H	-0.466678	3.655655	1.927399
H	0.233537	4.448711	0.505585
H	-1.498363	4.585161	0.824362
C	-1.222814	2.728840	-1.931341
H	-2.267958	3.009752	-2.108753
H	-0.602020	3.566297	-2.264375
H	-0.993209	1.863304	-2.562356
H	3.865209	-0.013388	-1.094509
H	2.545330	0.095964	-2.271602

H	0.379940	1.022276	1.209201
C	-3.530567	-0.070592	-1.657557
H	-3.652331	-1.067761	-2.091519
H	-4.518030	0.362421	-1.466168
H	-2.998818	0.547267	-2.384247
C	-3.668969	-1.168874	0.969751
H	-4.630395	-0.660760	1.097399
H	-3.841874	-2.160250	0.539596
H	-3.199767	-1.299984	1.948795
C	2.447692	-2.812763	-1.722023
H	3.532958	-2.837665	-1.865322
H	2.119371	-3.777402	-1.323297
H	1.958214	-2.657038	-2.687350
C	2.896981	-1.886066	0.945197
H	2.470694	-2.779445	1.408671
H	3.956137	-2.057950	0.725051
H	2.809405	-1.067686	1.663837
Ru	-0.325285	-0.978264	-0.314112
H	-0.368073	-0.737256	-1.880529
H	-0.245377	-1.094191	1.652485
C	-0.214974	-0.576226	2.715478
H	-1.245822	-0.729961	3.093508
O	0.204872	0.667561	2.678791
O	0.614259	-1.450373	3.483811
H	1.370680	-0.895252	3.707613

B6

	Coordinates (Angstroms)		
	X	Y	Z

N	0.777304	-0.874029	-0.193610
C	-2.180812	2.067690	0.161181
O	-2.989740	2.898369	0.288868
C	2.422667	1.460367	-0.242006
H	3.211246	2.066887	-0.702615
H	2.729013	1.245755	0.790304
C	-1.658643	-2.422518	-0.838052
P	-2.472471	-0.980766	-0.055984
P	0.824509	2.354900	-0.187017
Si	0.146772	-2.533410	-0.289440
Si	2.171381	-0.212839	-1.076464
C	0.309311	-3.252922	1.435829

H	-0.253979	-4.185861	1.552257
H	1.362662	-3.465843	1.654208
H	-0.042041	-2.538229	2.188639
C	1.063038	-3.603610	-1.527390
H	2.088271	-3.814183	-1.206597
H	0.544821	-4.566013	-1.621538
H	1.099125	-3.156729	-2.526661
C	3.727594	-1.242845	-0.897538
H	3.907198	-1.493433	0.152979
H	3.682109	-2.168898	-1.480121
H	4.596113	-0.675784	-1.255179
C	1.727378	-0.044511	-2.889392
H	2.495988	0.524038	-3.426815
H	1.656215	-1.025990	-3.372013
H	0.763594	0.458868	-3.015384
H	-2.214933	-3.353549	-0.671053
H	-1.655152	-2.227414	-1.918739
H	0.854200	-0.656239	0.815798
C	0.875039	3.457897	-1.644099
H	-0.064203	4.015866	-1.702464
H	1.710824	4.163844	-1.589604
H	0.965882	2.859374	-2.554638
C	0.960639	3.505979	1.223262
H	1.908806	4.053648	1.208169
H	0.131490	4.220322	1.195665
H	0.878364	2.917539	2.141604
C	-4.027405	-0.752826	-0.992433
H	-4.596208	-1.686484	-1.056390
H	-4.642410	0.008346	-0.502371
H	-3.789226	-0.399916	-1.999157
C	-3.087198	-1.626936	1.546313
H	-3.631821	-0.832218	2.065816
H	-3.756717	-2.482014	1.403963
H	-2.249721	-1.932203	2.178611
Ru	-0.914626	0.774086	-0.039863
H	-1.170630	0.858444	-1.637454
H	1.507154	-0.033844	3.051964
C	2.484521	-0.475956	3.336585
H	2.651096	-0.749525	4.398655
O	3.360579	-0.666457	2.515351
O	-0.171493	0.433168	2.029801
H	-0.900986	0.205834	2.611327

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	Coordinates (Angstroms)		
	X	Y	Z
N	0.469930	1.185397	0.279863
C	-1.039738	-2.686924	-0.232953
O	-1.464078	-3.765648	-0.364545
C	-2.350019	1.677916	0.656622
H	-3.238011	2.283753	0.438257
H	-2.237835	1.634291	1.747852
C	2.822573	-0.244527	-0.833359
P	1.859141	-1.675319	-0.218408
P	-2.532756	-0.047586	0.067082
Si	2.200883	1.369988	-0.068286
Si	-0.756796	2.420452	-0.037902
C	3.084451	1.722350	1.546835
H	4.170570	1.779487	1.409128
H	2.747517	2.675896	1.971011
H	2.875231	0.941622	2.286538
C	2.531195	2.738628	-1.309572
H	2.210617	3.725339	-0.958613
H	3.612010	2.794737	-1.490543
H	2.049899	2.540116	-2.272836
C	-0.382620	4.014433	0.885225
H	-0.246757	3.819779	1.955532
H	0.529523	4.496735	0.515743
H	-1.200540	4.737560	0.779294
C	-0.912953	2.735696	-1.880162
H	-1.901106	3.149322	-2.114168
H	-0.168328	3.455067	-2.235963
H	-0.787576	1.805723	-2.445170
H	3.901790	-0.387880	-0.695166
H	2.629693	-0.184411	-1.912351
H	0.353954	0.828393	1.262823
C	-3.494796	0.089838	-1.482472
H	-3.658710	-0.915411	-1.882237
H	-4.461304	0.579579	-1.321541
H	-2.921088	0.651262	-2.223736
C	-3.748542	-0.807012	1.207752
H	-4.662846	-0.207901	1.276731
H	-4.003765	-1.810063	0.851809
H	-3.307595	-0.905021	2.203705
C	2.329719	-3.059863	-1.317071

H	3.415531	-3.200340	-1.341661
H	1.859789	-3.982436	-0.963230
H	1.963570	-2.858067	-2.327406
C	2.640256	-2.108789	1.374502
H	2.286343	-3.097016	1.684361
H	3.733300	-2.117779	1.309691
H	2.294860	-1.397380	2.129462
Ru	-0.385905	-0.996184	-0.058160
H	-0.445107	-0.896761	-1.673140
O	-0.024894	-0.640279	2.116873
H	-0.781694	-0.809554	2.681637

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	Coordinates (Angstroms)		
	X	Y	Z

N	0.406035	1.156182	0.251091
C	-0.923138	-2.756676	-0.091679
O	-1.287017	-3.863056	-0.127902
C	-2.430864	1.574456	0.632396
H	-3.330539	2.151389	0.385204
H	-2.356899	1.538333	1.727238
C	2.820060	-0.132943	-0.858080
P	1.920692	-1.604175	-0.253724
P	-2.538033	-0.150798	0.031698
Si	2.103292	1.442596	-0.078057
Si	-0.830949	2.357606	-0.024346
C	3.001036	1.827773	1.527446
H	4.077437	1.966100	1.369653
H	2.606566	2.749743	1.972355
H	2.862125	1.027837	2.262886
C	2.423599	2.839260	-1.299543
H	2.075953	3.811987	-0.934220
H	3.504226	2.926228	-1.469980
H	1.952840	2.649325	-2.270087
C	-0.522817	3.944461	0.942449
H	-0.395047	3.733246	2.010709
H	0.379337	4.462303	0.596838
H	-1.360302	4.645206	0.837280
C	-1.038211	2.764843	-1.850494
H	-2.032119	3.182876	-2.051327
H	-0.302271	3.505112	-2.182064

H	-0.910134	1.867741	-2.466366
H	3.904163	-0.230339	-0.719816
H	2.625181	-0.071959	-1.936855
H	0.281216	0.606552	1.362949
C	-3.458284	-0.035662	-1.544395
H	-3.577445	-1.040842	-1.959391
H	-4.444475	0.419326	-1.402438
H	-2.886578	0.557440	-2.261990
C	-3.753472	-0.970480	1.130628
H	-4.684532	-0.397318	1.195683
H	-3.974513	-1.971035	0.746028
H	-3.326678	-1.081436	2.131652
C	2.408383	-2.968286	-1.370248
H	3.496959	-3.076840	-1.418673
H	1.971782	-3.905908	-1.012503
H	2.015768	-2.771845	-2.371621
C	2.740857	-2.039511	1.320927
H	2.374043	-3.015291	1.654343
H	3.830166	-2.078283	1.216809
H	2.454004	-1.308517	2.080817
Ru	-0.348749	-1.018608	-0.055407
H	-0.457206	-1.048444	-1.647859
O	0.113843	-0.380988	2.133149
H	-0.640497	-0.286534	2.720637

B8

	Coordinates (Angstroms)		
	X	Y	Z

N	0.246883	1.153216	0.172971
C	-0.570763	-2.844870	-0.110080
O	-0.800974	-3.985581	-0.172009
C	-2.608781	1.271207	0.629136
H	-3.570372	1.737361	0.383171
H	-2.536539	1.231469	1.724820
C	2.819186	0.215834	-0.880306
P	2.110076	-1.347357	-0.267610
P	-2.495148	-0.442891	0.007737
Si	1.872886	1.671080	-0.099553
Si	-1.090770	2.223902	-0.013873
C	2.727147	2.164996	1.509955
H	3.788832	2.394238	1.354543

H	2.252610	3.060219	1.931231
H	2.662327	1.376779	2.268852
C	2.073214	3.124109	-1.291507
H	1.636347	4.051435	-0.903153
H	3.139946	3.317309	-1.463562
H	1.613611	2.915190	-2.264189
C	-0.958657	3.798883	1.019822
H	-0.772525	3.569803	2.076041
H	-0.149870	4.453756	0.674829
H	-1.889523	4.377842	0.963003
C	-1.426683	2.740112	-1.801749
H	-2.476414	3.019866	-1.955058
H	-0.815840	3.606207	-2.082103
H	-1.183758	1.928800	-2.497269
H	3.905904	0.261883	-0.737174
H	2.619009	0.249428	-1.959303
H	0.178991	0.382124	1.838579
C	-3.373782	-0.419821	-1.596191
H	-3.362995	-1.428126	-2.020202
H	-4.410105	-0.084228	-1.482840
H	-2.853112	0.242054	-2.291974
C	-3.637776	-1.424645	1.053939
H	-4.622379	-0.950050	1.122677
H	-3.753804	-2.427839	0.631920
H	-3.221392	-1.530094	2.060286
C	2.718266	-2.657147	-1.391222
H	3.807469	-2.615921	-1.496716
H	2.433121	-3.639190	-1.001424
H	2.254149	-2.532515	-2.373351
C	3.021203	-1.700339	1.280853
H	2.688414	-2.662740	1.680938
H	4.102698	-1.732828	1.111092
H	2.791974	-0.937116	2.027927
Ru	-0.210755	-1.039450	-0.045165
H	-0.294742	-1.046083	-1.618913
O	0.103397	-0.484557	2.320120
H	-0.705351	-0.450610	2.839045

C1

Coordinates (Angstroms)		
X	Y	Z

N	-0.481380	-1.002133	0.033141
C	1.177674	2.674549	-0.326521
O	1.649796	3.734358	-0.431442
C	2.268056	-1.746883	0.567785
H	3.109913	-2.419258	0.364688
H	2.165127	-1.656746	1.656834
C	-2.813738	0.447525	-1.007684
P	-1.782694	1.773595	-0.310817
P	2.543366	-0.072403	-0.101557
Si	-2.162562	-1.215583	-0.351299
Si	0.599589	-2.350582	-0.111135
C	-3.188870	-1.704256	1.153613
H	-4.238496	-1.867973	0.878648
H	-2.813541	-2.633806	1.598158
H	-3.158324	-0.939067	1.936199
C	-2.530347	-2.493083	-1.693839
H	-2.281239	-3.515165	-1.386072
H	-3.604912	-2.478408	-1.918409
H	-1.993471	-2.277803	-2.624264
C	0.068069	-3.840594	0.916953
H	-0.082456	-3.566701	1.967456
H	-0.865229	-4.283053	0.548289
H	0.833468	-4.626268	0.882124
C	0.871599	-2.946951	-1.886038
H	1.836052	-3.460673	-1.987754
H	0.093965	-3.656557	-2.188984
H	0.851769	-2.114785	-2.598836
H	-3.882195	0.608973	-0.819510
H	-2.653767	0.460769	-2.093434
H	-0.586070	-0.817640	1.903093
H	0.388065	1.175077	2.152583
C	3.444635	-0.329305	-1.672365
H	3.655054	0.643061	-2.127015
H	4.386391	-0.864091	-1.509529
H	2.822690	-0.898922	-2.366399
C	3.829471	0.689339	0.959958
H	4.700962	0.032916	1.054791
H	4.146019	1.645262	0.531316
H	3.418056	0.881058	1.955320
C	-2.177638	3.286657	-1.258573
H	-3.257865	3.463793	-1.287991
H	-1.685457	4.150202	-0.800545
H	-1.799669	3.181904	-2.279370
C	-2.514244	2.119815	1.333856

H	-2.022466	2.995295	1.769398
H	-3.589815	2.313716	1.262008
H	-2.343561	1.269460	2.001176
Ru	0.429982	0.986806	-0.208881
H	0.475254	0.977849	-1.766742
C	0.375017	0.458038	3.001125
H	1.392361	0.056233	3.120447
H	0.136075	1.048311	3.891705
O	-0.585896	-0.548382	2.852627

D1

	Coordinates (Angstroms)		
	X	Y	Z

N	0.712419	1.052365	0.153868
C	-1.544527	-2.364642	-0.674011
O	-2.171280	-3.296499	-0.976768
C	-1.954301	2.085912	0.576163
H	-2.706257	2.869853	0.423957
H	-1.817685	1.957357	1.658100
C	2.735596	-0.801965	-1.013565
P	1.508931	-1.982285	-0.349102
P	-2.490346	0.468085	-0.090503
Si	2.428709	0.933740	-0.322375
Si	-0.264995	2.506856	-0.155695
C	3.463209	1.226311	1.211462
H	4.532422	1.104356	1.001617
H	3.307538	2.240959	1.596236
H	3.189092	0.534375	2.014598
C	2.905369	2.157207	-1.662952
H	2.771696	3.201890	-1.362754
H	3.971282	2.017622	-1.883994
H	2.354990	1.988641	-2.594121
C	0.446310	3.998605	0.732650
H	0.572749	3.796020	1.801993
H	1.422647	4.285252	0.325593
H	-0.217887	4.865349	0.630415
C	-0.414577	2.842972	-1.995209
H	-1.316153	3.434466	-2.195072
H	0.437636	3.413996	-2.375710
H	-0.485152	1.910686	-2.565314
H	3.765082	-1.142493	-0.845329

H	2.570546	-0.761215	-2.097700
H	0.691914	0.906316	1.191346
C	-3.445160	0.859189	-1.599193
H	-3.848418	-0.071251	-2.010425
H	-4.272300	1.543748	-1.383359
H	-2.791441	1.301890	-2.353889
C	-3.779963	-0.127367	1.058771
H	-4.551030	0.632047	1.226215
H	-4.246304	-1.029717	0.651381
H	-3.305873	-0.391351	2.007615
C	1.685727	-3.485022	-1.375460
H	2.725931	-3.824975	-1.410916
H	1.063292	-4.285441	-0.964167
H	1.339402	-3.271007	-2.390344
C	2.207617	-2.502991	1.260264
H	1.557797	-3.262098	1.704360
H	3.216568	-2.913367	1.144467
H	2.240226	-1.652120	1.946228
Ru	-0.563353	-0.876600	-0.248336
H	-0.431903	-0.600141	-1.818044
C	-0.236156	-0.540252	2.953724
O	0.498205	0.469387	2.869795
O	-0.759365	-1.200502	2.013949
H	-0.465938	-0.918000	3.972105

D2

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.020365	1.193786	-0.062638
C	0.300292	-2.955400	0.176086
O	0.361325	-4.113037	0.185658
C	-2.740328	0.486030	-0.610551
H	-3.630861	0.507543	-1.249489
H	-3.019397	0.873190	0.378010
C	2.797035	0.805435	-0.790034
P	2.533155	-0.836992	-0.037458
P	-2.130320	-1.213177	-0.360356
Si	1.560106	2.019354	-0.034059
Si	-1.328567	1.585249	-1.213108
C	1.969971	2.378114	1.757046
H	3.040088	2.576651	1.890140

H	1.414564	3.257768	2.098461
H	1.681969	1.554140	2.417322
C	1.615848	3.611898	-1.024304
H	0.930589	4.362819	-0.617945
H	2.628852	4.029892	-0.968863
H	1.381690	3.464675	-2.084206
C	-1.880440	3.371263	-1.071908
H	-1.915509	3.666791	-0.017384
H	-1.220688	4.060048	-1.608932
H	-2.888319	3.490074	-1.488329
C	-0.785245	1.207329	-2.968545
H	-1.637476	1.260977	-3.656776
H	-0.047174	1.941036	-3.313858
H	-0.336571	0.213288	-3.057355
H	3.838438	1.138274	-0.703172
H	2.562733	0.707299	-1.858230
H	-0.466308	1.436496	0.863609
C	-2.511408	-2.068045	-1.933000
H	-2.156050	-3.101464	-1.882049
H	-3.589108	-2.070358	-2.127664
H	-1.996998	-1.571491	-2.759901
C	-3.257328	-2.013226	0.828150
H	-4.294298	-1.958614	0.480124
H	-2.972867	-3.063301	0.950500
H	-3.157775	-1.498240	1.787630
C	3.407613	-2.021609	-1.122029
H	4.449130	-1.720717	-1.274909
H	3.389249	-3.019489	-0.673623
H	2.897212	-2.072415	-2.087043
C	3.572979	-0.859095	1.468981
H	3.489915	-1.843963	1.938798
H	4.624746	-0.663143	1.234625
H	3.221846	-0.114658	2.186700
Ru	0.190676	-1.112142	0.111989
H	0.348849	-1.228687	-1.466686
C	-1.975262	1.416362	2.954576
O	-1.297915	2.160596	2.192876
O	-2.142138	0.180738	2.860431
H	-2.480678	1.930511	3.805193
H	-0.429706	-0.753072	1.923092
H	0.356095	-0.906726	1.982174

TSD2-3

	Coordinates (Angstroms)		
	X	Y	Z
N	0.536566	1.086310	-0.016122
C	-1.014115	-2.785811	-0.316338
O	-1.453295	-3.851337	-0.467759
C	-2.305550	1.669833	-0.085753
H	-3.143944	2.229894	-0.517231
H	-2.323704	1.829475	0.999512
C	2.924394	-0.520442	-0.812507
P	1.902890	-1.813686	-0.026801
P	-2.468461	-0.130631	-0.367413
Si	2.293510	1.200292	-0.347222
Si	-0.627283	2.242341	-0.727417
C	3.122273	1.832418	1.207445
H	4.211933	1.850396	1.085417
H	2.790486	2.853199	1.428549
H	2.885981	1.221170	2.084037
C	2.717666	2.325686	-1.787579
H	2.428181	3.369175	-1.627940
H	3.808008	2.309078	-1.913177
H	2.279257	1.980114	-2.728743
C	-0.292824	3.976457	-0.097762
H	-0.239547	3.976553	0.996626
H	0.648648	4.383804	-0.482459
H	-1.093555	4.663372	-0.397682
C	-0.593042	2.179283	-2.601874
H	-1.570499	2.478854	-2.998716
H	0.148129	2.866903	-3.020528
H	-0.375253	1.169542	-2.964883
H	3.992695	-0.646062	-0.595484
H	2.788200	-0.636388	-1.895068
H	0.438322	1.229313	1.009022
C	-3.260281	-0.287310	-2.009574
H	-3.441311	-1.347645	-2.211534
H	-4.211684	0.253553	-2.053621
H	-2.587836	0.089641	-2.783596
C	-3.792676	-0.682474	0.765599
H	-4.714298	-0.111974	0.608671
H	-3.995350	-1.744879	0.597496
H	-3.451782	-0.553310	1.796197
C	2.373300	-3.371960	-0.860510
H	3.458293	-3.518959	-0.848828

H	1.894359	-4.217652	-0.357742
H	2.019938	-3.345748	-1.894991
C	2.626406	-2.011298	1.642852
H	2.123935	-2.838610	2.152598
H	3.702811	-2.210152	1.601790
H	2.445432	-1.106213	2.228650
Ru	-0.330587	-1.092142	-0.129541
H	-0.145797	-1.035714	-1.747164
C	-0.841010	1.243193	3.360738
O	0.098587	1.765291	2.743434
O	-1.445717	0.155545	3.065825
H	-1.226619	1.745780	4.267983
H	-0.845475	-0.540377	2.136475
H	-0.335550	-1.189623	1.656771

D3

Coordinates (Angstroms)			
	X	Y	Z

N	0.432120	1.148117	-0.039485
C	-0.707585	-2.884034	-0.298874
O	-1.029431	-3.999348	-0.400379
C	-2.450706	1.424032	-0.177963
H	-3.334386	1.887363	-0.633597
H	-2.506193	1.606341	0.902717
C	2.996674	-0.228747	-0.739267
P	2.072609	-1.619823	0.008594
P	-2.415698	-0.391100	-0.437064
Si	2.179000	1.421901	-0.319694
Si	-0.828474	2.166030	-0.793809
C	2.875750	2.141047	1.264945
H	3.960845	2.279236	1.191819
H	2.425238	3.118565	1.472828
H	2.674295	1.499244	2.129174
C	2.521646	2.583112	-1.753014
H	2.075692	3.575003	-1.627447
H	3.607637	2.723314	-1.825609
H	2.183147	2.167059	-2.707009
C	-0.698403	3.934097	-0.174991
H	-0.684497	3.955419	0.920439
H	0.208358	4.433287	-0.534039
H	-1.555534	4.529136	-0.512975

C	-0.730412	2.091638	-2.663452
H	-1.713429	2.313608	-3.095612
H	-0.026686	2.826677	-3.065950
H	-0.426696	1.095614	-3.002034
H	4.060082	-0.246318	-0.468256
H	2.926460	-0.363268	-1.825813
H	0.287159	1.257028	0.973583
C	-3.180034	-0.629768	-2.083696
H	-3.246422	-1.703971	-2.282730
H	-4.181737	-0.189947	-2.139635
H	-2.540341	-0.191245	-2.852863
C	-3.716405	-1.049911	0.671485
H	-4.680396	-0.561174	0.493106
H	-3.824080	-2.126034	0.502297
H	-3.420581	-0.899685	1.712872
C	2.719191	-3.111975	-0.830633
H	3.813408	-3.145964	-0.800124
H	2.322058	-4.007858	-0.343727
H	2.380783	-3.110854	-1.870251
C	2.796420	-1.773433	1.684548
H	2.327011	-2.618833	2.195820
H	3.881101	-1.924572	1.650985
H	2.572273	-0.873390	2.263559
Ru	-0.208664	-1.129496	-0.164409
H	0.022877	-1.040089	-1.817359
C	-1.081981	1.235350	3.496029
O	-0.333311	1.867428	2.770012
O	-1.437793	-0.015373	3.340772
H	-1.547024	1.682030	4.386561
H	-0.982784	-0.436523	2.527522
H	-0.322952	-1.125459	1.554294

D4

	Coordinates (Angstroms)		
	X	Y	Z

N	0.358932	1.156219	0.103641
C	-0.781331	-2.754870	-0.271275
O	-1.107173	-3.872454	-0.334441
C	-2.505447	1.516733	0.409001
H	-3.400820	2.063503	0.089025
H	-2.524099	1.470034	1.505537

C	2.872156	0.041992	-0.916456
P	2.021063	-1.487513	-0.406659
P	-2.488722	-0.197034	-0.222232
Si	2.036510	1.525541	-0.066644
Si	-0.868754	2.343849	-0.104552
C	2.854584	1.819532	1.611036
H	3.937702	1.970165	1.521789
H	2.433192	2.718390	2.079620
H	2.685022	0.986306	2.302733
C	2.438049	3.029168	-1.138895
H	2.062426	3.965170	-0.709697
H	3.525783	3.134545	-1.240164
H	2.019859	2.926872	-2.146691
C	-0.651759	3.857051	1.006120
H	-0.610006	3.572235	2.064519
H	0.270141	4.403622	0.774767
H	-1.484268	4.561561	0.882884
C	-1.051409	2.967689	-1.880481
H	-2.045158	3.396724	-2.060533
H	-0.314805	3.750433	-2.096744
H	-0.891063	2.158779	-2.602403
H	3.956114	-0.015185	-0.757608
H	2.694802	0.156992	-1.993917
H	0.220406	0.329233	1.796947
H	-1.763375	-0.117673	2.927982
C	-3.247945	-0.070346	-1.883609
H	-3.305949	-1.068331	-2.327785
H	-4.252853	0.362262	-1.830847
H	-2.620904	0.549747	-2.528579
C	-3.790490	-1.092955	0.708995
H	-4.739489	-0.546414	0.688696
H	-3.940189	-2.082794	0.266221
H	-3.480296	-1.232197	1.748105
C	2.512252	-2.767507	-1.618732
H	3.600798	-2.816267	-1.728253
H	2.140896	-3.744424	-1.293075
H	2.059697	-2.538342	-2.587211
C	2.899795	-2.023453	1.107826
H	2.469197	-2.966505	1.457743
H	3.969965	-2.162250	0.921132
H	2.759938	-1.281887	1.897383
Ru	-0.267258	-0.988497	-0.181691
C	-0.842689	-0.657700	3.181196
H	-0.439456	-0.244669	4.114316

H	-1.085457	-1.711015	3.339277
O	0.119521	-0.588848	2.146406
H	-0.328026	-0.953099	-1.760214

D5

	Coordinates (Angstroms)		
	X	Y	Z

N	-0.068617	1.146914	-0.094463
C	0.215967	-2.936783	0.310982
O	0.280985	-4.094571	0.383619
C	-2.836617	0.541765	-0.568426
H	-3.648063	0.453514	-1.299938
H	-3.230115	1.049437	0.320065
C	2.714906	0.820795	-0.889160
P	2.431501	-0.865148	-0.263116
P	-2.246734	-1.108051	-0.051749
Si	1.450858	1.943061	-0.007198
Si	-1.347686	1.558699	-1.173639
C	2.029398	2.169785	1.776933
H	3.102851	2.393176	1.820412
H	1.503301	3.006091	2.251700
H	1.846132	1.278617	2.386813
C	1.557202	3.642074	-0.821579
H	0.872637	4.360807	-0.357656
H	2.574226	4.038611	-0.706841
H	1.337576	3.608346	-1.895025
C	-1.874118	3.371354	-1.101331
H	-1.945184	3.722805	-0.065338
H	-1.184995	4.030848	-1.639220
H	-2.864137	3.493400	-1.559516
C	-1.018396	1.151652	-2.988306
H	-1.888699	1.390245	-3.613391
H	-0.171990	1.736004	-3.370909
H	-0.777561	0.092202	-3.128825
H	3.765313	1.122355	-0.799757
H	2.447633	0.820743	-1.953975
H	-1.016044	1.353253	1.525874
H	-0.841314	3.041110	3.172830
C	-2.866342	-2.241776	-1.347171
H	-2.584727	-3.271946	-1.109527
H	-3.956155	-2.179507	-1.435109

H	-2.412022	-1.975550	-2.305345
C	-3.246904	-1.565580	1.409062
H	-4.318348	-1.527135	1.185043
H	-2.981454	-2.575514	1.737534
H	-3.017912	-0.857571	2.210584
C	3.129519	-2.006057	-1.512234
H	4.175485	-1.760920	-1.725153
H	3.071228	-3.037478	-1.150958
H	2.545854	-1.933139	-2.433485
C	3.612424	-1.060254	1.124970
H	3.497143	-2.058885	1.557645
H	4.646995	-0.932970	0.788777
H	3.400171	-0.324761	1.904801
Ru	0.113563	-1.089058	0.158638
H	0.067965	-1.264172	-1.418360
C	-1.093794	1.994050	3.394956
H	-0.191431	1.492978	3.775389
H	-1.843305	1.991479	4.192408
O	-1.647498	1.333195	2.284723
H	0.537107	-0.784879	1.996035
H	-0.257894	-0.723274	1.999365

TSD5-6

	Coordinates (Angstroms)		
	X	Y	Z

N	0.289732	1.188926	0.028013
C	-0.737978	-2.850967	0.038086
O	-1.053115	-3.968158	0.009314
C	-2.540144	1.467089	-0.292760
H	-3.409321	1.772695	-0.886066
H	-2.616111	1.915982	0.705660
C	2.787477	-0.011720	-0.947849
P	2.034668	-1.548571	-0.308235
P	-2.497378	-0.341874	-0.041051
Si	2.035031	1.458482	-0.022306
Si	-0.884164	2.062305	-0.971751
C	2.671103	1.530138	1.739725
H	3.760885	1.412596	1.772553
H	2.427606	2.497911	2.192085
H	2.220370	0.757234	2.369875
C	2.550559	3.027627	-0.918082

H	2.198660	3.923171	-0.395356
H	3.645894	3.079033	-0.956042
H	2.186655	3.068787	-1.950750
C	-0.807214	3.923049	-0.712810
H	-0.712063	4.157085	0.353675
H	0.025409	4.393918	-1.245101
H	-1.732685	4.389829	-1.072246
C	-0.664522	1.674464	-2.794638
H	-1.457667	2.151651	-3.383416
H	0.292077	2.055689	-3.171546
H	-0.694370	0.597273	-2.985625
H	3.883551	-0.039657	-0.913289
H	2.485827	0.075910	-2.000071
H	-0.077874	1.330707	1.064541
H	0.354919	2.331684	3.614522
C	-3.479183	-1.021245	-1.426858
H	-3.531781	-2.110891	-1.345028
H	-4.495655	-0.613913	-1.428312
H	-2.990206	-0.775195	-2.373408
C	-3.536788	-0.650578	1.426754
H	-4.537899	-0.223709	1.303387
H	-3.618915	-1.726686	1.608942
H	-3.035476	-0.177350	2.276860
C	2.419759	-2.839765	-1.545123
H	3.495782	-2.889889	-1.742230
H	2.080002	-3.813746	-1.179038
H	1.889049	-2.621082	-2.475309
C	3.090654	-2.050335	1.101125
H	2.709900	-2.990826	1.510798
H	4.132996	-2.189776	0.795044
H	3.047719	-1.298312	1.892008
Ru	-0.246178	-1.073239	0.046832
H	-0.300744	-1.122035	-1.547855
C	-0.315668	1.448482	3.581544
H	0.295762	0.591083	3.949067
H	-1.086651	1.619977	4.358318
O	-0.868982	1.224840	2.339916
H	-0.027590	-1.111136	1.934635
H	-0.427397	-0.383216	1.959573

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Coordinates (Angstroms)

	X	Y	Z
N	0.332823	1.224767	-0.010434
C	-0.775101	-2.836094	0.062860
O	-1.112431	-3.951291	0.107097
C	-2.518252	1.486566	-0.201246
H	-3.408730	1.843558	-0.732494
H	-2.566624	1.871706	0.825850
C	2.797218	-0.099546	-0.986446
P	1.994827	-1.600396	-0.301413
P	-2.486495	-0.345501	-0.100745
Si	2.097707	1.431140	-0.139007
Si	-0.900170	2.126865	-0.929143
C	2.718281	1.584432	1.624158
H	3.813035	1.550640	1.670668
H	2.393687	2.534024	2.066122
H	2.326272	0.776953	2.250647
C	2.601934	2.949703	-1.121907
H	2.316008	3.875997	-0.612466
H	3.692935	2.960697	-1.236801
H	2.171568	2.963639	-2.129043
C	-0.800980	3.969701	-0.572069
H	-0.724552	4.156310	0.505672
H	0.054372	4.445504	-1.062852
H	-1.706763	4.474240	-0.930397
C	-0.724185	1.819717	-2.765910
H	-1.607996	2.190540	-3.298728
H	0.145713	2.346512	-3.174541
H	-0.609097	0.752961	-2.978348
H	3.891950	-0.150225	-0.930027
H	2.519131	-0.049336	-2.047156
H	0.105552	1.397223	0.978370
H	0.000375	2.407072	4.182476
C	-3.423333	-0.868321	-1.584938
H	-3.439087	-1.961121	-1.635716
H	-4.451840	-0.491088	-1.567157
H	-2.912564	-0.499520	-2.478412
C	-3.652162	-0.755987	1.250779
H	-4.629918	-0.285774	1.099288
H	-3.777305	-1.842402	1.301409
H	-3.229282	-0.417864	2.200651
C	2.384140	-2.925043	-1.503800
H	3.462296	-3.010306	-1.677156
H	2.008103	-3.880451	-1.123885

H	1.874598	-2.712411	-2.446834
C	3.054280	-2.080583	1.115250
H	2.655382	-3.002397	1.549343
H	4.094507	-2.245168	0.813325
H	3.019001	-1.310943	1.889101
Ru	-0.263944	-1.083125	0.001243
H	-0.285188	-1.061640	-1.673978
C	-0.184701	1.346428	3.990385
H	0.773007	0.811939	4.035237
H	-0.836908	0.956780	4.783474
O	-0.794550	1.230626	2.719779
H	-0.144538	-1.016493	1.722577
H	-0.700819	0.300818	2.408859

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	Coordinates (Angstroms)		
	X	Y	Z

N	0.031559	1.175677	0.125163
C	-0.120219	-2.902423	0.081744
O	-0.187738	-4.059579	-0.010966
C	-2.814146	0.879625	0.591149
H	-3.826359	1.152843	0.269467
H	-2.785755	0.926236	1.687718
C	2.716313	0.666405	-0.843250
P	2.294947	-0.999284	-0.249691
P	-2.387286	-0.822347	0.113797
Si	1.574914	1.902595	0.052517
Si	-1.436060	2.031800	-0.047811
C	2.294221	2.269034	1.764498
H	3.371269	2.477900	1.738367
H	1.796261	3.146340	2.197040
H	2.123180	1.435848	2.456437
C	1.684146	3.508783	-0.940183
H	1.124656	4.330866	-0.479812
H	2.729785	3.834394	-1.015288
H	1.305063	3.374447	-1.960088
C	-1.557428	3.606874	0.991926
H	-1.368421	3.394801	2.051195
H	-0.837460	4.369222	0.673260
H	-2.556826	4.053702	0.911132
C	-1.838117	2.509352	-1.835130

H	-2.902171	2.733595	-1.983178
H	-1.271959	3.401224	-2.131632
H	-1.558673	1.705090	-2.525834
H	3.790204	0.872112	-0.760449
H	2.441070	0.708179	-1.904986
H	-0.283746	-0.849684	2.057334
H	0.501908	-0.945838	2.001203
C	-3.155941	-1.051844	-1.529650
H	-2.947376	-2.063604	-1.889065
H	-4.239285	-0.897243	-1.484533
H	-2.721473	-0.342776	-2.238734
C	-3.401796	-1.921178	1.172858
H	-4.465767	-1.673773	1.093745
H	-3.255484	-2.964568	0.876413
H	-3.086907	-1.816945	2.215308
C	2.938119	-2.178879	-1.492430
H	3.998128	-1.992381	-1.694965
H	2.818195	-3.204583	-1.130107
H	2.368748	-2.073404	-2.419463
C	3.430953	-1.281363	1.161149
H	3.249627	-2.273042	1.586623
H	4.477687	-1.215884	0.845143
H	3.252466	-0.535755	1.940476
Ru	-0.032772	-1.049365	0.156596
H	-0.133131	-1.031761	-1.424910

References

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