Supplementary Information

Oxo vs. Imido Alkylidene d^0-Metal Species:

How and why do they differ in structure, activity and efficiency in alkene metathesis?

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Table S1. Gibbs Energies, in kcal mol^{-1} relative to the separated reactants (**I** + C_2H_4) of intermediates and transition states for the reaction of Figure 1.[a,b]

Complex[a]	**I + C_2H_4**	**TSI**	**II**	**TSII**	**TBP**	**TSIII**	**IV**	**TSIV**	**V**
W-N-1	0.0	11.2	12.1	14.1	0.4	17.8	12.3	10.4	-2.3
W-N-1'	0.0	13.2	14.2	15.9	2.6	21.5	--[c]	--[c]	-0.9
W-O-1	0.0	--[c]	11.2	16.9	6.0	19.7	7.6	--[c]	-2.1
W-O-2	0.0	--[c]	9.9	14.0	3.5	17.1	7.6	--[c]	-2.0
W-N-3	0.0	14.1	--[c]	--[c]	-1.5	17.1	14.9	14.4	-1.7
W-N-3'	0.0	14.8	--[c]	--[c]	1.7	20.5	17.3	16.8	-1.9
W-O-3	0.0	12.1	13.0	--[c]	4.0	17.0	12.3	10.7	-1.7
W-O-4	0.0	10.2	--[c]	--[c]	0.8	13.3	12.0	--[c]	-1.1
W-N-5	0.0	15.6	--[c]	--[c]	-2.7	--[c]	--[c]	14.5	-2.7
W-O-5	0.0	14.2	--[c]	--[c]	1.7	16.3	13.1	12.2	-2.4
Mo-N-1	0.0	11.9	13.6	17.6	4.4	21.4	13.5	12.6	-1.0
Mo-N-1'	0.0	14.4	15.8	19.4	7.6	25.0	--[c]	--[c]	-0.7
Mo-O-1	0.0	--[c]	11.1	20.8	10.7	23.2	8.6	--[c]	-0.8
Mo-O-2	0.0	--[c]	10.5	17.9	8.8	20.6	9.2	--[c]	-0.7
Mo-N-3	0.0	13.0	14.2	15.2	4.6	20.1	16.8	15.4	-1.4
Mo-N-3'	0.0	14.7	14.3	15.6	7.3	23.4	18.7	17.4	-1.5
Mo-O-3	0.0	12.1	13.9	16.0	11.8	21.7	13.7	12.2	-0.1
Mo-O-4	0.0	11.0	12.6	13.8	8.0	18.0	11.0	--[c]	0.1
Mo-N-5	0.0	15.8	--[c]	--[c]	3.6	19.1	17.0	16.3	-1.2
Mo-O-5	0.0	14.7	15.5	18.0	8.8	21.1	15.2	13.7	-0.8

[a] See Scheme 3 for labelling definition.

[b] See Figure 1a for intermediate and transition state definition.

[c] Not located

Table S2. Gibbs Energies in kcal mol^{-1}, relative to the separated reactants (**I** + C_2H_4) of the intermediates and transition states for the pathway of Figure 2.[a]

Complex[a]	**TBP**	**TSA**	**SP (E_{SP}-E_{TBP})**	**TSB**	**B**	**TSC**	**C**
W-N-1	0.4	19.0	–1.7 (–2.1)	20.1	2.2	30.2	0.8
W-N-1'	2.6	18.7	–1.9 (–4.5)	21.8	1.6	32.2	2.0
W-O-1	6.0	20.8	–2.0 (–8.0)	27.8	2.3	35.8	0.1
W-O-2	3.5	16.4	–2.6 (-6.1)	27.1	3.6	35.8	-1.2
W-N-3	-1.5	9.2	–3.2 (-1.7)	26.2	4.7	33.4	-2.3
W-N-3'	1.7	8.8	–3.7 (–2.0)	27.3	3.6	33.7	-1.3
W-O-3	4.0	11.7	–3.6 (–7.6)	32.2	5.7	40.6	-2.1
W-O-4	0.8	9.2	–5.3 (–6.1)	32.2	4.6	39.7	-3.8
W-N-5	-2.7	7.5	–6.5 (–3.8)	23.8	2.4	30.8	-5.7
W-O-5	1.7	10.5	–7.0 (–8.7)	33.5	5.0	38.4	-5.1
Mo-N-1	4.4	24.5	1.6 (–2.8)	22.5	3.1	33.5	6.6
Mo-N-1'	7.6	25.0	1.8 (-5.8)	24.4	3.7	35.7	7.0
Mo-O-1	10.7	25.1	0.3 (–10.4)	28.1	3.9	36.0	3.7
Mo-O-2	8.8	20.8	–0.5 (–9.3)	28.0	4.5	39.8	2.6
Mo-N-3	4.6	15.7	0.8 (–3.8)	27.4	8.2	38.3	4.6
Mo-N-3'	7.3	15.5	0.2 (-7.1)	29.2	6.2	37.4	5.2
Mo-O-3	11.8	19.5	0.1 (–11.7)	33.4	8.7	44.2	4.2
Mo-O-4	8.0	15.9	–2.0 (–10.0)	32.8	7.6	43.1	1.5
Mo-N-5	3.6	14.3	-1.8 (-5.4)	26.3	7.5	34.9	1.8
Mo-O-5	8.8	18.3	–2.1 (–10.9)	37.4	9.9	44.2	2.9

[a] See Scheme 3 for labelling definition and Figure 2a for intermediate and transition state definition

Table S3. ΔG + D energies, in kcal mol^{-1} relative to the separated reactants (**I** + C_2H_4) of intermediates and transition states for the reaction of Figure 1.[a,b]

Complex[a]	**I + C_2H_4**	**TSI**	**II**	**TSII**	**TBP**	**TSIII**	**IV**	**TSIV**	**V**
W-N-1	0.0	5.0	2.8	4.2	-9.6	6.6	3.3	4.2	-1.6
W-N-1'	0.0	6.9	4.3	5.3	-8.4	9.4	--[c]	--[c]	0.0
W-O-1	0.0	--[c]	3.9	8.0	-2.3	10.5	1.5	--[c]	-1.5
W-O-2	0.0	--[c]	2.0	4.8	-4.6	7.4	0.3	--[c]	-1.3
W-N-3	0.0	7.2	--[c]	--[c]	-13.3	5.7	3.9	7.1	-0.9
W-N-3'	0.0	7.4	--[c]	--[c]	-11.5	7.7	5.1	8.6	-0.9
W-O-3	0.0	6.2	4.3	--[c]	-5.1	7.6	4.0	5.0	-1.1
W-O-4	0.0	4.7	--[c]	--[c]	-8.5	3.5	2.5	--[c]	-0.6
W-N-5	0.0	8.4	--[c]	--[c]	-12.6	--[c]	--[c]	7.5	-1.9
W-O-5	0.0	8.2	--[c]	--[c]	-5.8	8.7	5.9	6.3	-1.8
Mo-N-1	0.0	5.4	4.0	6.4	-6.5	9.0	4.0	5.8	-0.2
Mo-N-1'	0.0	7.2	3.4	7.0	-4.3	11.6	--[c]	--[c]	0.2
Mo-O-1	0.0	--[c]	3.7	10.8	1.6	12.9	2.4	--[c]	-0.2
Mo-O-2	0.0	--[c]	2.5	7.7	-0.1	9.8	1.4	--[c]	0.0
Mo-N-3	0.0	5.9	2.9	3.8	-8.1	7.3	5.0	7.5	-0.5
Mo-N-3'	0.0	6.8	1.9	2.9	-6.8	9.0	5.6	8.4	-0.5
Mo-O-3	0.0	5.1	4.5	6.5	1.7	10.8	4.5	5.6	0.4
Mo-O-4	0.0	4.4	2.4	3.4	-2.1	7.0	2.7	--[c]	0.7
Mo-N-5	0.0	8.2	--[c]	--[c]	-7.2	8.0	6.7	9.2	-0.3
Mo-O-5	0.0	8.0	7.5	8.6	0.6	12.4	7.4	6.9	-0.3

[a] See Scheme 3 for labelling definition.

[b] See Figure 1a for intermediate and transition state definition.

[c] Not located

Table S4. ΔG + D Energies in kcal mol^{-1}, relative to the separated reactants (**I** + C_2H_4) of the intermediates and transition states for the pathway of Figure 2.[a]

Complex[a]	TBP	TSA	SP (E_{SP}-E_{TBP})	TSB	B	TSC	C
W-N-1	-9.6	9.8	–11.4 (–1.8)	10.0	-2.8	13.8	-14.3
W-N-1'	-8.4	9.0	–11.7 (–3.4)	12.0	-3.6	15.0	-13.6
W-O-1	-2.3	12.5	–11.2 (–8.9)	20.4	-2.6	22.1	-14.2
W-O-2	-4.6	7.4	–11.6 (-7.0)	18.1	-3.4	21.6	-16.4
W-N-3	-13.3	-0.3	–13.0 (+0.3)	16.5	-1.1	16.9	-17.4
W-N-3'	-11.5	-1.4	–13.7 (–2.2)	17.4	-2.4	16.5	-10.2
W-O-3	-5.1	3.6	–12.4 (–7.3)	24.6	0.0	25.8	-16.5
W-O-4	-8.5	0.3	–14.5 (–6.0)	23.4	-0.7	24.2	-20.2
W-N-5	-12.6	-1.0	–15.4 (–2.8)	14.9	-4.0	15.6	-20.4
W-O-5	-5.8	2.8	–15.2 (–8.7)	25.5	-0.6	25.0	-18.5
Mo-N-1	-6.5	14.1	-9.3 (–2.8)	11.5	-2.2	16.0	-9.9
Mo-N-1'	-4.3	0.2	-9.4 (-4.9)	13.1	-2.0	17.3	-10.7
Mo-O-1	1.6	15.6	-10.0 (–11.6)	19.9	-1.3	22.0	-12.4
Mo-O-2	-0.1	10.7	–10.8 (–10.7)	18.3	-2.7	26.6	-16.8
Mo-N-3	-8.1	5.3	-10.5 (–2.2)	17.6	2.1	20.2	-12.4
Mo-N-3'	-6.8	4.1	-11.5 (-4.7)	18.4	-0.1	18.6	-14.3
Mo-O-3	1.7	9.9	-10.3 (–12.0)	24.9	2.5	28.4	-12.4
Mo-O-4	-2.1	5.7	–12.6 (–10.5)	23.4	2.0	26.6	-16.8
Mo-N-5	-7.2	5.1	-12.1 (-4.9)	16.3	0.7	18.2	-14.9
Mo-O-5	0.6	9.6	–11.6 (–12.2)	30.3	3.9	30.1	-11.7

[a] See Scheme 3 for labelling definition and Figure 2a for intermediate and transition state definition

Table S5. M-L bond distances (Å) and L-M-L angles (degrees) of the *syn* and *anti* W alkyl alkylidene isomers.

	W-N-1		**W-N-1'**		**W-O-1**		**W-O-2**	
	syn	*anti*	*Syn*	*anti*	*syn*	*anti*	*syn*	*anti*
$M{=}C_{ene}$	1.894	1.908	1.899	1.911	1.900	1.909	1.899	1.908
M-E	1.752	1.753	1.741	1.739	1.700	1.700	1.700	1.700
M-X	2.141	2.134	2.140	2.139	2.138	2.139	2.136	2.138
M-Y	1.907	1.906	1.912	1.913	1.894	1.892	1.904	1.901
C_{ene}-H_{α}	1.109	1.092	1.109	1.091	1.104	1.093	1.103	1.093
E-M-C_{ene}	103.8	103.2	104.1	103.2	105.6	105.7	105.8	105.7
E-M-X	102.8	103.1	103.5	103.2	104.5	103.6	104.2	103.6
E-M-Y	126.7	128.5	126.2	127.3	125.3	125.5	127.6	127.4
C_{ene}-M-X	100.3	99.4	100.2	99.2	99.6	99.8	98.7	100.0
C_{ene}-M-Y	112.3	112.8	112.9	113.4	111.8	112.6	110.3	111.3
X-M-Y	107.6	105.8	106.5	106.7	106.8	106.3	105.6	105.3
M-C_{ene}-H_{α}	106.1	123.7	105.7	125.2	109.2	119.3	109.5	119.1
M-C_{ene}-C_{β}	139.4	121.6	140.1	120.3	136.0	125.9	135.7	126.0

Table S6. M-L bond distances (Å) and L-M-L angles (degrees) of the *syn* and *anti* W pyrrolyl alkylidene isomers.

	W-N-3		**W-N-3'**		**W-O-3**		**W-O-4**	
	syn	*anti*	*syn*	*anti*	*syn*	*anti*	*syn*	*anti*
$M=C_{ene}$	1.892	1.905	1.894	1.908	1.895	1.905	1.897	1.905
M-E	1.748	1.747	1.735	1.733	1.698	1.699	1.699	1.699
M-X	2.017	2.016	2.024	2.024	2.005	2.004	2.004	2.003
M-Y	1.901	1.888	1.906	1.905	1.888	1.885	1.898	1.896
C_{ene}-H_{α}	1.110	1.091	1.110	1.090	1.105	1.093	1.103	1.093
E-M-C_{ene}	102.7	102.0	103.3	102.2	104.5	104.7	104.8	104.8
E-M-X	109.3	109.0	109.3	109.1	110.4	109.1	109.1	109.1
E-M-Y	118.6	119.8	117.8	118.9	117.5	119.9	121.9	121.8
C_{ene}-M-X	102.3	102.2	102.6	102.4	102.0	101.5	101.8	101.7
C_{ene}-M-Y	109.9	119.8	110.1	110.0	110.3	109.4	107.9	108.3
X-M-Y	112.4	112.3	112.4	112.5	110.9	110.4	109.3	109.3
M-C_{ene}-H_{α}	105.8	124.4	104.6	125.9	108.2	120.3	109.3	119.9
M-C_{ene}-C_{β}	139.2	120.4	140.7	119.0	136.5	124.2	135.3	124.7

Table S7. M-L bond distances (Å) and L-M-L angles (degrees) of the *syn* and *anti* bisiloxy Mo and W alkylidene isomers.

	W-N-5		**W-O-5**		**Mo-N-5**		**Mo-O-5**	
	syn	*anti*	*syn*	*anti*	*syn*	*anti*	*syn*	*anti*
$M{=}C_{ene}$	1.894	1.904	1.896	1.904	1.872	1.881	1.876	1.885
M-E	1.746	1.745	1.696	1.695	1.724	1.722	1.669	1.668
M-X	1.911	1.909	1.899	1.896	1.913	1.911	1.897	1.894
M-Y	1.911	1.909	1.899	1.896	1.913	1.911	1.897	1.894
C_{ene}-H_{α}	1.108	1.091	1.104	1.091	1.107	1.091	1.103	1.092
E-M-C_{ene}	101.6	100.9	102.9	102.8	100.5	100.0	102.2	102.4
E-M-X	114.7	115.1	114.5	114.7	114.6	114.9	115.4	115.5
E-M-Y	114.7	115.1	114.5	114.6	114.6	114.9	115.4	115.5
C_{ene}-M-X	107.5	107.6	107.6	107.9	107.2	107.1	107.0	107.0
C_{ene}-M-Y	107.5	107.6	107.6	108.0	107.2	107.1	107.0	107.1
X-M-Y	110.0	109.8	109.2	108.4	111.6	111.5	109.0	108.5
M-C_{ene}-H_{α}	107.0	124.7	109.0	120.9	106.5	125.2	109.1	120.1
M-C_{ene}-C_{β}	138.4	120.2	135.8	123.8	138.3	119.0	135.2	124.0

Table S8. M-L bond distances (Å) and L-M-L angles (degrees) of the *syn* and *anti* Mo alkyl alkylidene isomers.

	Mo-N-1		**Mo-N-1'**		**Mo-O-1**		**Mo-O-2**	
	syn	*anti*	*syn*	*anti*	*syn*	*anti*	*syn*	*anti*
$M=C_{ene}$	1.874	1.886	1.878	1.890	1.882	1.891	1.882	1.890
M-E	1.732	1.733	1.717	1.715	1.675	1.674	1.676	1.675
M-X	2.133	2.126	2.131	2.131	2.132	2.134	2.131	2.133
M-Y	1.910	1.909	1.915	1.918	1.893	1.890	1.903	1.899
C_{ene}-H_{α}	1.108	1.092	1.108	1.091	1.103	1.094	1.103	1.094
E-M-C_{ene}	102.6	102.4	103.1	102.3	105.2	105.6	105.4	105.7
E-M-X	102.2	102.4	103.0	102.5	104.8	103.9	104.5	103.6
E-M-Y	127.9	129.7	127.1	128.4	126.9	126.7	129.1	128.6
C_{ene}-M-X	99.6	98.6	99.6	98.4	98.7	99.0	98.9	99.2
C_{ene}-M-Y	112.4	112.9	113.2	113.5	111.2	111.9	109.7	110.7
X-M-Y	108.4	106.3	107.1	107.3	106.3	106.0	105.2	105.0
M-C_{ene}-H_{α}	105.7	124.0	105.4	125.5	109.3	118.7	109.6	118.6
M-C_{ene}-C_{β}	139.3	120.8	139.9	119.4	135.4	126.1	135.1	126.1

Table S9. M-L bond distances (Å) and L-M-L angles (degrees) of the *syn* and *anti* Mo pyrrolyl alkylidene isomers.

	Mo-N-3		**Mo-N-3'**		**Mo-O-3**		**Mo-O-4**	
	syn	*anti*	*syn*	*anti*	*syn*	*anti*	*syn*	*anti*
$M{=}C_{ene}$	1.869	1.883	1.872	1.885	1.878	1.886	1.878	1.886
M-E	1.725	1.724	1.710	1.708	1.673	1.673	1.674	1.674
M-X	2.014	2.013	2.021	2.021	1.998	1.999	1.999	1.999
M-Y	1.904	1.902	1.909	1.909	1.886	1.884	1.899	1.896
C_{ene}-H_{α}	1.108	1.091	1.109	1.091	1.103	1.093	1.103	1.093
E-M-C_{ene}	101.5	100.9	102.2	101.4	104.2	104.6	104.6	104.7
E-M-X	108.6	108.5	108.9	108.3	109.6	109.3	109.3	109.1
E-M-Y	119.6	120.2	117.9	119.4	121.5	121.6	123.7	123.7
C_{ene}-M-X	101.8	101.8	102.0	101.9	100.9	100.9	101.1	101.0
C_{ene}-M-Y	109.8	109.4	110.3	110.0	108.6	108.7	107.4	107.6
X-M-Y	113.7	113.7	113.8	113.8	109.8	109.7	108.3	108.4
M-C_{ene}-H_{α}	105.4	125.0	104.2	126.4	108.9	119.8	109.2	119.5
M-C_{ene}-C_{β}	139.2	119.2	140.5	117.7	135.2	124.2	134.9	124.5

Table S10. NPA Charges, ellipticity (ε) and electron density (ρ) at the bond critical point of W siloxy carbenes (**I**) and the two isomeric forms (**TBP** and **SBP**) of the metallacycle intermediates.

	W-O-1			**W-N-1**			**W-O-3**			**W-N-3**			**W-O-5**			**W-N-5**		
	I	**TBP**	**SBP**	**I**	**TBP**	**SBP**	**I**	**TBP**	**SBP**	**I**	**TBP**	**SBP**	**I**	**TBP**	**SBP**	**I**	**TBP**	**SBP**
M	+1.29	+1.15	+1.36	+1.09	+0.96	+1.14	+1.40	+1.25	+1.47	+1.20	+1.05	+1.27	+1.49	+1.28	+1.56	+1.29	+1.09	+1.36
E[a]	-0.53	-0.49	-0.51	-0.34	-0.28	-0.32	-0.52	-0.48	-0.50	-0.32	-0.24	-0.29	-0.53	-0.51	-0.51	-0.33	-0.28	-0.31
X[a]	-0.21	-0.17	-0.17	-0.20	-0.19	-0.16	-0.37	-0.28	-0.33	-0.38	-0.36	-0.36	-0.37	-0.33	-0.34	-0.37	-0.35	-0.34
Y[a]	-0.37	-0.41	-0.34	-0.37	-0.42	-0.34	-0.36	-0.39	-0.32	-0.36	-0.41	-0.32	-0.37	-0.41	-0.34	-0.37	-0.43	-0.34
Carbene[a]	-0.18			-0.17			-0.15			-0.15			-0.22			-0.21		
$C_3H_5(Me)$[a]		-0.07	-0.35		-0.08	-0.33		-0.02	-0.32		-0.04	-0.30		-0.03	-0.37		-0.04	-0.36
$\varepsilon_{M=C}$	0.58			0.53			0.62			0.57			0.63			0.58		
$\rho_{M=C}$	0.19			0.19			0.19			0.19			0.19			0.19		
$\varepsilon_{M=E}$	0.01	0.01	0.03	0.02	0.01	0.04	0.01	0.04	0.01	0.03	0.07	0.02	0.01	0.04	0.01	0.03	0.04	0.02
$\rho_{M=E}$	0.27	0.25	0.27	0.22	0.21	0.22	0.27	0.25	0.27	0.23	0.21	0.23	0.27	0.25	0.27	0.23	0.21	0.23

[a] Sum of the NPA charges of all atoms of the ligand.

Table S11. NPA Charges, ellipticity (ε) and electron density (ρ) at the bond critical point of W siloxy carbenes (**I**) and the two isomeric forms (**TBP** and **SBP**) of the metallacycle intermediates.

	Mo-O-1			**Mo-N-1**			**Mo-O-3**			**Mo-N-3**			**Mo-O-5**			**Mo-N-5**		
	I	**TBP**	**SBP**	**I**	**TBP**	**SBP**	**I**	**TBP**	**SBP**	**I**	**TBP**	**SBP**	**I**	**TBP**	**SBP**	**I**	**TBP**	**SBP**
M	+1.04	+0.87	+1.08	+0.82	+0.67	+0.84	+1.14	+0.97	+1.19	+0.93	+0.76	+0.98	+1.23	+1.00	+1.28	+1.01	+0.80	+1.07
E[a]	-0.44	-0.40	-0.42	-0.22	-0.15	-0.21	-0.43	-0.37	-0.41	-0.19	-0.10	-0.17	-0.43	-0.41	-0.42	-0.20	-0.14	-0.18
X[a]	-0.18	-0.09	-0.10	-0.16	-0.12	-0.09	-0.35	-0.32	-0.30	-0.36	-0.33	-0.33	-0.36	-0.30	-0.32	-0.37	-0.33	-0.33
Y[a]	-0.35	-0.40	-0.33	-0.37	-0.42	-0.34	-0.34	-0.37	-0.30	-0.36	-0.40	-0.32	-0.36	-0.39	-0.32	-0.36	-0.41	0.33
Carbene[a]	-0.06			-0.06			-0.02			-0.02			-0.08			-0.08		
$C_3H_5(Me)$[a]		+0.01	-0.23		+0.01	-0.20		+0.01	-0.28		+0.07	-0.17		+0.09	-0.22		+0.08	-0.23
$\varepsilon_{M=C}$	0.53			0.49			0.57			0.51			0.58			0.51		
$\rho_{M=C}$	0.19			0.19			0.19			0.19			0.19			0.19		
$\varepsilon_{M=E}$	0.01	0.01	0.03	0.01	0.02	0.04	0.00	0.04	0.01	0.02	0.09	0.09	0.00	0.03	0.00	0.01	0.07	0.02
$\rho_{M=E}$	0.28	0.26	0.28	0.23	0.22	0.23	0.28	0.26	0.29	0.23	0.22	0.24	0.28	0.26	0.29	0.23	0.21	0.24

[a] Sum of the NPA charges of all atoms of the ligand.

Coordinates of all optimized extrema with E and G in

W-N-1-I

W	.423737	.525926	.329648
O	.422784	.482536	2.235478
C	2.464417	.521985	-.316911
N	-.325924	-.638070	-.746119
C	-.145580	2.200307	-.350783
H	.210624	2.962222	.371111
Si	-.114696	.692298	3.814555
H	2.874830	-.436464	.047628
H	2.514075	.478414	-1.409838
C	3.308275	1.688811	.207047
H	4.369868	1.557524	-.040402
H	1.022268	.414642	4.740864
H	-.590560	2.095932	4.004689
H	-1.233698	-.256790	4.094141
H	3.248115	1.789952	1.297561
H	2.979074	2.637241	-.230081
C	-.949008	2.751825	-1.488174
H	-.342147	3.428670	-2.105205
H	-1.320737	1.951812	-2.133172
H	-1.809589	3.334031	-1.132321
C	-1.008313	-1.642166	-1.396547
C	-1.852366	-2.521428	-.694391
C	-2.533151	-3.527476	-1.370859
C	-2.385036	-3.676709	-2.750504
C	-1.548110	-2.808525	-3.452382
C	-.863370	-1.797354	-2.786824
H	-1.961245	-2.398694	.379355
H	-3.183230	-4.199822	-.817519
H	-2.918250	-4.464410	-3.274848
H	-1.427757	-2.918928	-4.526715
H	-.209803	-1.115430	-3.321986

E = -592.238748563
G = -592.049314

W-N-1-Ianti

H	2.418620	2.948961	2.367360
O	2.008444	1.152391	-1.277861
Si	3.114316	1.448063	-2.509127
H	4.273170	2.212735	-1.960035
H	3.594996	0.154478	-3.082090
H	2.438393	2.247454	-3.573078
C	-1.023834	0.773790	-0.246367
H	-1.254784	0.275829	-1.204870
H	-1.034359	1.856987	-0.456876
C	-2.102057	0.439209	0.781862
H	-2.128620	-0.634978	0.987866
H	-1.907033	0.949930	1.729702
H	-3.100202	0.736217	0.433394
C	1.462248	2.711942	1.882272
H	1.464325	3.203812	0.902357
H	0.670831	3.185507	2.479241
C	1.241060	1.217609	1.803161
H	1.259780	0.703561	2.766374
C	1.117071	-2.728927	0.756205
C	0.283027	-3.400319	1.668345
C	2.076344	-3.465618	0.037678
C	0.408810	-4.773316	1.850962
H	-0.453406	-2.825642	2.221261
C	2.194206	-4.837510	0.230281
H	2.720268	-2.944353	-0.664869
C	1.362385	-5.498149	1.135367
H	-0.241985	-5.280661	2.558034
H	2.939873	-5.394861	-0.3
H	1.457144	-6.570162	1.2
N	0.987484	-1.368939	0.5
W	1.028200	0.324384	0.1

E = -592.236206127
G = -592.045256

W-N-1-TSrot1

W	-0.752612	-0.308584	-0.16
O	-1.833091	1.234834	0.04
C	-1.277754	-1.482479	-1.82
N	0.882276	0.274267	-0.57
C	-0.754554	-1.323510	1.44
H	-0.459046	-0.748844	2.34
Si	-2.081010	2.649396	0.92
H	-0.963203	-1.036143	-2.77
H	-0.624606	-2.365261	-1.68
C	-2.757979	-1.884530	-1.84
H	-2.952234	-2.646951	-2.61
H	-3.405914	3.202373	0.51
H	-2.083288	2.353032	2.38
H	-1.001485	3.634588	0.61
H	-3.398417	-1.025468	-2.07
H	-3.088554	-2.300564	-0.88
C	-0.871936	-2.812876	1.69
H	-1.648995	-3.019981	2.43
H	-1.144545	-3.368541	0.78
H	0.064093	-3.245573	2.06
C	2.202513	0.485226	-0.21
C	2.960801	1.440076	-0.91
C	4.293057	1.661607	-0.58
C	4.892712	0.937049	0.44
C	4.148038	-0.015190	1.14
C	2.815738	-0.243459	0.82
H	2.481984	1.994037	-1.71
H	4.867537	2.402905	-1.13
H	5.933942	1.111217	0.70
H	4.610767	-0.584468	1.94
H	2.224348	-0.982741	1.35

E = -592.204614623
G = -592.015168

W-N-1-TSrot2

W	-0.803984	-0.335008	-0.11
O	-1.932285	1.192229	-0.04
C	-1.233983	-1.582072	-1.79
N	0.846883	0.217154	-0.46
C	-0.846471	-1.346351	1.44
H	-0.927128	-2.199979	0.68
Si	-2.000149	2.862041	0.15
H	-1.122518	-0.913637	-2.66
H	-0.462965	-2.354085	-1.91
C	-2.635495	-2.205257	-1.76
H	-2.863116	-2.706336	-2.71
H	-3.275993	3.341857	-0.45
H	-1.977874	3.205601	1.60
H	-0.836220	3.502206	-0.53
H	-3.418119	-1.454932	-1.60
H	-2.732191	-2.951807	-0.97
C	-0.616179	-1.740271	2.86
H	0.284171	-2.353566	2.99
H	-0.496772	-0.840718	3.47

H	-1.466336	-2.300090	3.273832
C	2.188046	0.380104	-0.173298
C	2.831196	1.590414	-0.487761
C	4.184192	1.758089	-0.211381
C	4.921153	0.725073	0.368739
C	4.291151	-0.482519	0.674532
C	2.937804	-0.658357	0.408964
H	2.250572	2.384690	-0.947214
H	4.667602	2.700462	-0.455074
H	5.978699	0.858180	0.577876
H	4.859103	-1.293373	1.123304
H	2.437628	-1.593507	0.644139

E = -592.212039846
G = -592.022739

W-N-1-TSI

W	.435767	.592770	.312468
O	.401154	.568606	2.224594
C	2.551476	.589325	-.002382
N	-.030225	-.532468	-.959431
C	-2.811643	-.590760	1.215466
C	.036079	2.309474	-.394664
C	-2.930407	.670658	.795642
H	.247697	3.036914	.412264
Si	.157778	.116364	3.819243
H	-3.024146	1.499280	1.492815
H	-2.953758	.918397	-.261379
H	-2.805375	-.841377	2.273483
H	2.895497	-.381561	.395847
H	2.755838	.567800	-1.077726
C	3.322914	1.732096	.661950
H	4.407079	1.603345	.544055
H	1.365262	.482218	4.617839
H	-1.036104	.830667	4.364239
H	-.068055	-1.359018	3.911788
H	3.121146	1.796821	1.737109
H	3.053132	2.696299	.217797
C	-.475837	2.928444	-1.657900
H	.271630	3.606397	-2.092729
H	-.713762	2.169341	-2.406791
H	-1.377293	3.530567	-1.477990
H	-2.727086	-1.417624	.515561
C	-.475425	-1.586786	-1.722106
C	-.608561	-2.878328	-1.176437
C	-1.060106	-3.931863	-1.964337
C	-1.389961	-3.722534	-3.303832
C	-1.258384	-2.446393	-3.852972
C	-.803300	-1.386578	-3.076245
H	-.346888	-3.036212	-.133878
H	-1.155174	-4.923144	-1.529040
H	-1.743839	-4.547501	-3.915249
H	-1.509255	-2.275365	-4.896467
H	-.690958	-.392463	-3.497400

E = -670.798800370
G = -670.561758

W-N-1-II

W	.051137	.521492	.396726
O	.059656	.577099	2.345995
C	2.209762	.507073	.488822
N	-.058716	-.485760	-1.053147
C	-2.278997	-.456919	.956872
C	-.286886	2.283283	-.281847
C	-2.585488	.845813	.716096
H	-.194535	3.008194	.545954
Si	.565806	.143355	3.873330
H	-2.608711	1.577387	1.518058
H	-2.943503	1.173594	-.254120
H	-2.073877	-.802068	1.965187
H	2.483164	-.432966	1.000859
H	2.603067	.416225	-.530315
C	2.886469	1.686265	1.192561
H	3.974288	1.552931	1.263403
H	1.866790	-.593746	3.823793
H	.723092	1.365789	4.719949
H	-.459804	-.747296	4.507565
H	2.512036	1.830372	2.212331
H	2.705037	2.621989	.650395
C	-.587181	2.912422	-1.603633
H	.231149	3.582174	-1.902082
H	-.716676	2.164104	-2.387927
H	-1.492022	3.534711	-1.555423
H	-2.397583	-1.210348	.183994
C	-.167657	-1.522029	-1.947964
C	-.085073	-2.863896	-1.525940
C	-.209544	-3.899816	-2.445268
C	-.416806	-3.624891	-3.797432
C	-.495317	-2.298818	-4.225520
C	-.371846	-1.254924	-3.315707
H	.083978	-3.073076	-.473287
H	-.142607	-4.929332	-2.103571
H	-.513531	-4.437121	-4.511969
H	-.652700	-2.075744	-5.277430
H	-.427311	-.220994	-3.641886

E = -670.802414541
G = -670.560373

W-N-1-TSII

W	-.003840	-.170424	-.608832
N	-.010763	-.157901	1.160547
C	2.162280	-.216142	-.748106
H	2.565817	-.673799	.163380
H	2.481052	.841742	-.714459
C	2.782920	-.891879	-1.974844
H	2.573661	-1.968431	-1.981419
H	2.390034	-.483476	-2.911933
H	3.874655	-.774812	-2.000020
O	.070687	.679500	-2.376925
Si	.518268	1.850097	-3.469902
H	.510785	1.277563	-4.851672
H	-.454478	2.992141	-3.425424
H	1.882115	2.388605	-3.169668
C	-.716141	-1.930798	-.989346
H	-.708273	-2.112605	-2.075579
C	-1.192968	-3.093822	-.182603
H	-.475092	-3.920363	-.273341
H	-2.153868	-3.478197	-.551023
H	-1.288645	-2.842741	.875629
C	-2.522015	-.196813	-.946856
H	-2.710401	-.414078	-1.993520
H	-2.979129	-.866207	-.225950
C	-2.048160	1.049032	-.560033
H	-1.914032	1.825485	-1.306255
H	-2.163295	1.369178	.471334
C	.003210	.170136	2.493425
C	.064678	1.513993	2.912754
C	.064472	1.828930	4.267105
C	.006338	.819282	5.228428
C	-.048298	-.514853	4.822322
C	-.049490	-.842288	3.471200

H	.118481	2.296389	2.161003
H	.112971	2.870312	4.574059
H	.007584	1.069667	6.285258
H	-.088273	-1.307572	5.564652
H	-.084395	-1.878157	3.148065

E = -670.801989205
G = -670.557170

W-N-1-TBP

W	.628295	-.014849	.026414
C	.819294	.708845	1.969033
C	.886189	-3.014296	.076098
N	-1.141833	-.044925	.026749
C	.720174	-1.919125	-.984884
O	2.594143	-.096728	-.032636
H	1.792804	-2.869783	.676057
H	.962893	-4.009693	-.380622
H	.033109	-3.046854	.764872
H	-.184209	-2.101287	-1.576390
H	1.580483	-1.923251	-1.667354
H	1.750862	.459525	2.476869
C	.900898	2.083943	1.194050
C	.796421	2.013490	-.406132
H	1.775596	2.235144	-.838902
H	.071067	2.708615	1.528662
H	1.859539	2.547461	1.431189
Si	4.186309	-.431176	-.362413
H	4.848288	.767512	-.971339
H	4.914285	-.783936	.897967
H	4.311938	-1.576260	-1.320549
C	-.287776	2.887074	-1.004115
H	-1.268809	2.657889	-.578958
H	-.079427	3.952452	-.834925
H	-.346703	2.737190	-2.087201
H	-.038675	.653669	2.635581
C	-2.508213	-.150941	-.011510
C	-3.221406	.186781	-1.178161
C	-4.607453	.080806	-1.207063
C	-5.307185	-.360614	-.083257
C	-4.607355	-.700036	1.075709
C	-3.221445	-.599320	1.117591
H	-2.668599	.528474	-2.047873
H	-5.145498	.343895	-2.113828
H	-6.389907	-.441872	-.110969
H	-5.145484	-1.048190	1.953288
H	-2.668878	-.866707	2.013295

E = -670.826373168
G = -670.578966

W-N-1-TSIII

W	.674712	-.118939	-.365932
O	2.503923	.069466	.330468
C	.862573	1.981237	-.869021
N	-1.090498	-.040964	-.308144
C	1.086739	-2.571586	.140130
C	.932879	-1.273515	-1.898811
C	.684937	-1.856550	1.270345
H	1.953267	-1.442140	-2.257096
H	.165492	-1.766989	-2.492322
Si	3.911320	.846432	.760823
H	5.062363	-.093759	.576464
H	4.157712	2.065888	-.071923
H	3.860037	1.254411	2.201321
H	1.484598	-1.479012	1.905143
H	2.140979	-2.706763	-.073780
H	.133618	2.234506	-1.648699
H	1.859700	2.150940	-1.298653
C	.660454	2.904158	.340697
H	.836912	3.957736	.087220
H	-.361097	2.836016	.732074
H	1.343789	2.662274	1.165661
C	-.639499	-2.118893	1.945815
H	-1.021007	-1.238422	2.469179
H	-1.401201	-2.436396	1.228983
H	-.521352	-2.916946	2.690456
H	.403414	-3.267854	-.337794
C	-2.431509	.153538	-.085190
C	-3.371045	-.318863	-1.021575
C	-4.731763	-.128984	-.807920
C	-5.183342	.532960	.334692
C	-4.258885	1.007242	1.266175
C	-2.895732	.821783	1.064134
H	-3.010456	-.826941	-1.910778
H	-5.445116	-.498297	-1.539863
H	-6.247140	.680304	.496760
H	-4.601990	1.526923	2.156792
H	-2.172429	1.191852	1.784740

E = -670.796376011
G = -670.551233

W-N-1-IV

W	-.705762	-.184743	-.403725
O	-2.244614	.445802	.582490
C	-1.069538	-2.173229	.328427
N	1.048995	-.285846	-.274669
C	-.198058	2.716339	-.062406
C	-1.039094	-.490187	-2.255134
C	-.823051	2.525931	-1.242138
H	-2.093536	-.478537	-2.562834
H	-.343433	-.690995	-3.067990
Si	-3.279219	.587439	1.888249
H	-.277986	2.554204	-2.181450
H	-1.902148	2.428809	-1.302613
H	-.254205	-2.825614	-.000735
H	-.978762	-2.097388	1.426445
C	-2.414805	-2.802966	-.037481
H	-2.561046	-3.766550	.468596
H	-3.041747	-.511119	2.874515
H	-3.044971	1.902086	2.566222
H	-4.694464	.534161	1.412487
H	-2.479425	-2.981809	-1.116555
H	-3.261552	-2.162995	.235500
C	1.256842	3.024916	.097625
H	1.733487	2.371638	.834795
H	1.797766	2.925467	-.846801
H	1.377590	4.054980	.456567
H	-.802033	2.730601	.844890
C	2.369884	-.341446	.099548
C	2.747077	-.384791	1.455850
C	4.090537	-.452727	1.809691
C	5.080894	-.473898	.827027
C	4.715252	-.432232	-.519318
C	3.375433	-.369232	-.885439
H	1.971960	-.373657	2.216994
H	4.365890	-.489597	2.860391
H	6.128762	-.525560	1.108024
H	5.480239	-.452673	-1.290983
H	3.080790	-.343012	-1.930031

E = -670.801659134
G = -670.560090

W-N-1-TSIV

W	-.797858	-.412121	-.292493
O	-2.159136	.619953	.562098
C	-1.287762	-2.307759	.565133
N	.948569	-.522039	-.137824
C	.255435	3.077298	-.559390
C	-1.141758	-.812124	-2.119274
C	-.491142	2.657880	-1.587571
H	-.468529	-1.086619	-2.929023
H	-2.194077	-.722647	-2.423725
Si	-3.010104	1.544313	1.674328
H	-.243061	3.349494	.372429
H	-.044078	2.388672	-2.541217
H	-1.572996	2.598732	-1.520500
H	-.547925	-3.049265	.248526
H	-1.142066	-2.168784	1.650845
C	-2.703028	-2.817599	.284065
H	-2.918928	-3.727782	.859206
H	-4.218818	.789050	2.118629
H	-2.148131	1.846329	2.858031
H	-3.428212	2.824505	1.028206
H	-2.826805	-3.057259	-.777232
H	-3.470170	-2.080608	.547289
C	1.742328	3.240040	-.581897
H	2.020041	4.283447	-.386311
H	2.221913	2.633004	.194141
H	2.163410	2.948617	-1.548044
C	2.285381	-.478133	.182647
C	2.718583	-.097163	1.466776
C	4.075640	-.072694	1.771200
C	5.023054	-.420316	.807505
C	4.600519	-.799645	-.467341
C	3.246425	-.833374	-.781705
H	1.976672	.170292	2.213876
H	4.395282	.219992	2.767831
H	6.081767	-.398405	1.048968
H	5.331741	-1.075214	-1.222600
H	2.906993	-1.132811	-1.768367

E = -670.800643729
G = -670.563167

W-N-1-V

W	.210190	-.719853	.348934
O	.283729	-.460977	2.228926
C	2.184008	-1.217390	-.301002
N	-.296701	.458607	-.840824
C	-.737913	-2.289680	-.140866
H	-1.407817	-2.494729	-.974014
H	-.653214	-3.115327	.580670
Si	-.126814	-.013948	3.799572
H	2.220387	-1.270019	-1.393860
H	2.797453	-.344387	-.014594
C	2.763932	-2.496063	.312840
H	3.827250	-2.609686	.064434
H	1.120192	.016870	4.618412
H	-.756702	1.340187	3.787313
H	-1.083831	-1.010166	4.365098
H	2.236502	-3.380094	-.059220
H	2.692035	-2.504891	1.407300
C	-.749260	1.486078	-1.637333
C	-1.267011	2.667947	-1.077861
C	-1.717183	3.692173	-1.903381
C	-1.658810	3.558494	-3.291320
C	-1.146231	2.387853	-3.851594
C	-.693959	1.355951	-3.036526
H	-1.308944	2.763202	.003246
H	-2.116079	4.600794	-1.460633
H	-2.011174	4.361647	-3.932021
H	-1.098772	2.276957	-4.931486
H	-.294337	.439383	-3.459148

E = -552.933008276
G = -552.769794

W-N-1-TSA

W	-0.741020	0.240361	0.081676
C	-1.366527	0.184300	-1.970128
C	-0.358689	-1.236137	2.912691
N	1.002120	0.299779	-0.047243
C	-0.917669	0.019345	2.246459
O	-1.841926	-1.404414	0.289263
H	-0.810875	-2.130180	2.472882
H	-0.564328	-1.255866	3.991092
H	0.727442	-1.307918	2.785004
H	-0.421531	0.917929	2.650330
H	-1.991993	0.108582	2.468354
H	-2.349376	-0.203724	-2.244275
C	-1.384697	1.719078	-1.700864
C	-1.449217	2.150104	-0.138161
H	-2.509175	2.159602	0.157999
H	-0.516035	2.212748	-2.139728
H	-2.303102	2.129201	-2.127868
Si	-2.375846	-2.632409	-0.699043
H	-3.663928	-2.265919	-1.377190
H	-1.379200	-2.984882	-1.763759
H	-2.622329	-3.850542	0.134373
C	-0.777045	3.472598	0.166227
H	0.275660	3.457238	-0.129632
H	-1.266934	4.307615	-0.352296
H	-0.819783	3.678579	1.240314
H	-0.621123	-0.096520	-2.714062
C	2.338215	-0.027339	-0.146921
C	3.310307	0.874725	0.319357
C	4.660477	0.557334	0.217173
C	5.060414	-0.652758	-0.350629
C	4.098319	-1.550347	-0.816247
C	2.745230	-1.246778	-0.717461
H	2.986186	1.812553	0.759637
H	5.404676	1.259619	0.582512
H	6.116077	-0.895442	-0.429856
H	4.403830	-2.494547	-1.258500
H	1.988995	-1.938999	-1.075122

E = -670.796710688
G = -670.549434

W-N-1-SBP

W	-.637340	-.001849	-.029621
C	-.982255	-.165384	2.100901
H	-2.046119	.035597	2.290583
C	-.662289	-1.649667	2.213721
C	-1.062816	-2.023723	.790947
H	-2.165154	-2.070516	.749321
H	.416526	-1.794636	2.346851
H	-1.174578	-2.199709	3.020431
C	-1.221552	-1.007826	-1.824830
O	-1.726942	1.542114	-.209050
Si	-2.739916	2.855156	.083254
H	-3.705914	2.517174	1.170872
H	-1.915986	4.032449	.488296

H	-3.481664	3.165474	-1.173908
N	1.113271	-.054018	-.070373
H	-.539976	-1.815076	-2.105497
H	-.984444	-.161543	-2.505090
C	-2.679063	-1.425615	-2.003506
H	-3.375926	-.633262	-1.706248
H	-2.899059	-1.671647	-3.050176
H	-2.915067	-2.312382	-1.406875
C	2.465503	.205728	-.120429
C	2.964484	1.502865	.096617
C	4.333449	1.741635	.049463
C	5.224151	.700387	-.214904
C	4.734167	-.587774	-.432567
C	3.367356	-.839996	-.386100
H	2.264346	2.307519	.302109
H	4.707412	2.747520	.220122
H	6.292657	.891737	-.250751
H	5.421543	-1.403624	-.639114
H	2.975386	-1.838357	-.552477
C	-.478112	-3.310447	.231826
H	-.735009	-4.161108	.879985
H	-.846666	-3.548185	-.770782
H	.615067	-3.257660	.182301
H	-.380881	.535028	2.694626

E = -670.827992396
G = -670.582336

W-N-1-TSB

C	0.256177	-1.535367	-1.634590
C	2.287591	-1.611702	-0.385890
C	1.009979	-2.235091	-0.607051
H	2.745871	-1.236967	-1.304744
H	0.728655	-3.213049	-0.209966
H	0.201259	-1.680275	0.547716
O	1.695419	1.444071	-0.479534
Si	3.260118	2.036121	-0.619968
H	4.017305	1.255305	-1.646540
H	3.196749	3.467406	-1.041763
H	3.966173	1.937683	0.694147
C	0.805381	-0.198622	2.091418
H	0.980397	0.870425	2.303492
H	1.745039	-0.718706	2.310279
C	-0.311862	-0.716126	2.988909
H	-1.252757	-0.193112	2.793498
H	-0.490445	-1.785613	2.827809
H	-0.067143	-0.581707	4.050782
H	0.823879	-1.226190	-2.515032
C	-2.511417	0.504318	-0.156359
C	-3.151005	1.669626	-0.618033
C	-3.293272	-0.609945	0.201765
C	-4.536589	1.710679	-0.724649
H	-2.540829	2.526248	-0.887980
C	-4.678603	-0.555737	0.096008
H	-2.791891	-1.501170	0.567896
C	-5.305670	0.601554	-0.368313
H	-5.020478	2.614252	-1.085444
H	-5.273157	-1.420842	0.377233
H	-6.388152	0.639592	-0.450142
N	-1.139206	0.469358	-0.055102
W	0.559924	-0.047186	-0.059443
C	3.256880	-2.160577	0.632738
H	3.848018	-2.995558	0.231189
H	3.966623	-1.398410	0.972385
H	2.734923	-2.535040	1.520540
H	-0.760509	-1.854332	-1.850726

E = -670.790955884
G = -670.547696

W-N-1-TSB*$_{TransX}$*

O	1.024317	-1.539133	-1.150380
C	1.894462	0.939390	1.799750
C	-0.027986	-0.343009	2.161931
C	1.405161	-0.292885	2.337635
H	-0.540059	0.587615	2.409133
Si	1.921802	-2.960797	-1.094237
H	1.395158	-3.858849	-0.019468
H	1.797727	-3.643271	-2.418055
H	3.365139	-2.673039	-0.824803
H	1.996256	-1.011005	2.907221
H	1.719809	-1.280300	1.118273
H	1.295832	1.824102	2.012557
N	-0.772701	0.651541	-0.383532
C	-2.115452	0.948806	-0.390021
C	-2.571161	2.195813	0.078698
C	-3.055107	0.025802	-0.889915
C	-3.927572	2.503048	0.052879
H	-1.842838	2.910872	0.449982
C	-4.408631	0.342868	-0.907034
H	-2.699248	-0.929640	-1.263979
C	-4.852499	1.580026	-0.436458
H	-4.264903	3.470012	0.416745
H	-5.122772	-0.379263	-1.294028
H	-5.910823	1.823824	-0.454551
W	0.775411	-0.079112	0.086443
C	-0.806418	-1.604591	2.438142
H	-0.916802	-1.783451	3.516559
H	-1.811260	-1.548154	2.009804
H	-0.305991	-2.483927	2.013350
H	2.962945	1.122062	1.723553
C	2.055241	1.373865	-0.884255
H	2.031560	2.357796	-0.408086
H	3.080072	0.991292	-0.751713
C	1.712938	1.492854	-2.371613
H	2.448649	2.128146	-2.884097
H	1.707657	0.521029	-2.874303
H	0.724747	1.939932	-2.512194

E = -670.781595530
G = -670.536831

W-N-1-B

C	1.807017	-0.720831	-1.102182
C	4.067548	-0.104778	-0.165729
C	3.082354	-0.989628	-0.386679
H	1.886693	0.158446	-1.765651
H	3.192928	-1.997205	0.018557
H	1.483601	-1.576229	-1.699880
H	0.758622	-1.702920	0.636786
O	1.010682	1.601752	0.783197
Si	1.510896	3.155343	1.180453
H	2.935518	3.329284	0.769544
H	0.657736	4.150855	0.464191
H	1.381403	3.351966	2.655235
C	-0.313679	-0.649136	2.290829
H	-0.924137	0.230984	2.569758
H	0.596473	-0.607723	2.909978
C	-1.086217	-1.930358	2.576857
H	-1.995808	-1.986519	1.970996
H	-0.481004	-2.811237	2.340468

H	-1.380854	-1.997465	3.632342
H	3.961054	0.906540	-0.562841
C	5.332465	-0.397874	0.578932
H	6.215030	-0.244352	-0.055543
H	5.452941	0.267267	1.443938
H	5.353968	-1.430029	0.942123
N	-1.183211	-0.385731	-0.562572
C	-2.379943	-0.381310	-1.246847
C	-2.729667	-1.485933	-2.042692
C	-3.261780	0.709853	-1.157086
C	-3.936032	-1.490833	-2.734669
H	-2.044017	-2.325456	-2.101094
C	-4.466610	0.690868	-1.851176
H	-2.987317	1.560360	-0.539753
C	-4.808957	-0.406158	-2.642790
H	-4.196924	-2.348976	-3.348087
H	-5.142095	1.538547	-1.774056
H	-5.750642	-0.415824	-3.183916
W	0.300437	-0.100031	0.312465

E = -670.815785330
G = -670.576108

W-N-1-TSC

C	1.089398	-1.374432	-0.952456
C	3.499682	-1.901418	-1.469983
C	2.351778	-2.137346	-0.816736
H	1.087958	-0.807400	-1.901987
H	2.322427	-2.989981	-0.132852
H	0.243006	-2.066218	-0.995264
H	0.867884	-0.951753	1.431324
O	0.874274	1.947726	-0.678421
Si	0.333548	3.180977	-1.668977
H	0.351808	4.467453	-0.907594
H	1.242938	3.293556	-2.849906
H	-1.060354	2.920352	-2.151612
C	-0.072595	1.078287	2.267151
H	-0.666081	1.963755	1.981943
H	0.834299	1.466045	2.750541
C	-0.870611	0.230189	3.249639
H	-1.806980	-0.117649	2.803245
H	-0.307861	-0.658832	3.558270
H	-1.122701	0.790755	4.159661
C	2.393710	-0.476039	1.756248
H	2.741941	-1.469473	1.491634
H	2.139536	-0.332237	2.802567
C	2.744473	0.597831	0.955741
H	2.723435	1.612494	1.340297
H	3.299570	0.423031	0.038888
H	3.536456	-1.068672	-2.176013
C	4.752312	-2.709794	-1.330938
H	5.053104	-3.149922	-2.290489
H	5.595907	-2.093069	-0.994635
H	4.625165	-3.526547	-0.613156
W	0.409398	0.332792	0.278465
N	-1.268662	-0.070586	-0.056709
C	-2.546868	-0.525977	-0.270969
C	-2.969718	-1.741946	0.297928
C	-3.442736	0.210668	-1.067723
C	-4.260758	-2.205348	0.071226
H	-2.270111	-2.299586	0.913150
C	-4.731266	-0.263334	-1.285385
H	-3.107668	1.146480	-1.504178
C	-5.145594	-1.469975	-0.718810
H	-4.578926	-3.145097	0.514196
H	-5.416993	0.311653	-1.901592
H	-6.153641	-1.835340	-0.892398

E = -749.354925499
G = -749.061947

W-N-1-C

C	-1.237547	0.563102	-1.644611
C	-3.586006	-0.300309	-1.969460
C	-2.719541	0.663612	-1.620357
H	-0.920157	-0.347664	-2.185053
H	-3.135573	1.619660	-1.295192
H	-0.780463	1.422093	-2.143347
H	1.323867	3.138959	0.201532
O	-1.334825	-1.411408	0.607172
Si	-2.577866	-2.438675	1.102354
H	-1.974990	-3.544932	1.903297
H	-3.561043	-1.684593	1.934552
H	-3.250109	-3.001624	-0.102716
C	-0.065453	0.557753	2.381103
H	0.137240	-0.478250	2.716746
H	-1.044621	0.834645	2.800230
C	1.031705	1.466867	2.923514
H	2.018140	1.141602	2.579207
H	0.897422	2.505001	2.604109
H	1.044182	1.467840	4.021213
C	0.354633	3.215236	-0.301236
H	0.515005	2.954972	-1.353142
H	0.048750	4.270051	-0.270635
C	-0.691292	2.318228	0.371913
H	-0.802212	2.645908	1.410259
H	-1.664686	2.502269	-0.098816
H	-3.193102	-1.255529	-2.323020
C	-5.077124	-0.162322	-1.945362
H	-5.506942	-0.296504	-2.946580
H	-5.543830	-0.921181	-1.303990
H	-5.382881	0.822257	-1.577763
N	1.393238	0.057597	-0.192645
C	2.674141	-0.328817	-0.527109
C	3.575772	0.620656	-1.038765
C	3.097688	-1.659429	-0.358572
C	4.871572	0.241108	-1.372529
H	3.239649	1.644702	-1.165143
C	4.396560	-2.025338	-0.693496
H	2.397001	-2.388840	0.037578
C	5.288236	-1.079408	-1.201189
H	5.560879	0.982189	-1.767811
H	4.714738	-3.055378	-0.557563
H	6.301753	-1.370223	-1.461730
W	-0.289465	0.126864	0.274550

E = -749.401898211
G = -749.108807

W-N-1'-I

O	2.004769	-0.765371	-0.297429
Si	3.375134	-1.685596	0.002854
H	4.116374	-1.130312	1.176230
H	2.982480	-3.098878	0.287733
H	4.250661	-1.646617	-1.206386
C	0.353043	1.721366	-1.583185
H	0.244725	1.156125	-2.525195
H	1.376981	2.132886	-1.593998
C	-0.655876	2.867485	-1.549897
H	-1.682438	2.488633	-1.538908
H	-0.524256	3.475891	-0.650145
H	-0.552699	3.525781	-2.423104
C	0.464973	1.357002	1.495362

C	-2.433904	-1.172547	-0.057376
N	-1.221508	-0.393704	-0.033735
W	0.399423	0.240717	-0.038994
C	-0.417335	1.833610	2.607547
H	-0.047487	1.506633	3.589170
H	-0.459393	2.930987	2.636709
H	-1.438287	1.463215	2.486247
H	1.518828	1.690951	1.579145
C	-2.556929	-1.854732	-1.429680
H	-1.708026	-2.523064	-1.604996
H	-3.477939	-2.445219	-1.482269
H	-2.579463	-1.108157	-2.229165
C	-2.370436	-2.230673	1.055780
H	-2.248371	-1.753074	2.032331
H	-3.290420	-2.824967	1.072663
H	-1.525327	-2.907403	0.895604
C	-3.628871	-0.233542	0.172821
H	-3.668756	0.534180	-0.605103
H	-4.568160	-0.796791	0.154103
H	-3.543787	0.265550	1.142293

E = -518.479444240
G = -518.258448

W-N-1'-Ianti

O	1.847973	-0.946787	-0.268977
Si	2.781235	-2.335919	-0.398070
H	3.427431	-2.628599	0.916419
H	1.926436	-3.495213	-0.798719
H	3.831713	-2.112494	-1.435605
C	0.392741	1.658606	-1.564700
H	0.217341	1.089715	-2.494602
H	1.446335	1.985465	-1.605164
C	-0.520809	2.881829	-1.527345
H	-1.573085	2.584392	-1.489069
H	-0.322309	3.485806	-0.636843
H	-0.385095	3.519953	-2.411005
C	0.572455	1.383753	1.506562
C	-2.635253	-0.827640	0.168763
N	-1.325319	-0.233033	0.101025
W	0.353340	0.213396	0.011609
C	1.946761	1.901973	1.875054
H	1.962475	3.000559	1.855899
H	2.234671	1.592642	2.888982
H	2.738176	1.559390	1.196914
H	-0.224366	1.693607	2.184564
C	-3.314715	-0.672941	-1.201300
H	-2.738306	-1.184952	-1.977993
H	-4.321364	-1.103771	-1.177128
H	-3.395853	0.383380	-1.472739
C	-2.505756	-2.315725	0.530538
H	-2.005898	-2.432160	1.497111
H	-3.493460	-2.785164	0.593383
H	-1.919850	-2.845519	-0.227242
C	-3.444916	-0.088910	1.246627
H	-3.526811	0.974084	1.002627
H	-4.453803	-0.508778	1.321447
H	-2.958392	-0.180924	2.222156

E = -518.477068862
G = -518.255385

W-N-1'-TSI

W	-0.288430	-0.300334	0.098275
N	1.395082	-0.072888	-0.306151
C	-0.639238	-2.110695	-0.998778
H	-0.707524	-1.797250	-2.055511
H	0.235921	-2.763392	-0.928542
C	-1.901860	-2.878194	-0.599184
H	-2.796734	-2.246106	-0.626219
H	-1.812046	-3.274866	0.417844
H	-2.085957	-3.726153	-1.272594
O	-1.927370	0.608670	-0.345830
Si	-3.160748	1.413422	-1.136260
H	-4.380022	1.434222	-0.271989
H	-3.478947	0.725362	-2.424672
H	-2.748869	2.822559	-1.427231
C	-0.257912	-1.035170	1.852896
H	-1.312701	-1.137882	2.174687
C	0.735824	-1.479019	2.881673
H	0.604185	-0.944581	3.833138
H	0.617862	-2.548404	3.106340
H	1.760811	-1.320512	2.538193
C	-0.309999	2.467934	2.063034
H	0.420072	2.149179	2.801251
H	-1.348489	2.228081	2.272402
C	0.047634	3.132694	0.962511
H	1.085476	3.383764	0.761571
H	-0.683115	3.456997	0.226946
C	2.685764	0.290878	-0.828970
C	3.548982	0.831849	0.322607
H	3.083092	1.713276	0.772372
H	4.542599	1.112618	-0.043205
H	3.667842	0.073634	1.101916
C	3.337240	-0.968626	-1.423623
H	3.442741	-1.742693	-0.658131
H	4.330354	-0.734355	-1.822417
H	2.724424	-1.371097	-2.235680
C	2.525818	1.363480	-1.918646
H	3.500786	1.654588	-2.324507
H	2.041359	2.255948	-1.511043
H	1.911051	0.983963	-2.741064

E = -597.037235518
G = -596.767728

W-N-1'-II

W	-0.241645	0.187045	0.040856
N	1.454839	-0.255658	0.019448
C	-0.724395	-0.973028	1.812133
H	-0.917022	-2.000747	1.455376
H	0.160466	-1.040533	2.454743
C	-1.915730	-0.496154	2.647712
H	-2.826146	-0.387580	2.047874
H	-1.711788	0.482798	3.097903
H	-2.148855	-1.190656	3.466222
O	-2.074349	-0.224151	-0.543245
Si	-3.401787	-1.197755	-0.774145
H	-4.644345	-0.478336	-0.352508
H	-3.293360	-2.475005	-0.000376
H	-3.530320	-1.544269	-2.228425
C	-0.186170	1.975326	0.745233
H	-1.217271	2.349847	0.870993
C	0.860729	2.944027	1.191273
H	0.758849	3.911058	0.677961
H	0.752893	3.154786	2.264364
H	1.867604	2.558379	1.019290
C	-0.268505	1.791624	-2.056249
H	0.574829	2.461545	-1.927974
H	-1.257153	2.233499	-1.979826
C	-0.102791	0.508740	-2.488286

H	0.884054	0.127237	-2.727371
H	-0.956276	-0.091152	-2.785165
C	2.736394	-0.898046	-0.103452
C	3.681298	0.019045	-0.898262
H	4.672742	-0.437794	-0.988435
H	3.790562	0.985250	-0.397024
H	3.295612	0.197825	-1.906862
C	3.298903	-1.126304	1.309919
H	3.403409	-0.174798	1.839240
H	4.282379	-1.606253	1.257926
H	2.630294	-1.768232	1.890218
C	2.576753	-2.245879	-0.826733
H	1.892737	-2.896658	-0.273384
H	3.542027	-2.756045	-0.916149
H	2.172840	-2.100239	-1.833826

E = -597.040503696
G = -596.766106

W-N-1'-TSII

W	-0.278518	-0.183451	-0.114519
O	-2.176638	0.001568	0.411791
N	1.433212	0.165537	0.055938
C	-0.404551	-2.329121	1.302578
C	-0.235825	-1.735219	-1.264255
C	-0.284316	-1.209249	2.095100
H	-1.262333	-2.041862	-1.523310
Si	-3.686842	0.691190	0.448514
H	-4.713219	-0.382440	0.648100
H	-4.011386	1.418351	-0.820493
H	-3.797110	1.659932	1.587126
H	-1.166160	-0.757252	2.536025
H	-1.380206	-2.750095	1.082010
H	0.454770	-2.946377	1.063806
C	2.753253	0.649937	0.359706
H	0.678315	-0.942312	2.518202
C	0.818677	-2.571277	-1.911934
H	0.671891	-3.640829	-1.705013
H	1.820806	-2.280332	-1.591459
H	0.762268	-2.460828	-3.003884
C	-0.679640	1.501366	-1.428559
H	0.078187	1.545210	-2.219908
H	-1.642474	1.325475	-1.928495
C	-0.729760	2.848341	-0.694089
H	-1.010357	3.672978	-1.363168
H	0.241929	3.107154	-0.256333
H	-1.459794	2.848423	0.125782
C	3.668500	-0.550662	0.655331
H	4.683926	-0.210735	0.886068
H	3.718351	-1.219483	-0.208943
H	3.295876	-1.122013	1.511395
C	3.279716	1.419848	-0.863416
H	4.291772	1.794288	-0.674193
H	2.631225	2.270728	-1.090024
H	3.308003	0.769321	-1.742359
C	2.703349	1.580452	1.583585
H	3.702011	1.966263	1.815435
H	2.332427	1.046466	2.464207
H	2.041635	2.430885	1.394432

E = -597.040641150
G = -596.763410

W-N-1'-TBP

W	-0.276996	-0.014004	-0.104831
C	-0.543552	-2.151858	0.104216
O	-2.261642	0.010182	-0.107502
C	-0.376193	1.632797	1.162708
H	-1.358984	1.668672	1.640315
C	-0.413226	1.486527	-1.543979
C	-0.448659	2.393470	-0.245132
H	-1.348238	1.530351	-2.101577
H	-1.383197	2.955855	-0.257945
H	0.411230	3.064360	-0.279252
Si	-3.852643	-0.354317	-0.389654
H	-4.366543	0.412892	-1.571729
H	-4.688899	0.007299	0.800104
H	-4.041741	-1.815764	-0.667975
H	0.299938	-2.719913	-0.301522
H	-1.447925	-2.458325	-0.436599
C	-0.706779	-2.447200	1.601470
H	0.180733	-2.154620	2.176867
H	-0.865630	-3.517697	1.787305
H	-1.567665	-1.920604	2.030550
C	0.712247	2.121809	2.095005
H	0.763745	1.491228	2.988568
H	0.520395	3.150260	2.431151
H	1.692369	2.097492	1.611168
H	0.449021	1.695482	-2.172971
N	1.474048	-0.149166	-0.164377
C	2.885528	-0.375656	-0.302322
C	3.470809	-0.750798	1.069533
H	2.998126	-1.660293	1.451785
H	3.304114	0.051987	1.793494
H	4.548941	-0.928056	0.991234
C	3.550908	0.907065	-0.829783
H	3.129330	1.189660	-1.799140
H	4.627835	0.752888	-0.956373
H	3.403997	1.738377	-0.133739
C	3.110092	-1.523400	-1.302262
H	4.181157	-1.711662	-1.433473
H	2.680315	-1.272343	-2.276689
H	2.640042	-2.444647	-0.946983

E = -597.064181754
G = -596.784739

W-N-1'-TSIII

O	2.212056	-0.119228	0.167120
C	0.404473	-2.129193	0.894827
C	0.310407	-0.804073	-2.103160
C	0.580217	-2.585696	-0.408294
H	1.281390	-0.938647	-2.591152
H	-0.539990	-1.094801	-2.717241
Si	3.717847	0.482812	0.524694
H	-0.220541	-3.109814	-0.922295
H	1.577371	-2.708092	-0.814957
H	3.984392	1.793293	-0.150890
H	3.869769	0.677060	2.003408
H	4.761090	-0.494286	0.073663
C	-0.811838	-2.477739	1.715946
H	-1.023157	-1.719590	2.474270
H	-1.700151	-2.593890	1.090275
H	-0.642005	-3.426917	2.241460
H	1.314151	-1.920554	1.454175
C	0.622760	2.093079	-0.375100
H	1.585731	2.278250	-0.869980
H	-0.144062	2.582989	-0.986070
C	0.641817	2.718938	1.026322
H	1.387850	2.248544	1.680090
H	0.882402	3.790050	0.996630

H	-0.329390	2.621536	1.526907
W	0.287724	-0.054330	-0.319937
N	-1.444441	0.125123	-0.102065
C	-2.825047	0.451597	0.141820
C	-3.710043	-0.626934	-0.506144
H	-4.769230	-0.380025	-0.375998
H	-3.502395	-0.699977	-1.577804
H	-3.529851	-1.606176	-0.052721
C	-3.107571	0.530996	1.650580
H	-2.460575	1.274697	2.125291
H	-4.149084	0.820369	1.827611
H	-2.936076	-0.434518	2.133370
C	-3.115084	1.815071	-0.510569
H	-2.906361	1.779543	-1.583642
H	-4.166553	2.087529	-0.368443
H	-2.492103	2.596141	-0.066249

E = -597.033187925
G = -596.754622

W-N-1'-V

W	0.343263	-0.261841	0.175528
O	1.725377	0.979545	-0.247891
C	0.655470	-2.022845	-1.003342
N	-1.357290	0.032552	-0.012166
C	0.483187	-0.973114	1.933040
H	-0.259613	-1.208840	2.692134
H	1.522628	-1.104113	2.269936
Si	2.671459	2.369027	-0.248185
H	0.604667	-1.676168	-2.050897
H	-0.176277	-2.722017	-0.872722
C	1.990371	-2.730935	-0.746711
H	2.167826	-3.528084	-1.480686
H	3.706601	2.233628	-1.315302
H	3.333247	2.526983	1.081362
H	1.818375	3.563293	-0.527278
H	2.846132	-2.047409	-0.810204
H	2.004890	-3.183891	0.249704
C	-2.718958	0.470373	-0.184462
C	-3.501787	0.116060	1.089755
H	-3.473994	-0.962522	1.268591
H	-4.547396	0.427354	0.992611
H	-3.069048	0.620028	1.958864
C	-2.749685	1.987945	-0.422904
H	-3.779610	2.334758	-0.559548
H	-2.177430	2.249202	-1.318628
H	-2.318166	2.519970	0.430508
C	-3.312383	-0.270022	-1.393678
H	-4.355990	0.025622	-1.545072
H	-3.276668	-1.351771	-1.236459
H	-2.751309	-0.035163	-2.303329

E = -479.174358940
G = -478.976711

W-N-1'-TSA

O	-1.818271	-1.025607	0.263394
C	-0.771634	0.105222	-2.072175
H	-1.805725	-0.064323	-2.377598
C	-0.437742	2.210656	-0.415417
C	-0.436468	1.619296	-1.931690
H	-1.468482	2.520635	-0.185654
H	-1.214793	2.193073	-2.440018
H	0.540272	1.850941	-2.358651
Si	-2.625241	-2.159353	-0.644262
H	-3.222980	-3.182743	0.270668
H	-3.743701	-1.536286	-1.430002
H	-1.726293	-2.868847	-1.614063
C	0.540899	3.346170	-0.202076
H	0.520914	3.669839	0.843201
H	1.563200	3.035310	-0.435202
H	0.296883	4.217514	-0.824837
H	-0.084239	-0.410684	-2.741050
C	-0.558084	0.189991	2.192255
H	-0.363067	-0.824067	2.567624
H	0.247857	0.829194	2.589424
C	-1.920479	0.668740	2.694225
H	-2.720486	0.044761	2.285382
H	-1.991976	0.627680	3.789396
H	-2.124340	1.707808	2.402670
N	1.416428	-0.183419	0.019330
C	2.663109	-0.908433	0.087506
C	2.379140	-2.417788	0.096260
H	1.842685	-2.712638	-0.810654
H	3.315385	-2.983829	0.145350
H	1.766106	-2.687688	0.961274
C	3.503347	-0.530894	-1.142641
H	3.697606	0.545581	-1.163008
H	4.464437	-1.055007	-1.117517
H	2.984301	-0.807835	-2.065115
C	3.387771	-0.490028	1.376257
H	4.346402	-1.013077	1.457484
H	3.578269	0.587167	1.379017
H	2.783408	-0.734398	2.254301
W	-0.272922	0.216406	0.017564

E = -597.038103619
G = -596.758993

W-N-1'-SBP

O	1.790533	-1.151784	-0.073555
C	0.688766	1.109511	-1.835507
C	0.476784	0.387410	2.122058
C	0.095144	2.138250	0.719267
C	-0.249906	1.725218	2.145389
H	1.138596	2.499411	0.716328
Si	3.074337	-2.184928	0.257034
H	3.837147	-1.686331	1.440623
H	2.551045	-3.555081	0.540125
H	3.969830	-2.227082	-0.936827
H	0.048297	2.429903	2.939902
H	-1.331713	1.567474	2.233969
H	0.738562	0.212602	-2.489371
H	-0.169173	1.687105	-2.188502
C	1.982272	1.911953	-1.962859
H	2.188236	2.177753	-3.007809
H	1.928529	2.847693	-1.397268
H	2.853432	1.356107	-1.596372
N	-1.365152	-0.399517	-0.139489
C	-2.645175	-1.053150	-0.259303
C	-2.966720	-1.758025	1.067726
H	-2.987746	-1.037443	1.890362
H	-3.944173	-2.248945	1.011283
H	-2.211394	-2.516996	1.293812
C	-2.581337	-2.077544	-1.403335
H	-3.547136	-2.580603	-1.520356
H	-2.333544	-1.584552	-2.348288
H	-1.820074	-2.837018	-1.198862
C	-3.708185	0.014407	-0.563503
H	-3.475469	0.533870	-1.497561
H	-4.696229	-0.448219	-0.660074

H	-3.748256	0.754711	0.240432
H	1.545613	0.506663	2.351080
H	0.076428	-0.424688	2.741871
C	-0.801302	3.180870	0.071333
H	-1.827642	2.811443	-0.029136
H	-0.838620	4.093114	0.685178
H	-0.457341	3.478680	-0.924115
W	0.310295	0.044823	-0.012590

E = -597.069067387
G = -596.791762

W-N-1'-TSB

C	0.380499	-1.474531	-1.817910
C	2.358972	-1.236153	-0.512757
C	1.257068	-2.099890	-0.831148
H	2.701926	-0.635348	-1.358582
H	1.207467	-3.158946	-0.565981
H	0.318826	-1.878452	0.315446
O	1.094317	1.589781	-0.466455
Si	0.920912	3.239997	-0.690466
H	1.494401	3.616460	-2.018469
H	-0.521984	3.635351	-0.647912
H	1.660517	3.963032	0.388461
H	0.885304	-0.973870	-2.647080
C	3.438793	-1.648729	0.455034
H	4.229825	-2.233697	-0.035467
H	3.921440	-0.781311	0.919043
H	3.039576	-2.270878	1.264006
H	-0.527501	-1.996007	-2.108297
C	0.642103	-0.489374	2.035522
H	-0.136593	-1.125713	2.464558
H	1.597314	-0.993457	2.204842
C	0.635632	0.873796	2.743706
H	0.740270	0.742902	3.829575
H	1.458443	1.515281	2.412455
H	-0.300040	1.419077	2.574754
N	-1.441165	-0.005927	-0.003011
C	-2.859343	-0.260689	0.026519
C	-3.463155	0.189616	-1.313838
H	-3.028260	-0.376216	-2.143128
H	-4.546635	0.029410	-1.317040
H	-3.269311	1.252667	-1.484348
C	-3.466360	0.556584	1.179209
H	-4.549636	0.401945	1.226575
H	-3.032273	0.253369	2.136583
H	-3.273991	1.623951	1.036520
C	-3.110020	-1.759810	0.250658
H	-4.184246	-1.970741	0.288807
H	-2.672297	-2.348720	-0.560921
H	-2.658148	-2.086449	1.191912
W	0.310829	-0.129260	-0.097798

E = -597.028200050
G = -596.753988

W-N-1'-B

C	0.956319	-1.652104	-0.884710
C	3.451410	-1.322945	-0.669673
C	2.293027	-1.874729	-0.272795
H	1.038103	-1.270197	-1.917612
H	2.307132	-2.526137	0.603222
H	0.356386	-2.564674	-0.898710
H	0.165213	-1.338353	1.214370
O	1.043268	1.426401	-0.486045
Si	2.203429	2.621791	-0.692002
H	3.063515	2.270733	-1.861451
H	1.522486	3.926215	-0.950479
H	3.047338	2.737352	0.535373
C	-0.151741	0.666770	2.175627
H	-0.512085	1.702434	2.029757
H	0.895902	0.747085	2.509898
C	-0.984779	-0.027155	3.245091
H	-2.030504	-0.116417	2.934451
H	-0.614535	-1.040073	3.431716
H	-0.964201	0.520613	4.196588
H	3.446686	-0.667422	-1.542859
C	4.778741	-1.554041	-0.016522
H	5.495947	-2.003068	-0.715900
H	5.228697	-0.613775	0.327732
H	4.688967	-2.220184	0.847185
N	-1.696881	-0.256184	-0.244148
C	-3.062630	-0.225682	-0.707239
W	-0.024254	-0.027561	0.148678
C	-3.067019	-0.137346	-2.241656
H	-2.551393	-0.997532	-2.678769
H	-4.095177	-0.123279	-2.618477
H	-2.564599	0.775350	-2.577105
C	-3.753892	-1.518541	-0.246615
H	-3.735532	-1.595282	0.844034
H	-4.796711	-1.532240	-0.581173
H	-3.244120	-2.393713	-0.659252
C	-3.765927	0.999673	-0.103067
H	-3.276471	1.923948	-0.425341
H	-4.812394	1.033644	-0.424158
H	-3.740879	0.958079	0.989608

E = -597.057687313
G = -596.786203

W-N-1'-TSC

W	0.015584	0.148152	0.319976
C	1.287240	-0.976587	-1.111413
C	3.774089	-0.620338	-1.339395
C	2.713956	-1.337816	-0.937756
H	1.180655	-0.241849	-1.930331
H	2.908083	-2.300138	-0.456291
H	0.717974	-1.862367	-1.403576
H	0.711024	-1.224414	1.243531
O	0.129799	2.017024	-0.176484
Si	-0.641374	3.244705	-1.007688
H	0.233780	3.701919	-2.130716
H	-1.952855	2.787668	-1.569877
H	-0.885930	4.390119	-0.078320
C	-0.864294	0.220506	2.315351
H	-1.664300	0.958674	2.138097
H	-0.158283	0.701950	3.004927
C	-1.457323	-1.022804	2.966388
H	-2.204962	-1.490444	2.318663
H	-0.687719	-1.778716	3.162164
H	-1.941923	-0.792052	3.924669
C	1.970397	-0.501297	1.914179
H	2.622656	-1.268685	1.508898
H	1.581899	-0.701398	2.909230
C	2.089460	0.800313	1.448895
H	1.737086	1.639130	2.040517
H	2.771958	1.017738	0.633150
H	3.598699	0.332703	-1.843695
C	5.204586	-1.029519	-1.170348
H	5.714459	-1.115550	-2.138676
H	5.769405	-0.290887	-0.586816

H	5.287640	-1.994946	-0.660845
N	-1.430033	-0.511784	-0.401863
C	-2.583580	-1.112428	-1.018649
C	-2.558311	-2.629067	-0.769796
H	-3.429619	-3.106150	-1.230991
H	-1.655155	-3.075102	-1.196369
H	-2.571012	-2.844923	0.302105
C	-2.531592	-0.822132	-2.528519
H	-2.547773	0.255644	-2.714302
H	-1.620444	-1.235684	-2.970834
H	-3.393869	-1.273510	-3.030644
C	-3.848879	-0.489625	-0.406102
H	-3.893327	-0.678849	0.670208
H	-3.861647	0.592225	-0.567440
H	-4.743102	-0.920130	-0.869155

E = -675.594068794
G = -675.267867

W-N-1'-C

C	-1.099988	1.175644	-1.210231
C	-3.583084	0.716863	-1.281163
C	-2.518089	1.395817	-0.824992
H	-1.036798	0.509214	-2.088282
H	-2.704298	2.192668	-0.101365
H	-0.602904	2.114679	-1.466996
H	2.118643	2.700857	0.723003
O	-1.149303	-1.472434	0.108685
Si	-2.511334	-2.434863	0.353065
H	-3.490848	-1.750326	1.246388
H	-3.139401	-2.731125	-0.967265
H	-2.062602	-3.709672	0.989722
C	0.487372	-0.422537	2.315023
H	0.468421	-1.527961	2.277301
H	-0.383639	-0.120660	2.916925
C	1.783133	0.015306	2.990727
H	2.654790	-0.389766	2.467108
H	1.890648	1.104658	3.008143
H	1.832419	-0.330037	4.031758
C	1.092496	3.023126	0.520378
H	0.997021	3.122688	-0.566225
H	0.969661	4.027051	0.949892
C	0.081077	2.036168	1.114922
H	0.256089	1.990606	2.194130
H	-0.928730	2.453066	1.005315
H	-3.426123	-0.066544	-2.025560
C	-5.001351	0.971492	-0.872190
H	-5.619855	1.261973	-1.731419
H	-5.467056	0.074337	-0.444043
H	-5.065707	1.770529	-0.126841
W	0.051581	-0.009923	0.229968
N	1.620206	-0.081887	-0.504772
C	2.807248	-0.462844	-1.234696
C	2.490318	-0.415623	-2.737822
H	3.377266	-0.683939	-3.321461
H	1.689039	-1.118756	-2.985579
H	2.172870	0.588590	-3.032978
C	3.928859	0.531780	-0.897988
H	3.639225	1.548032	-1.178468
H	4.144575	0.519773	0.174186
H	4.843718	0.268078	-1.439249
C	3.216483	-1.885348	-0.822481
H	3.420334	-1.931613	0.251343
H	2.419866	-2.599054	-1.054532
H	4.121165	-2.191320	-1.358529

E = -675.643073598
G = -675.315953

W-O-1-I

O	1.590019	0.090779	0.382491
C	-1.346780	-0.764991	1.099042
H	-0.993999	-0.407956	2.082069
Si	3.250249	-0.213813	0.439062
H	3.945512	1.084412	0.673653
H	3.526623	-1.156287	1.561923
H	3.701997	-0.811655	-0.852066
C	-2.531701	-1.681268	1.153414
H	-3.402595	-1.161808	1.575370
H	-2.804224	-2.044967	0.159691
H	-2.337148	-2.548913	1.797513
O	-0.625909	-0.943082	-1.672789
C	-0.982759	1.848434	-0.505647
H	-0.319173	2.335598	-1.241983
H	-1.960677	1.759696	-0.993486
C	-1.093720	2.709087	0.755286
H	-0.142519	2.777735	1.296195
H	-1.396467	3.735384	0.511272
H	-1.836153	2.295646	1.445205
W	-0.181997	-0.117739	-0.254762

E = -381.161417660
G = -381.054605

W-O-1-Ianti

W	-0.202516	-0.421289	-0.020090
O	1.452502	0.491309	0.067775
C	-1.364544	0.025385	1.426784
H	-2.043609	-0.735098	1.821976
Si	3.140485	0.585058	0.011194
H	3.509930	1.582403	-1.034059
H	3.632860	1.030721	1.346329
H	3.712731	-0.751087	-0.327814
C	-1.376570	1.331202	2.181892
H	-1.131158	1.175483	3.240654
H	-0.671473	2.068346	1.783530
H	-2.376996	1.782623	2.148749
O	-0.396644	-2.092000	-0.265433
C	-1.286256	0.455254	-1.642228
H	-0.648304	0.291574	-2.528796
H	-2.192327	-0.138845	-1.808250
C	-1.640834	1.938575	-1.513450
H	-0.761763	2.560203	-1.306639
H	-2.090098	2.320401	-2.439059
H	-2.358061	2.100912	-0.703363

E = -381.159026279
G = -381.051612

W-O-1-TSrot1

W	0.155577	-0.058498	0.228393
O	-1.497972	0.371002	-0.552300
C	0.961576	-1.501886	-0.729012
H	0.297421	-2.362034	-0.892335
Si	-3.150646	0.004631	-0.518283
H	-3.816725	0.926833	-1.481335
H	-3.361318	-1.413385	-0.935676
H	-3.672255	0.218242	0.862258
C	2.430035	-1.819579	-0.915073
H	2.622293	-2.124156	-1.952671

H	3.083194	-0.962854	-0.713805
H	2.759249	-2.643846	-0.267468
O	-0.209720	-0.546138	1.839514
C	1.475823	1.567028	0.423409
H	1.150265	2.260221	1.208349
H	2.409901	1.107442	0.796135
C	1.709774	2.289266	-0.911493
H	0.810991	2.820526	-1.240818
H	2.512667	3.030126	-0.820010
H	1.998960	1.598988	-1.712413

E = -381.116970212
G = -381.012385

W-O-1-TSrot2

W	-0.228871	-0.004574	0.249897
O	1.470806	-0.450495	-0.417460
C	-0.987391	1.473490	-0.600472
H	-1.933059	0.856325	-0.374010
Si	3.137322	-0.160224	-0.444941
H	3.765525	-1.262658	-1.227615
H	3.403401	1.151814	-1.104856
H	3.658235	-0.149169	0.952403
C	-1.219807	2.912814	-0.888978
H	-1.728205	3.436719	-0.068545
H	-0.258240	3.408084	-1.057368
H	-1.814977	3.053836	-1.800202
O	-0.081854	0.300709	1.936656
C	-1.576213	-1.656888	0.132203
H	-1.091220	-2.465191	0.698523
H	-2.513456	-1.437973	0.659900
C	-1.851213	-2.091968	-1.313324
H	-0.927531	-2.299783	-1.865461
H	-2.450309	-3.010375	-1.334763
H	-2.400124	-1.326413	-1.871393

E = -381.125311107
G = -381.020697

W-O-1-II

O	1.489940	-0.260458	0.487127
C	-0.013608	-2.726555	-0.356394
C	-1.584227	0.387997	1.117779
C	-0.790660	-2.552577	0.732624
H	-1.111667	0.577272	2.095705
H	-0.364528	-2.475533	1.728970
H	-1.873764	-2.569706	0.664656
H	1.066512	-2.797078	-0.272704
C	-3.079219	0.477379	1.132677
H	-3.398558	1.487708	1.422437
H	-3.510690	0.252626	0.154676
H	-3.512051	-0.208660	1.874028
H	-0.448251	-2.875431	-1.339999
O	-1.161818	-0.298183	-1.659912
C	0.253716	2.048360	-0.735546
H	1.057197	1.959314	-1.487452
H	-0.596718	2.502221	-1.257066
C	0.709927	2.953618	0.408999
H	1.541894	2.515186	0.971072
H	1.044816	3.932847	0.042756
H	-0.105259	3.129138	1.120385
Si	3.159438	-0.376306	0.428107
H	3.711320	-0.146804	1.796572
H	3.554991	-1.745189	-0.033655
H	3.719171	0.635229	-0.518497
W	-0.278474	0.027499	-0.234783

E = -459.723367629
G = -459.567073

W-O-1-TSII

O	1.413765	-0.525335	0.490700
C	-0.512866	-2.153516	-0.656513
C	-1.508827	0.127283	1.248875
C	-1.338534	-2.022578	0.478484
H	-0.998559	-0.014385	2.211013
H	-0.973615	-2.353894	1.446042
H	-2.417133	-2.008184	0.360236
H	0.460814	-2.618116	-0.541937
C	-2.971017	0.426381	1.366998
H	-3.092061	1.404620	1.850176
H	-3.459313	0.469934	0.391063
H	-3.489577	-0.302735	2.002942
H	-0.982041	-2.238681	-1.632273
O	-1.312902	0.386642	-1.602346
C	0.787131	1.972320	-0.557209
H	1.532792	1.767838	-1.345789
H	0.080105	2.685821	-0.999441
C	1.478018	2.605686	0.652723
H	2.187998	1.918262	1.123637
H	2.033076	3.511716	0.376491
H	0.751199	2.895941	1.421050
Si	3.008382	-1.010778	0.410260
H	3.567401	-1.083418	1.794453
H	3.101161	-2.369762	-0.217619
H	3.822625	-0.057202	-0.404835
W	-0.279089	0.107017	-0.268727

E = -459.719520769
G = -459.557979

W-O-1-TBP

O	1.438837	-0.690994	0.014411
C	-0.867317	-1.310491	-1.534159
H	-0.073946	-1.903661	-1.987039
C	-1.087954	-1.023956	1.148754
C	-1.366546	-1.911377	-0.151385
H	-0.311501	-1.492984	1.756338
H	-0.865684	-2.868834	-0.004070
H	-2.448109	-2.037748	-0.217046
Si	2.975816	-1.233472	0.366864
H	3.975287	-0.132710	0.195851
H	3.035473	-1.723116	1.780730
H	3.338388	-2.361320	-0.547674
C	-2.317341	-0.673465	1.960883
H	-2.050346	-0.011500	2.790790
H	-3.063880	-0.160359	1.349155
H	-2.773589	-1.573641	2.394089
H	-1.685107	-1.113960	-2.223999
O	-1.716003	1.147207	-0.449582
C	0.924004	2.027292	-0.374879
H	1.928269	1.784779	-0.741988
H	0.459275	2.737101	-1.069170
C	0.993019	2.626212	1.034110
H	1.439431	1.931291	1.756620
H	1.609008	3.534466	1.051732
H	-0.000168	2.905462	1.403882
W	-0.265190	0.239194	-0.295174

E = -459.738129116

G = -459.575478

W-O-1-TSIII

O	-1.098920	1.072536	-0.239582
C	1.492286	1.390944	0.739495
C	1.159360	-0.239759	-1.917907
C	1.952799	1.454582	-0.590342
H	0.758091	0.366491	-2.733109
H	2.060614	-0.794532	-2.174859
Si	-2.561868	1.812875	0.076624
H	2.958332	1.116978	-0.825782
H	1.523777	2.182456	-1.270861
H	-3.709066	0.936295	-0.313682
H	-2.676281	2.141420	1.532845
H	-2.631173	3.082409	-0.711380
C	2.398324	0.954281	1.867375
H	1.830905	0.545068	2.707264
H	3.104357	0.186655	1.541954
H	2.968686	1.815874	2.237692
H	0.710681	2.100408	1.001158
O	1.191197	-1.452185	0.687661
C	-1.468064	-1.685582	-0.194942
H	-2.230559	-1.309680	-0.889969
H	-1.135604	-2.659680	-0.577481
C	-2.064922	-1.862645	1.206582
H	-2.383542	-0.908437	1.646893
H	-2.949763	-2.511849	1.194766
H	-1.337516	-2.311514	1.891906
W	0.235774	-0.356653	-0.210490

E = -459.714783689
G = -459.553591

W-O-1-IV

O	-0.344919	1.425468	-0.422772
C	2.845813	0.425090	0.428134
C	-0.168465	-1.469669	-1.791748
C	2.689319	0.231353	-0.889937
H	-0.405637	-0.992567	-2.749107
H	0.164584	-2.503588	-1.882135
Si	-0.281581	3.065584	-0.053841
H	2.988984	-0.700176	-1.363074
H	2.307245	1.011157	-1.541768
H	-1.651461	3.642605	-0.180610
H	0.221340	3.262071	1.339657
H	0.642588	3.733584	-1.017277
C	3.414347	-0.571058	1.385794
H	2.665454	-0.853420	2.133853
H	3.737494	-1.481077	0.873475
H	4.272847	-0.146745	1.919997
H	2.552877	1.386248	0.854251
O	0.332455	-1.435904	1.072866
C	-2.370775	-0.721845	0.208687
H	-2.921073	-0.266480	-0.626441
H	-2.613720	-1.788832	0.188823
C	-2.788785	-0.097926	1.545051
H	-2.579940	0.977775	1.584215
H	-3.866005	-0.218939	1.717849
H	-2.268326	-0.568322	2.386244
W	-0.282894	-0.460860	-0.181092

E = -459.725808131
G = -459.572903

W-O-1-V

O	-1.544498	0.343820	0.301019
C	0.940403	-1.291628	1.353625
H	0.581777	-1.122980	2.375237
H	1.631472	-2.127849	1.253425
Si	-3.205845	0.516905	0.025931
H	-3.566648	1.935285	0.309028
H	-3.518163	0.177043	-1.392961
H	-3.934460	-0.399380	0.948973
O	0.721298	-0.964745	-1.502846
C	1.446529	1.490082	0.105793
H	1.119840	2.145175	-0.720383
H	1.140987	1.989984	1.037894
C	2.965465	1.323208	0.072988
H	3.288234	0.803501	-0.834101
H	3.472858	2.295914	0.099237
H	3.307494	0.735105	0.929503
W	0.213914	-0.240960	-0.053361

E = -341.855618417
G = -341.774653

W-O-1-TSA

O	-1.642105	0.090304	-0.462053
C	0.049253	-2.050845	-0.358370
H	-0.638544	-2.322743	-1.156411
C	1.829930	-0.068688	-0.937132
C	1.470604	-1.674824	-0.858639
H	1.575349	0.273330	-1.947935
H	1.565951	-2.000722	-1.895167
H	2.244862	-2.127637	-0.237930
Si	-3.123242	-0.648122	-0.304292
H	-3.839931	-0.162474	0.918119
H	-3.946393	-0.317150	-1.509134
H	-3.004905	-2.141695	-0.200955
C	3.267994	0.245368	-0.574174
H	3.438722	1.324328	-0.636620
H	3.504078	-0.070989	0.445733
H	3.973516	-0.243818	-1.257952
H	0.067058	-2.796369	0.435612
O	0.638943	-0.201763	1.913320
C	-0.258465	2.106283	0.384373
H	-1.079938	2.234057	1.102746
H	0.640275	2.539382	0.855523
C	-0.588986	2.820400	-0.922684
H	-1.455079	2.357583	-1.404259
H	-0.824967	3.879224	-0.756258
H	0.248058	2.786733	-1.631656
W	0.198116	-0.020430	0.285490

E = -459.715580377
G = -459.551809

W-O-1-SBP

O	1.833050	0.078355	-0.136478
C	-0.163723	-1.786255	0.952391
C	-1.800029	-0.213338	0.935895
C	-1.672807	-1.719758	1.149433
H	-1.483388	0.290293	1.862859
Si	3.343230	-0.053754	0.611736
H	4.043123	-1.254677	0.072585
H	4.115685	1.182289	0.297930
H	3.166840	-0.184220	2.088892
H	-2.056468	-2.107347	2.106223
H	-2.185698	-2.259269	0.344264

H	0.374680	-1.530486	1.874820
C	-3.162470	0.306626	0.501647
H	-3.933535	0.001589	1.223578
H	-3.199644	1.398308	0.434297
H	-3.449386	-0.099415	-0.474457
H	0.266583	-2.703129	0.530186
O	-0.676762	-0.741181	-1.835202
C	-0.568464	1.956453	-0.364367
H	-1.535265	2.113774	-0.852636
H	0.194488	2.294430	-1.097112
C	-0.457024	2.773774	0.918944
H	-0.520047	3.848961	0.710967
H	-1.263938	2.531026	1.616783
H	0.492618	2.602128	1.438988
W	-0.028852	-0.107758	-0.399090

E = -459.750730486
G = -459.588213

W-O-1-TSB

C	2.091563	-0.283763	-1.271557
C	1.666741	1.432684	0.274983
C	2.429719	0.249448	0.042247
H	1.530370	2.064204	-0.604553
H	3.256060	-0.094002	0.668601
H	1.610632	-0.808401	0.762987
O	-1.113561	1.014012	0.283702
Si	-2.494020	1.740926	-0.351927
H	-2.094376	2.831177	-1.293506
H	-3.338512	0.742070	-1.070504
H	-3.251942	2.327497	0.793103
H	2.055631	0.434164	-2.091359
W	0.173170	-0.313584	-0.184861
C	1.610810	2.127827	1.608337
H	2.405324	2.877926	1.717057
H	0.652333	2.641197	1.737065
H	1.717041	1.416843	2.436371
H	2.479537	-1.259873	-1.559686
O	-0.530030	-1.124225	-1.530340
C	-0.292246	-1.789754	1.322546
H	0.330229	-2.683150	1.186969
H	-0.008371	-1.375320	2.301772
C	-1.776172	-2.168554	1.304070
H	-1.999478	-2.888336	2.102493
H	-2.419531	-1.296848	1.459452
H	-2.057025	-2.622524	0.349774

E = -459.699935422
G = -459.540595

W-O-1-TSB$_{transX}$

O	-1.516783	-1.046283	-0.258581
C	1.268895	0.520815	1.716224
C	0.653836	2.084230	0.085449
C	0.403488	1.627081	1.429110
H	1.708608	2.102282	-0.199344
Si	-3.080290	-0.815444	0.325160
H	-3.630326	0.481584	-0.174846
H	-3.923162	-1.946579	-0.162276
H	-3.079119	-0.801170	1.821272
H	-0.266953	2.102600	2.144536
H	-0.951300	0.859389	0.959104
H	2.306423	0.643740	1.409556
W	0.132820	-0.076145	-0.165921
C	-0.229648	3.086078	-0.600687
H	-0.037595	4.109545	-0.252030
H	-0.069681	3.062212	-1.682345
H	-1.289410	2.870758	-0.410859
H	1.136912	-0.057251	2.628228
O	0.640308	0.085623	-1.800884
C	1.280184	-1.864383	0.240417
H	1.023720	-2.232330	1.241227
H	0.815651	-2.547036	-0.485345
C	2.790570	-1.846644	0.033920
H	3.206968	-2.856561	0.138438
H	3.048765	-1.484144	-0.965715
H	3.303733	-1.213851	0.765402

E = -459.699342935
G = -381.020697

W-O-1-B

C	1.342169	-1.204167	-0.933670
C	3.347794	-0.094745	0.107738
C	2.452399	-1.091301	0.048324
H	3.286497	0.708163	-0.629552
H	2.513679	-1.891246	0.788280
H	0.007093	-1.742653	0.773411
O	-0.076460	1.374760	-0.073591
Si	0.054391	3.030263	-0.379896
H	1.417917	3.298236	-0.921091
H	-0.981109	3.442045	-1.372387
H	-0.145169	3.760861	0.904380
H	1.509777	-0.557858	-1.813278
W	-0.536426	-0.451931	-0.184397
C	4.456519	0.003241	1.108240
H	5.437857	0.017134	0.616815
H	4.388389	0.930019	1.692443
H	4.441560	-0.838348	1.807545
H	1.210042	-2.231563	-1.285620
O	-1.614503	-1.113188	-1.312181
C	-1.702741	-0.612438	1.613890
H	-2.058173	-1.633394	1.778502
H	-1.054408	-0.371092	2.467506
C	-2.882514	0.364424	1.513668
H	-3.504406	0.307179	2.416707
H	-2.558045	1.406101	1.415409
H	-3.531519	0.132993	0.661862

E = -459.736963530
G = -459.581372

W-O-1-TSC

C	1.069867	-0.554012	-1.516703
C	3.354159	-0.279618	-0.498630
C	2.324791	-1.046599	-0.890447
H	1.224025	0.401653	-2.037606
H	2.394037	-2.125138	-0.732972
H	0.667664	-1.267877	-2.242721
H	0.014772	-1.738808	0.140280
O	0.147503	1.596018	0.664972
Si	-0.108192	3.201478	0.198689
H	-1.519651	3.596898	0.481350
H	0.820859	4.039815	1.014796
H	0.194170	3.393159	-1.251772
C	-2.264603	-1.208950	0.474360
H	-2.987224	-0.427503	0.756515
H	-2.103254	-1.827435	1.362053
C	-2.841862	-2.062686	-0.652154
H	-3.080300	-1.454549	-1.529173

H	-2.134997	-2.840432	-0.967869
H	-3.760963	-2.572700	-0.334168
C	0.427409	-1.714702	1.768165
H	1.487336	-1.823452	1.553460
H	-0.134829	-2.641584	1.839337
C	-0.037162	-0.544442	2.333873
H	-1.009327	-0.502288	2.814360
H	0.648137	0.268273	2.542048
H	3.286380	0.799367	-0.649369
C	4.617171	-0.786119	0.123624
H	5.492456	-0.521645	-0.483129
H	4.782151	-0.342406	1.114005
H	4.603800	-1.874741	0.236714
W	-0.491253	-0.045018	-0.106195
O	-1.512063	0.548330	-1.340209

E = -538.268124405
G = -538.058323

W-O-1-C

C	-0.925167	1.379508	-1.053045
C	-3.193456	1.109632	0.010731
C	-1.965802	1.651755	-0.027864
H	-3.493613	0.433118	-0.791808
H	-1.687972	2.347731	0.765511
O	-0.590859	-1.449117	-0.466735
Si	-1.865305	-2.465397	-0.006893
H	-2.999756	-2.244661	-0.947756
H	-1.381031	-3.872086	-0.109137
H	-2.281841	-2.168648	1.394264
H	-1.343647	0.827219	-1.910665
W	0.598510	0.007549	-0.344409
C	-4.221396	1.390926	1.062255
H	-5.125959	1.833708	0.626071
H	-4.540049	0.471745	1.570360
H	-3.840762	2.081029	1.821461
H	-0.458841	2.293430	-1.432737
O	1.879085	0.057631	-1.454345
C	1.354261	-0.749548	1.536918
H	2.088115	-0.099235	2.015683
H	0.479931	-0.773183	2.207107
C	1.944587	-2.154752	1.353946
H	2.284910	-2.555285	2.317670
H	1.223977	-2.867679	0.941300
H	2.812773	-2.143018	0.685831
C	1.065360	1.850689	0.810722
H	0.525688	2.713899	0.408450
H	0.706129	1.723038	1.841002
C	2.558739	2.212294	0.820820
H	2.743913	3.082746	1.463821
H	3.196898	1.400126	1.184203
H	2.907075	2.461773	-0.186137

E = -538.327574255
G = -538.115192

W-O-2-I

W	-0.897720	-0.185770	-0.176445
O	0.812877	0.387257	0.433563
C	-2.079449	-0.411407	1.293465
H	-1.786286	0.271486	2.108984
C	-3.228927	-1.317483	1.615064
H	-4.138542	-0.733668	1.810384
H	-3.439735	-2.007713	0.794636
H	-3.029927	-1.906670	2.519946
O	-1.244981	-1.458540	-1.248965
C	2.151177	0.175160	0.283111
C	3.033489	1.098403	0.849236
C	2.637544	-0.936356	-0.411503
C	4.405758	0.907090	0.712015
H	2.631050	1.950823	1.387304
C	4.012789	-1.115780	-0.538865
H	1.941195	-1.651871	-0.842654
C	4.901527	-0.197555	0.019712
H	5.090644	1.626745	1.151770
H	4.388674	-1.981055	-1.077569
H	5.972662	-0.343168	-0.082349
C	-1.785747	1.527726	-1.092908
H	-1.110939	1.781543	-1.929873
H	-2.732512	1.217943	-1.551024
C	-2.001267	2.750125	-0.198050
H	-1.080434	3.058306	0.310588
H	-2.348880	3.612984	-0.780485
H	-2.750216	2.542015	0.572803

E = -606.991763620
G = -606.821829

W-O-2-Ianti

W	-0.940235	-0.410403	-0.024528
O	0.722061	0.493849	0.158229
C	-2.140499	0.055509	1.383139
H	-2.869022	-0.683262	1.728226
C	-2.137242	1.348261	2.159650
H	-1.930098	1.165572	3.222294
H	-1.396017	2.068086	1.797206
H	-3.121411	1.831693	2.103150
O	-1.187862	-2.067854	-0.311076
C	2.073796	0.320216	0.092548
C	2.884642	1.457288	0.082592
C	2.640501	-0.956670	0.041680
C	4.267627	1.310886	0.015399
H	2.419752	2.437069	0.126839
C	4.025436	-1.087597	-0.023734
H	1.999135	-1.834788	0.055948
C	4.843627	0.041762	-0.038010
H	4.897539	2.195991	0.006498
H	4.464622	-2.080439	-0.062540
H	5.922785	-0.066916	-0.088596
C	-1.917237	0.535985	-1.674010
H	-1.240574	0.367225	-2.530693
H	-2.834159	-0.021484	-1.897169
C	-2.222829	2.028443	-1.529124
H	-1.334370	2.609200	-1.254694
H	-2.600437	2.448565	-2.470058
H	-2.980914	2.200881	-0.759308

E = -606.989637639
G = -606.819364

W-O-2-TSrot1

W	-0.901606	-0.209826	-0.112148
O	0.745809	0.099991	0.758680
C	-2.148753	-0.710230	1.247108
H	-1.757637	-1.515048	1.886816
C	-3.649183	-0.542792	1.319719
H	-3.944382	-0.248140	2.335658
H	-4.025666	0.233539	0.644394
H	-4.181683	-1.474474	1.084613
O	-0.616759	-1.510568	-1.204565

C	2.076262	0.057826	0.436633
C	2.955719	0.781368	1.245701
C	2.548618	-0.693792	-0.641251
C	4.319156	0.752172	0.966584
H	2.558796	1.349052	2.081434
C	3.917258	-0.712203	-0.904550
H	1.849209	-1.257482	-1.252028
C	4.806561	0.007695	-0.107906
H	5.003471	1.314340	1.596087
H	4.287182	-1.298155	-1.741495
H	5.871136	-0.012440	-0.321003
C	-1.643652	1.366047	-1.289764
H	-1.100509	1.453792	-2.238605
H	-2.661560	1.023659	-1.558210
C	-1.695575	2.705088	-0.539613
H	-0.690197	3.092976	-0.347170
H	-2.231135	3.461192	-1.125561
H	-2.209015	2.621877	0.425124

E = -606.947478903
G = -606.779487

W-O-2-TSrot2

W	0.958678	0.059571	-0.229079
O	-0.742315	-0.556009	0.293222
C	1.711757	1.270056	0.975473
H	2.664061	0.725925	0.629607
C	1.922432	2.579065	1.646054
H	2.453296	3.302249	1.012676
H	0.951827	3.011867	1.908147
H	2.487365	2.470841	2.580787
O	0.808947	0.792699	-1.779203
C	-2.082064	-0.316983	0.197429
C	-2.927215	-0.908752	1.138088
C	-2.596717	0.481825	-0.826532
C	-4.300449	-0.695602	1.048686
H	-2.498407	-1.525493	1.921623
C	-3.972645	0.684732	-0.900719
H	-1.919627	0.929557	-1.548671
C	-4.828981	0.100254	0.032516
H	-4.959505	-1.155247	1.780034
H	-4.375343	1.306014	-1.695918
H	-5.900472	0.264372	-0.031506
C	2.299787	-1.573083	-0.528792
H	1.820079	-2.206203	-1.289052
H	3.244103	-1.229325	-0.970473
C	2.554770	-2.365052	0.760596
H	1.623550	-2.702583	1.229721
H	3.151661	-3.261437	0.553160
H	3.098108	-1.771087	1.502786

E = -606.955584424
G = -606.787804

W-O-2-II

W	-0.945214	0.001698	-0.225299
O	0.823990	0.195822	0.548719
C	0.031518	-2.524551	-0.389256
C	-2.279878	-0.012873	1.148899
C	-0.800222	-2.610247	0.673066
H	-1.856638	0.274616	2.124913
H	-0.437998	-2.483181	1.689324
H	-1.838659	-2.904364	0.558057
H	1.093880	-2.336610	-0.262580
C	-3.749069	-0.298612	1.177042
H	-4.304552	0.595080	1.492466
H	-4.125466	-0.604773	0.198444
H	-3.986941	-1.084244	1.907712
H	-0.319878	-2.743449	-1.392911
O	-1.745933	-0.506392	-1.644752
C	2.152842	0.111560	0.333638
C	3.016598	0.089316	1.436706
C	2.681746	0.045783	-0.963154
C	4.390777	-0.002825	1.238703
H	2.592561	0.147612	2.434525
C	4.059714	-0.045733	-1.146652
H	2.011551	0.078747	-1.818751
C	4.920640	-0.072345	-0.050512
H	5.053043	-0.019333	2.100133
H	4.459832	-0.093768	-2.155830
H	5.993917	-0.143285	-0.198883
C	-0.936117	2.097691	-0.702083
H	-0.156192	2.214442	-1.475021
H	-1.885681	2.334266	-1.196289
C	-0.677520	3.076955	0.443677
H	0.261251	2.855686	0.962351
H	-0.617237	4.112643	0.084631
H	-1.481610	3.034075	1.187643

E = -685.556411775
G = -685.336428

W-O-2-TSII

W	-0.971155	0.085025	-0.253420
O	0.836093	0.099975	0.510246
C	-0.327762	-2.087071	-0.729908
C	-2.109871	-0.401056	1.255611
C	-1.142297	-2.327760	0.390560
H	-1.579711	-0.380054	2.217270
H	-0.684506	-2.531825	1.353880
H	-2.152260	-2.701957	0.257465
H	0.750613	-2.154479	-0.620521
C	-3.577559	-0.671850	1.368158
H	-4.052733	0.170076	1.888513
H	-4.050384	-0.772932	0.388930
H	-3.784982	-1.567211	1.968582
H	-0.729760	-2.292065	-1.717804
O	-2.041272	-0.001749	-1.582492
C	-0.687913	2.223087	-0.449749
H	0.001608	2.352703	-1.302785
H	-1.645406	2.644547	-0.783499
C	-0.161309	2.999091	0.759321
H	0.807896	2.617207	1.093510
H	-0.036987	4.066112	0.533130
H	-0.850479	2.928855	1.609705
C	2.156280	-0.036019	0.310079
C	3.004913	-0.183940	1.417699
C	2.704090	-0.036148	-0.982060
C	4.374832	-0.333559	1.228579
H	2.571413	-0.174781	2.413288
C	4.077817	-0.187808	-1.156181
H	2.048374	0.093464	-1.839343
C	4.920668	-0.338546	-0.056145
H	5.022334	-0.446230	2.094201
H	4.489559	-0.184604	-2.161987
H	5.990969	-0.454985	-0.197221

E = -685.553635036
G = -685.329864

W-O-2-TBP

O	-0.885279	-0.046452	-0.297828
C	0.689574	-0.560192	1.889583
H	-0.336198	-0.526274	2.253905
C	1.370619	-1.805037	-0.416789
C	1.035482	-1.911705	1.155385
H	0.548354	-2.239947	-0.990773
H	0.178974	-2.579811	1.252205
H	1.923233	-2.337597	1.625235
W	1.039062	0.203420	-0.023410
C	2.713958	-2.382379	-0.816353
H	2.898043	-2.220572	-1.883162
H	3.527489	-1.909680	-0.259798
H	2.747939	-3.465354	-0.637835
H	1.414917	-0.296457	2.656067
O	2.676897	0.551160	0.352920
C	-2.216357	-0.131068	-0.181759
C	-2.897569	0.622151	0.786715
C	-2.940599	-0.981021	-1.031254
C	-4.280849	0.515994	0.902654
H	-2.330377	1.285863	1.432867
C	-4.323010	-1.076459	-0.903756
H	-2.405379	-1.551737	-1.784367
C	-5.001455	-0.332258	0.062075
H	-4.798628	1.104458	1.655564
H	-4.874613	-1.737146	-1.567436
H	-6.080475	-0.409863	0.155826
C	0.814023	2.027447	-1.135172
H	-0.019912	1.915300	-1.839217
H	1.734238	2.192500	-1.710039
C	0.563250	3.203150	-0.185455
H	0.438191	4.142791	-0.738622
H	-0.349897	3.065213	0.406309
H	1.398169	3.345794	0.509616

E = -685.571166563
G = -685.346532

W-O-2-TSIII

W	1.100116	0.196133	-0.046369
O	-0.766724	0.344067	0.519316
C	1.239916	-1.851995	1.427227
C	2.137763	0.255046	1.597180
C	0.579024	-2.088490	0.206002
H	1.678952	0.562462	2.539808
H	3.206866	0.058413	1.663643
H	-0.509198	-2.083576	0.248154
H	0.657853	-1.668314	2.324317
C	1.188609	-2.974904	-0.856126
H	0.818142	-2.727312	-1.854221
H	2.277137	-2.885296	-0.878392
H	0.929535	-4.022334	-0.654975
H	2.239234	-2.249674	1.582226
O	2.244880	-0.264935	-1.224274
C	-2.058512	0.094515	0.249612
C	-2.467237	-0.345273	-1.018330
C	-3.015356	0.276329	1.259150
C	-3.814160	-0.600988	-1.265077
H	-1.725254	-0.470573	-1.802950
C	-4.356878	0.017186	0.998103
H	-2.687431	0.624330	2.234058
C	-4.765526	-0.423456	-0.261765
H	-4.119352	-0.938615	-2.251970
H	-5.090123	0.162854	1.786959
H	-5.814415	-0.622719	-0.459450
C	0.753666	2.121455	-0.969523
H	0.120948	1.919750	-1.851489
H	1.716297	2.463444	-1.371413
C	0.114758	3.220058	-0.117123
H	-0.050409	4.136084	-0.699003
H	-0.852393	2.907085	0.287324
H	0.753393	3.490231	0.732368

E = -685.547978655
G = -685.324963

W-O-2-IV

W	-1.116368	-0.140521	-0.032991
O	0.678909	-0.543711	0.513671
C	0.149270	2.696708	0.286648
C	-2.405022	-0.317556	1.359199
C	-0.367965	2.303240	1.464551
H	-2.139972	-0.829308	2.290671
H	-3.423899	0.069222	1.337060
H	-1.336285	2.660679	1.804852
H	0.196295	1.681117	2.152857
C	-0.513266	3.631568	-0.672713
H	-0.662851	3.151233	-1.645230
H	-1.489163	3.959621	-0.305761
H	0.115703	4.515508	-0.833868
H	1.144488	2.343519	0.012233
O	-1.829731	0.804914	-1.257158
C	1.995647	-0.419488	0.226232
C	2.431005	-0.055467	-1.054240
C	2.929185	-0.670621	1.238117
C	3.795228	0.060639	-1.311751
H	1.700365	0.123198	-1.839426
C	4.288806	-0.549746	0.966782
H	2.571965	-0.959727	2.221660
C	4.729126	-0.183130	-0.305499
H	4.127092	0.340979	-2.307643
H	5.009070	-0.745816	1.756317
H	5.791234	-0.091910	-0.511673
C	-1.371248	-2.050511	-0.966066
H	-0.619315	-2.071434	-1.773973
H	-2.350146	-2.062337	-1.457340
C	-1.210934	-3.276203	-0.066737
H	-2.006251	-3.314324	0.685499
H	-1.256832	-4.206052	-0.648339
H	-0.252699	-3.271868	0.464152

E = -685.557898307
G = -685.340117

W-O-2-V

W	0.990692	-0.220200	0.131061
O	-0.753983	0.458517	0.429553
C	2.004870	-0.271611	1.736874
H	1.757213	0.426625	2.543889
H	2.785873	-0.989349	1.985658
O	1.409319	-1.611713	-0.747639
C	-2.079633	0.277764	0.159731
C	-2.549761	-0.916914	-0.392015
C	-2.960111	1.319988	0.456595
C	-3.911094	-1.060925	-0.648177
H	-1.853136	-1.722040	-0.612954
C	-4.318097	1.162287	0.192414
H	-2.568503	2.235537	0.888346
C	-4.799059	-0.025059	-0.359103
H	-4.276778	-1.990311	-1.075424
H	-5.003364	1.973375	0.421997

H	-5.859349	-0.143423	-0.560796
C	2.006907	1.342505	-0.899996
H	1.754640	2.269115	-0.362223
H	1.502111	1.402742	-1.879886
C	3.519373	1.241281	-1.092929
H	3.794325	0.310924	-1.598773
H	3.899491	2.075024	-1.696844
H	4.033219	1.256266	-0.127216

E = -567.685860183
G = -567.541723

W-O-2-TSA

O	0.881265	0.802356	0.216546
C	0.100672	-1.790944	0.371807
H	0.944060	-1.727868	1.056234
C	-2.211587	-0.568790	1.138972
C	-1.279227	-1.920645	1.077466
H	-1.993875	-0.063576	2.088186
H	-1.098327	-2.157943	2.126619
H	-1.893420	-2.688596	0.605740
W	-0.871553	-0.027797	-0.304170
C	-3.692737	-0.845364	0.968686
H	-4.253154	0.093561	1.009473
H	-3.906301	-1.319033	0.006279
H	-4.076119	-1.496547	1.764704
H	0.255959	-2.552309	-0.391138
O	-1.394124	-0.492413	-1.851334
C	2.150654	0.359765	0.157043
C	2.669553	-0.252401	-0.994102
C	2.993185	0.559676	1.262284
C	4.000726	-0.661533	-1.030436
H	2.022731	-0.391431	-1.856886
C	4.321852	0.148419	1.212611
H	2.588081	1.045925	2.145176
C	4.835230	-0.466178	0.069518
H	4.388126	-1.132159	-1.930578
H	4.961851	0.310674	2.076318
H	5.873065	-0.784047	0.035404
C	-1.183964	2.110453	-0.543965
H	-0.553507	2.450389	-1.376394
H	-2.227702	2.157077	-0.899430
C	-0.980223	3.009709	0.671412
H	0.053215	2.951580	1.022445
H	-1.194944	4.059071	0.432243
H	-1.636765	2.729676	1.504741

E = -685.552166208
G = -685.326004

W-O-2-SBP

O	1.045108	0.431688	-0.560708
C	-0.519174	-1.984824	-0.303076
C	-2.183816	-1.041838	0.939044
C	-1.909823	-2.350762	0.198316
H	-1.697904	-1.085658	1.926842
H	-1.984789	-3.269997	0.799570
H	-2.601136	-2.452927	-0.646791
H	0.259379	-2.190936	0.445532
W	-0.818236	0.146576	-0.339272
C	-3.647112	-0.651769	1.096810
H	-4.192631	-1.434993	1.642505
H	-3.786353	0.280352	1.653131
H	-4.129016	-0.532773	0.120612
H	-0.190422	-2.388063	-1.268774
O	-1.857190	0.438886	-1.651184
C	2.306723	0.115892	-0.164970
C	3.330588	0.151411	-1.116037
C	2.584585	-0.223896	1.163214
C	4.631084	-0.164244	-0.734233
H	3.088571	0.422815	-2.138749
C	3.891130	-0.534524	1.532150
H	1.782180	-0.234247	1.895663
C	4.916756	-0.508093	0.587619
H	5.425807	-0.139943	-1.474453
H	4.106594	-0.797438	2.563957
H	5.933530	-0.752024	0.880389
C	-1.184188	1.578130	1.211950
H	-2.247428	1.662448	1.450587
H	-0.683152	1.248253	2.133999
C	-0.638067	2.939185	0.744419
H	-0.854087	3.715772	1.489212
H	0.445545	2.924131	0.591298
H	-1.100699	3.266011	-0.194465

E = -685.582066216
G = -685.356396

W-O-2-TSB

C	-1.862540	-1.910446	-0.832648
C	-0.075565	-1.912973	0.694927
C	-1.477305	-2.138256	0.552060
H	0.530519	-2.271753	-0.138693
H	-2.118740	-2.572937	1.321405
H	-2.073194	-0.796851	1.008785
O	0.693760	0.768893	0.036981
H	-1.220013	-2.353289	-1.594342
W	-1.052206	0.029253	-0.205018
C	0.595097	-1.888731	2.044151
H	0.816830	-2.902295	2.404572
H	1.541952	-1.342902	2.007540
H	-0.038546	-1.407169	2.798754
H	-2.919283	-1.908712	-1.095180
O	-1.556506	0.662823	-1.724782
C	-2.137740	1.408656	1.054340
H	-3.215713	1.210480	1.017971
H	-1.833674	1.222687	2.095552
C	-1.842407	2.855698	0.648535
H	-2.313530	3.554921	1.351971
H	-0.768307	3.065220	0.641089
H	-2.226265	3.068552	-0.352784
C	2.016960	0.510892	-0.073252
C	2.883162	0.965817	0.927659
C	2.527061	-0.162829	-1.188868
C	4.251285	0.734791	0.811299
H	2.470791	1.499325	1.778553
C	3.897559	-0.390986	-1.288981
H	1.845503	-0.482933	-1.972201
C	4.765502	0.052907	-0.291846
H	4.919301	1.091193	1.590788
H	4.287908	-0.913751	-2.158017
H	5.833242	-0.125461	-0.376295

E = -685.531392745
G = -685.309047

W-O-2-TSB$_{transX}$

O	-0.934127	-0.820732	-0.413070
C	1.854656	0.077167	1.864997
C	1.585292	1.933882	0.457909

C	1.170468	1.321915	1.695969
H	2.652159	1.836310	0.238582
H	0.496152	1.773135	2.422624
H	-0.233185	0.837419	0.998415
H	2.920906	0.086193	1.645785
W	0.804942	-0.057522	-0.164952
C	0.913268	3.154640	-0.101379
H	1.252849	4.071440	0.398440
H	1.125298	3.253659	-1.169759
H	-0.175164	3.096094	0.025609
H	1.564560	-0.604851	2.661122
O	1.363027	0.314198	-1.752008
C	1.747457	-2.004513	-0.030489
H	1.431575	-2.503482	0.892808
H	1.240152	-2.510915	-0.864568
C	3.258362	-2.099362	-0.215863
H	3.579353	-3.148153	-0.253150
H	3.574014	-1.623129	-1.148989
H	3.809158	-1.628511	0.605471
C	-2.237156	-0.511842	-0.190441
C	-2.807971	0.627131	-0.767398
C	-3.016671	-1.372500	0.588037
C	-4.155245	0.906511	-0.550203
H	-2.192936	1.270374	-1.390322
C	-4.363105	-1.082235	0.794202
H	-2.557958	-2.259155	1.014983
C	-4.938397	0.056784	0.230543
H	-4.595058	1.792186	-1.000913
H	-4.965771	-1.753112	1.400552
H	-5.988742	0.277930	0.395072

E = -685.531479524
G = -685.309123

W-O-2-B

C	-1.091273	-1.929766	-0.885115
C	1.116281	-2.756738	0.008318
C	-0.221630	-2.654459	0.078514
H	1.634254	-2.299924	-0.836450
H	-0.733449	-3.113666	0.926118
H	-2.091712	-0.997482	0.897234
O	0.382678	0.742830	-0.565065
H	-0.599624	-1.791703	-1.862608
W	-1.354893	0.088197	-0.179520
C	1.971562	-3.490114	0.993016
H	2.505784	-4.319647	0.512224
H	2.739045	-2.832836	1.419854
H	1.377751	-3.902764	1.814433
H	-2.049584	-2.431092	-1.041749
O	-2.673699	0.683605	-1.057382
C	-1.595423	1.004180	1.752896
H	-2.611892	0.859936	2.130821
H	-0.935692	0.489791	2.466834
C	-1.260166	2.499231	1.657942
H	-1.418894	2.990176	2.626996
H	-0.219592	2.677876	1.368257
H	-1.900106	3.013784	0.932191
C	1.720962	0.817592	-0.357415
C	2.278632	0.494504	0.884031
C	2.535640	1.240801	-1.412006
C	3.656490	0.596352	1.061746
H	1.632319	0.174668	1.695272
C	3.911630	1.329417	-1.221953
H	2.076993	1.493283	-2.362937
C	4.477441	1.009052	0.012597
H	4.088820	0.351666	2.028015
H	4.543982	1.655184	-2.043051
H	5.550989	1.084395	0.157170

E = -685.567657430
G = -685.346478

W-O-2-TSC

C	-1.063013	-1.064422	-1.568338
C	-0.471421	-3.366929	-0.748300
C	-1.372772	-2.411040	-1.022207
H	-0.106171	-1.055656	-2.109446
H	-2.426984	-2.622185	-0.829503
H	-1.839947	-0.714258	-2.255941
H	-2.322636	-0.293488	0.178559
O	0.976718	-0.095187	0.619373
C	-2.140555	2.025113	0.617237
H	-1.472453	2.839025	0.939131
H	-2.721344	1.726248	1.494615
C	-3.083470	2.531262	-0.472185
H	-2.528900	2.924833	-1.328447
H	-3.737915	1.730739	-0.840022
H	-3.735002	3.330750	-0.094512
C	-2.185959	-0.764135	1.791345
H	-2.112110	-1.819103	1.538565
H	-3.195805	-0.376398	1.892466
C	-1.106218	-0.116779	2.359172
H	-1.231115	0.829862	2.874579
H	-0.184669	-0.656255	2.538385
H	0.582853	-3.157373	-0.937350
C	-0.795526	-4.726515	-0.214044
H	-0.461918	-5.513088	-0.902745
H	-0.286002	-4.915001	0.739816
H	-1.871150	-4.853121	-0.055693
W	-0.734860	0.468683	-0.074541
O	-0.334256	1.630549	-1.259292
C	2.290730	0.133474	0.332402
C	2.722579	1.183288	-0.484201
C	3.223452	-0.736230	0.910713
C	4.086127	1.350533	-0.717727
H	1.992299	1.851389	-0.929735
C	4.581231	-0.560245	0.661343
H	2.865921	-1.540303	1.546661
C	5.020834	0.484008	-0.152153
H	4.417023	2.169096	-1.351338
H	5.298657	-1.241802	1.110526
H	6.081173	0.622327	-0.341548

E = -764.097721572
G = -763.825534

W-O-2-C

C	0.782912	1.641919	-1.254193
C	-1.081283	2.980885	-0.215917
C	0.212011	2.629214	-0.302288
H	-1.793988	2.537713	-0.913007
H	0.917187	3.093455	0.389232
O	-0.769324	-0.723620	-0.534816
H	0.077620	1.422041	-2.071297
W	1.063332	-0.301617	-0.329107
C	-1.634364	3.975955	0.755897
H	-2.086259	4.830046	0.235287
H	-2.428274	3.535524	1.372559
H	-0.858556	4.361322	1.424763
H	1.723590	1.981400	-1.698071
O	2.101596	-1.241274	-1.285626

C	0.988094	-1.090055	1.687345
H	1.943143	-1.026712	2.211811
H	0.298217	-0.424610	2.231890
C	0.474472	-2.536057	1.707820
H	0.429303	-2.913306	2.737635
H	-0.528175	-2.631970	1.280855
H	1.137382	-3.206344	1.149495
C	2.626767	0.875314	0.699344
H	2.860557	1.772804	0.116006
H	2.228094	1.232905	1.658743
C	3.946413	0.123481	0.928064
H	4.656039	0.742572	1.492337
H	3.819753	-0.810561	1.485399
H	4.414376	-0.137531	-0.026022
C	-2.091116	-0.686884	-0.242501
C	-2.573420	0.026823	0.860287
C	-2.969886	-1.394524	-1.070185
C	-3.939742	0.023900	1.129832
H	-1.880681	0.579057	1.486216
C	-4.332966	-1.382216	-0.791938
H	-2.567647	-1.942894	-1.916249
C	-4.822719	-0.675843	0.307545
H	-4.315261	0.574224	1.987971
H	-5.015149	-1.930235	-1.435603
H	-5.887062	-0.671581	0.522806

E = -764.160103636
G = -763.884424

W-N-3-I

W	0.592479	-0.274197	0.134629
O	1.372873	-1.701938	-0.848427
N	-1.138791	-0.050362	0.049437
C	0.889938	-0.526683	1.985926
H	1.943874	-0.858574	2.080130
Si	1.910544	-3.287709	-1.022952
H	2.871956	-3.331842	-2.162509
H	2.587648	-3.729128	0.234385
H	0.747486	-4.180651	-1.305724
C	0.122602	-0.506824	3.270543
H	0.554209	0.223359	3.968299
H	-0.921981	-0.234435	3.101977
H	0.150188	-1.482318	3.773514
C	-2.495307	0.122249	-0.112422
C	-3.311505	-0.950236	-0.512721
C	-4.680575	-0.762802	-0.667579
C	-5.253742	0.486988	-0.428776
C	-4.446896	1.554288	-0.031801
C	-3.076668	1.380003	0.128414
H	-2.854659	-1.918250	-0.695087
H	-5.303922	-1.597285	-0.976900
H	-6.323626	0.628415	-0.551536
H	-4.887706	2.529666	0.154953
H	-2.436535	2.200751	0.437094
N	1.511157	1.488241	-0.210312
C	2.418198	2.212123	0.551783
C	1.402022	2.139697	-1.437827
C	2.878108	3.278826	-0.176319
H	2.646550	1.897359	1.559756
C	2.229232	3.232566	-1.448106
H	0.731046	1.770487	-2.203240
H	3.594528	4.017446	0.158398
H	2.355606	3.927916	-2.267397

E = -722.556534976
G = -722.361534

W-N-3-Ianti

H	2.147235	0.031582	3.641927
O	2.127634	0.603945	-0.231284
Si	3.666584	0.814437	-0.880756
H	3.802206	2.237605	-1.305702
H	4.689292	0.491111	0.158094
H	3.845108	-0.087166	-2.058230
C	1.234566	0.398539	3.154224
H	1.482669	1.346131	2.661506
H	0.512630	0.629647	3.949033
C	0.664098	-0.640546	2.214078
H	0.426638	-1.599677	2.678357
C	-0.136339	-3.082185	-0.877756
C	0.865928	-3.891237	-1.441676
C	-1.472882	-3.519995	-0.903373
C	0.532344	-5.111555	-2.018633
H	1.895629	-3.547825	-1.414603
C	-1.792732	-4.741307	-1.485848
H	-2.237788	-2.887825	-0.463060
C	-0.795010	-5.541507	-2.044506
H	1.313522	-5.730856	-2.450904
H	-2.827850	-5.071157	-1.502469
H	-1.050318	-6.495315	-2.497012
N	0.180515	-1.876139	-0.296152
W	0.558193	-0.295134	0.344099
N	-1.081438	0.872923	0.219655
C	-1.824402	1.523899	1.193672
C	-1.598491	1.263637	-1.014327
C	-2.772202	2.313010	0.594070
H	-1.610576	1.353203	2.238551
C	-2.627608	2.147562	-0.817273
H	-1.193838	0.865164	-1.936450
H	-3.495811	2.937064	1.101841
H	-3.218404	2.620262	-1.590734

E = -722.553727895
G = -722.357925

W-N-3-TSrot1

O	-0.754629	2.134061	0.411765
N	0.975625	-0.067702	-0.520429
C	-0.449665	-0.351180	2.139175
H	0.358865	0.223150	2.626643
Si	-0.176178	3.478222	-0.424194
H	-1.163670	4.582152	-0.243174
H	1.146137	3.884835	0.139116
H	-0.025024	3.166920	-1.878748
C	-1.031152	-1.451102	2.986743
H	-1.484759	-1.037852	3.897530
H	-1.806603	-2.011234	2.455782
H	-0.264028	-2.168411	3.308215
C	2.319230	-0.399763	-0.438917
C	3.242788	0.241935	-1.283142
C	4.592249	-0.089322	-1.223958
C	5.039823	-1.069728	-0.337199
C	4.126278	-1.718748	0.495261
C	2.776039	-1.389930	0.449501
H	2.879440	0.995034	-1.975989
H	5.298154	0.416734	-1.876958
H	6.093717	-1.329978	-0.298295
H	4.468859	-2.487128	1.183295
H	2.052506	-1.886504	1.089797
N	-1.907708	-0.786239	-0.676131
C	-3.266677	-0.755386	-0.330325
C	-1.785525	-1.601333	-1.801283

C	-3.963305	-1.538843	-1.205634
H	-3.608025	-0.176639	0.518470
C	-3.019857	-2.076932	-2.142190
H	-0.813241	-1.755716	-2.245410
H	-5.030229	-1.716721	-1.187781
H	-3.239442	-2.739469	-2.968728
W	-0.558323	0.235849	0.332818

E = -722.527782316
G = -722.331033

W-N-3-TSrot2

O	-0.815493	2.052636	0.526204
N	0.914360	-0.070293	-0.511360
C	-0.562492	-0.534175	2.110584
H	-1.140729	-1.477189	2.076382
Si	-0.190946	3.475326	-0.137235
H	-1.192011	4.557038	0.090828
H	1.092696	3.816852	0.544144
H	0.045014	3.295822	-1.601408
C	0.174688	-0.280889	3.394073
H	0.874742	-1.090645	3.638697
H	0.746055	0.651412	3.354392
H	-0.528297	-0.197599	4.233401
C	2.252014	-0.432445	-0.515249
C	3.125091	0.166226	-1.440317
C	4.468252	-0.194452	-1.469086
C	4.957927	-1.160053	-0.588922
C	4.093577	-1.765159	0.325682
C	2.750913	-1.407507	0.366988
H	2.728304	0.909781	-2.125109
H	5.135554	0.277436	-2.185160
H	6.006363	-1.442689	-0.617401
H	4.469478	-2.520977	1.010178
H	2.064410	-1.869270	1.070866
N	-1.945375	-0.855499	-0.715105
C	-3.294667	-0.937008	-0.354643
C	-1.804373	-1.504046	-1.939988
C	-3.971768	-1.625102	-1.323687
H	-3.647002	-0.503514	0.572439
C	-3.022302	-1.986620	-2.332543
H	-0.832802	-1.555655	-2.408961
H	-5.028634	-1.856187	-1.316058
H	-3.223226	-2.543393	-3.238070
W	-0.623740	0.174609	0.348654

E = -722.528789148
G = -722.332611

W-N-3-TSI

W	-0.683433	0.213027	0.339022
O	-1.828871	1.413756	-0.605856
N	1.021451	-0.184599	0.161455
C	0.986826	3.164665	-0.149137
C	-0.937078	0.352852	2.215506
C	0.535910	3.191814	1.107768
H	-1.962326	0.739299	2.370474
Si	-2.700517	2.163997	-1.827769
H	-0.425366	3.631336	1.359617
H	1.122775	2.795098	1.930956
H	0.406742	3.579205	-0.969235
H	-4.153514	1.875809	-1.649839
H	-2.469278	3.638734	-1.747301
H	-2.243269	1.668390	-3.161312
C	-0.153429	0.160158	3.474602
H	-0.615689	-0.613416	4.102847
H	0.872622	-0.148621	3.263267
H	-0.125296	1.078119	4.077641
H	1.953370	2.735423	-0.397857
C	2.333314	-0.386528	-0.191680
C	2.827815	0.034933	-1.441212
C	4.160094	-0.180858	-1.777559
C	5.022929	-0.811711	-0.880910
C	4.539340	-1.233646	0.358490
C	3.208484	-1.029424	0.704207
H	2.151477	0.522232	-2.137724
H	4.526530	0.145789	-2.747101
H	6.062727	-0.976952	-1.147364
H	5.203219	-1.731479	1.060099
H	2.820118	-1.365903	1.660241
N	-1.570185	-1.560551	0.000658
C	-2.497990	-2.256135	0.758842
C	-1.467284	-2.215113	-1.221038
C	-2.980488	-3.315317	0.031168
H	-2.725505	-1.932442	1.764195
C	-2.321881	-3.289452	-1.234447
H	-0.771466	-1.872808	-1.976027
H	-3.713747	-4.037090	0.366131
H	-2.452115	-3.988985	-2.049693

E = -801.112684948
G = -800.869394

W-N-3-TBP

O	-2.494978	-0.444417	0.137278
C	-0.458167	-1.904383	1.237038
H	-1.347171	-2.130963	1.823468
C	-0.597356	-1.668423	-1.494911
C	-0.479149	-2.602939	-0.183455
H	-1.606107	-1.760467	-1.904968
H	-1.344905	-3.264643	-0.209053
H	0.452495	-3.156770	-0.297156
Si	-4.034575	-0.968562	0.483980
H	-4.948155	0.197841	0.685638
H	-4.556984	-1.802464	-0.645560
H	-4.036592	-1.804158	1.728534
N	1.213425	-0.077759	-0.010241
C	2.578744	-0.027119	0.116439
C	3.395693	0.185114	-1.010552
C	3.178445	-0.181787	1.381533
C	4.778157	0.228283	-0.870143
H	2.927023	0.319793	-1.980386
C	4.562136	-0.138376	1.506679
H	2.541363	-0.323532	2.249229
C	5.367110	0.064169	0.384486
H	5.400240	0.394073	-1.745336
H	5.015325	-0.257912	2.486877
H	6.447623	0.099720	0.488206
W	-0.547498	-0.234868	-0.003903
N	-0.856727	1.780621	0.101333
C	-2.075677	2.448830	0.193300
C	0.131530	2.763149	0.081701
C	-1.857928	3.800998	0.228418
H	-2.998057	1.891414	0.219872
C	-0.446219	4.002640	0.157248
H	1.172297	2.484124	0.013482
H	-2.621907	4.564736	0.295815
H	0.077855	4.949613	0.161180
C	0.461898	-1.927054	-2.544600
H	0.343232	-2.921575	-2.995015
H	0.379368	-1.192431	-3.352080
H	1.469515	-1.857861	-2.126379
H	0.460052	-2.111769	1.781810

E = -801.149007091
G = -800.894227

W-N-3-TSIII

W	-0.662254	-0.494327	0.323138
O	-2.406705	-0.671647	-0.547156
N	1.093663	-0.290451	0.304426
C	-0.772646	-3.009559	0.366870
C	-0.895896	-1.183654	2.107811
C	-0.360979	-2.555165	-0.877951
H	-1.912636	-1.360576	2.474576
H	-0.115318	-1.419942	2.828631
Si	-3.965466	-0.081282	-0.734023
H	-4.897437	-1.252460	-0.647017
H	-4.324981	0.903558	0.327347
H	-4.127865	0.540350	-2.084345
H	-1.148012	-2.385852	-1.611261
H	-1.823861	-3.182260	0.568518
C	1.023248	-2.798468	-1.420691
H	1.353429	-1.998112	-2.087705
H	1.761926	-2.897222	-0.621656
H	1.021714	-3.730229	-2.001024
H	-0.064417	-3.472987	1.047683
C	2.406196	0.000283	0.028432
C	3.426387	-0.492482	0.863825
C	4.756683	-0.191812	0.593719
C	5.093165	0.601614	-0.503959
C	4.085555	1.097704	-1.332614
C	2.751636	0.802531	-1.075890
H	3.154441	-1.102967	1.719720
H	5.535888	-0.577248	1.245710
H	6.133679	0.834911	-0.710068
H	4.340291	1.722810	-2.184057
H	1.960057	1.196645	-1.705963
N	-1.073638	1.527674	0.349407
C	-0.730352	2.434476	1.330843
C	-1.551303	2.257781	-0.725766
C	-0.998452	3.713949	0.895883
H	-0.319614	2.092635	2.270736
C	-1.518648	3.601491	-0.422732
H	-1.871149	1.766054	-1.634979
H	-0.849465	4.624003	1.462381
H	-1.841449	4.407767	-1.068521

E = -801.116143246
G = -800.864587

W-N-3-IV

W	-0.618586	-0.517905	0.458027
O	-2.044422	-1.111175	-0.723344
N	1.089432	-0.078027	0.400107
C	0.266116	-2.854615	-0.477008
C	-0.911482	-0.784364	2.328926
C	-0.387021	-3.122019	0.686516
H	-1.922447	-1.062650	2.653594
H	-0.192877	-0.711261	3.143974
Si	-3.530814	-0.691044	-1.392342
H	0.159090	-3.368923	1.592144
H	-1.462555	-3.263482	0.703632
H	-4.275969	0.269792	-0.529881
H	-3.340023	-0.125060	-2.762406
H	-4.322622	-1.957083	-1.515346
C	1.750134	-2.948142	-0.653081
H	2.147718	-2.134533	-1.264731
H	2.273826	-2.945576	0.305998
H	1.985175	-3.887930	-1.169427
H	-0.334506	-2.742315	-1.378766
C	2.346513	0.345856	0.049569
C	2.654709	0.716584	-1.273939
C	3.934130	1.153719	-1.598663
C	4.926873	1.224992	-0.620644
C	4.628593	0.858887	0.692922
C	3.352671	0.423983	1.031546
H	1.875802	0.667518	-2.029355
H	4.156789	1.442935	-2.622143
H	5.924738	1.566772	-0.879377
H	5.395434	0.916781	1.460650
H	3.107950	0.145699	2.051963
N	-1.396535	1.368610	0.287015
C	-1.561458	2.021488	-0.923036
C	-1.764085	2.257830	1.277970
C	-2.030753	3.296671	-0.698725
H	-1.323515	1.531258	-1.858476
C	-2.162720	3.446079	0.710388
H	-1.701303	1.963881	2.316011
H	-2.258816	4.034177	-1.457273
H	-2.512801	4.321115	1.242102

E = -801.117358805
G = -800.868080

W-N-3-TSIV

W	-0.719467	0.253791	-0.542775
O	-1.764799	1.443661	0.523757
N	0.933128	-0.304365	-0.339147
C	1.089110	3.150287	-0.012524
C	-0.922632	0.470348	-2.421520
C	0.298710	3.287437	-1.085630
H	-0.230180	0.258043	-3.234019
H	-1.851202	0.963293	-2.741853
Si	-2.734760	1.903467	1.820076
H	0.634316	3.191782	0.977784
H	0.706059	3.268832	-2.093502
H	-0.767652	3.461694	-0.988167
H	-4.093000	1.305996	1.671652
H	-2.113400	1.447854	3.100697
H	-2.833533	3.393940	1.823456
C	2.574326	2.981502	-0.055550
H	3.069990	3.816507	0.455339
H	2.886782	2.065187	0.456706
H	2.943979	2.941572	-1.083892
C	2.180661	-0.745933	0.029705
C	2.612463	-0.683335	1.368269
C	3.876837	-1.145131	1.718408
C	4.732182	-1.668104	0.747917
C	4.309619	-1.732316	-0.580778
C	3.045821	-1.280481	-0.942799
H	1.942150	-0.273559	2.118586
H	4.196279	-1.095389	2.755870
H	5.719353	-2.025826	1.025406
H	4.968396	-2.142788	-1.341255
H	2.703320	-1.334587	-1.971296
N	-1.753606	-1.446948	-0.274223
C	-1.770520	-2.113484	0.945681
C	-2.678524	-2.072819	-1.095156
C	-2.696270	-3.125805	0.896227
H	-1.103265	-1.822042	1.746298
C	-3.275207	-3.099917	-0.408064
H	-2.814765	-1.728107	-2.109663
H	-2.925767	-3.817666	1.695971
H	-4.033318	-3.768342	-0.794239

E = -801.113396694
G = -800.868964

W-N-3-V

W	0.703361	0.339232	0.428952
O	1.468427	1.863033	-0.392342
N	-1.012979	0.075167	0.259280
C	0.923293	0.431187	2.308811
H	0.215160	0.276223	3.120942
H	1.906349	0.806991	2.628854
Si	1.730528	3.499521	-0.700987
H	2.787281	3.607853	-1.747343
H	0.464217	4.122643	-1.188258
H	2.176458	4.174022	0.554112
C	-2.356179	-0.144232	0.054796
C	-3.208653	0.914737	-0.303154
C	-4.564506	0.678457	-0.500742
C	-5.087354	-0.606259	-0.346897
C	-4.243769	-1.659680	0.008667
C	-2.886249	-1.437471	0.210929
H	-2.790979	1.910331	-0.418042
H	-5.217137	1.502266	-0.776249
H	-6.147207	-0.785397	-0.502718
H	-4.645732	-2.661697	0.130377
H	-2.217720	-2.246173	0.489429
N	1.673994	-1.353932	-0.061466
C	1.608485	-1.887948	-1.348137
C	2.600012	-2.110408	0.645325
C	2.481325	-2.939673	-1.447203
H	0.930908	-1.476438	-2.085525
C	3.113724	-3.081797	-0.173964
H	2.797570	-1.885396	1.683215
H	2.647260	-3.548279	-2.326248
H	3.854528	-3.820655	0.101720

E = -683.249795134
G = -683.081026

W-N-3-TSA

W	0.550653	-0.282303	0.220320
C	0.498529	-2.293524	1.012640
N	-1.184961	-0.036704	0.236442
O	1.818114	-0.946986	-1.094622
H	1.384000	-2.915272	0.854259
C	0.542730	-1.579159	2.400023
C	1.094583	-0.123158	2.222735
H	2.196589	-0.152581	2.223089
H	-0.459773	-1.520193	2.832427
H	1.197704	-2.124571	3.092092
Si	2.230439	-2.353138	-1.904797
H	2.904594	-1.978147	-3.184363
H	3.177312	-3.173112	-1.084821
H	1.016279	-3.172108	-2.209748
C	0.581477	0.921152	3.195311
H	-0.512296	0.953412	3.191463
H	0.909775	0.698499	4.219639
H	0.948693	1.917878	2.933528
H	-0.400622	-2.897282	0.881619
C	-2.508521	-0.007683	-0.148109
C	-3.480165	0.458269	0.754993
C	-4.819193	0.490802	0.381006
C	-5.207094	0.065379	-0.889801
C	-4.245435	-0.395563	-1.790650
C	-2.904384	-0.435706	-1.428454
H	-3.165057	0.788069	1.740045
H	-5.563632	0.851249	1.085374
H	-6.253904	0.093261	-1.177794
H	-4.542299	-0.726347	-2.781932
H	-2.149206	-0.791355	-2.123053
N	1.165788	1.535436	-0.522157
C	2.395604	1.900196	-1.054037
C	0.436528	2.718020	-0.352242
C	2.452723	3.260819	-1.193581
H	3.121126	1.137636	-1.294995
C	1.195666	3.786026	-0.742064
H	-0.574245	2.680730	0.028888
H	3.288054	3.828918	-1.582390
H	0.893460	4.825248	-0.729489

E = -801.130004969
G = -800.877259

W-N-3-SBP

O	1.261662	-1.313287	-1.336790
C	0.458921	-2.108034	1.254744
C	0.861649	-0.084967	2.223307
C	0.219917	-1.418698	2.591811
H	1.957608	-0.192772	2.307285
Si	2.032696	-2.648982	-2.020521
H	3.086658	-3.164292	-1.095549
H	1.024288	-3.719448	-2.278558
H	2.653322	-2.212059	-3.303679
H	0.636261	-1.924497	3.477083
H	-0.854334	-1.281237	2.762137
H	1.462447	-2.553516	1.201835
N	-1.224641	0.020194	0.024543
C	-2.570054	0.148987	-0.249639
C	-3.290959	1.227102	0.292477
C	-3.233302	-0.789148	-1.059876
C	-4.649249	1.358848	0.024271
H	-2.769567	1.945053	0.917643
C	-4.591856	-0.645807	-1.318881
H	-2.669841	-1.619244	-1.475108
C	-5.304873	0.425931	-0.779875
H	-5.199038	2.195268	0.446765
H	-5.096909	-1.375346	-1.945890
H	-6.365922	0.533095	-0.985373
W	0.490958	-0.291798	0.061866
N	1.523153	1.450133	-0.022258
C	2.807401	1.769378	0.384053
C	1.090305	2.478640	-0.858416
C	3.186760	2.956031	-0.193879
H	3.355907	1.118258	1.050206
C	2.089797	3.409624	-0.985888
H	0.092841	2.466674	-1.276582
H	4.141322	3.449130	-0.065030
H	2.039590	4.321525	-1.565951
C	0.413243	1.159608	2.971361
H	-0.670197	1.298214	2.886666
H	0.650242	1.074015	4.041757
H	0.899649	2.063253	2.592516
H	-0.272022	-2.854230	0.921948

E = -801.148059531
G = -800.897067

W-N-3-TSB

C	-0.306286	-1.199839	2.038394
C	2.025594	-0.859350	1.829791
C	0.835854	-0.398162	2.474677
H	2.042488	-1.939688	1.673932

H	0.807457	0.299100	3.315545
H	0.387976	0.767626	1.642651
O	1.120550	-1.687034	-0.933173
Si	0.974508	-2.795259	-2.186746
H	1.257466	-4.163886	-1.660024
H	-0.408252	-2.755095	-2.754592
H	1.965568	-2.449147	-3.248141
H	-0.130942	-2.277046	1.997049
C	-2.591489	0.244360	-0.270319
C	-3.449494	-0.435265	-1.155369
C	-3.139750	1.154758	0.653124
C	-4.820543	-0.212624	-1.106061
H	-3.019521	-1.128990	-1.871345
C	-4.513162	1.368068	0.691872
H	-2.468735	1.690537	1.318272
C	-5.359278	0.686600	-0.184036
H	-5.474098	-0.743089	-1.793242
H	-4.925595	2.074306	1.407427
H	-6.431218	0.858429	-0.151671
N	-1.234591	0.032234	-0.323985
W	0.432135	-0.302622	0.194471
N	1.394910	1.442472	-0.242083
C	1.797186	2.557414	0.468622
C	1.740085	1.663133	-1.571739
C	2.397268	3.454688	-0.380170
H	1.604694	2.630687	1.529584
C	2.364880	2.880311	-1.684848
H	1.515277	0.929026	-2.334189
H	2.809349	4.416035	-0.103305
H	2.754737	3.311780	-2.597278
C	3.371137	-0.203650	1.997068
H	3.848836	-0.486139	2.945844
H	4.048890	-0.500297	1.190722
H	3.299177	0.887262	1.966288
H	-1.303339	-0.923081	2.371894

E = -801.098347913
G = -800.850129

W-N-3-TSB$_{transX}$

O	1.365980	-1.476495	-1.183451
C	2.411912	-0.554970	1.589279
C	0.176638	-0.131538	2.280640
C	1.240036	-1.126434	2.172059
H	0.548462	0.848308	2.594633
Si	1.785825	-3.081978	-1.437380
H	0.593026	-3.854250	-1.901878
H	2.852334	-3.128403	-2.479785
H	2.293823	-3.692873	-0.167828
H	1.192104	-2.115081	2.634732
H	0.586557	-1.823591	0.991687
H	2.662427	0.444058	1.934100
N	-1.092837	-0.078678	-0.337034
C	-2.457539	0.092894	-0.383379
C	-3.048050	1.276966	0.096342
C	-3.274621	-0.904827	-0.945249
C	-4.425124	1.452667	0.011974
H	-2.411300	2.044739	0.526056
C	-4.650667	-0.720399	-1.014801
H	-2.809826	-1.811396	-1.320452
C	-5.231701	0.456761	-0.539917
H	-4.871347	2.371649	0.382085
H	-5.273922	-1.498257	-1.447341
H	-6.306870	0.597545	-0.601413
N	1.358892	1.594330	-0.285185
C	2.642025	2.121846	-0.163649
C	0.597827	2.566785	-0.950318
C	2.689161	3.364307	-0.734486
H	3.433138	1.546669	0.291014
C	1.378937	3.651641	-1.233157
H	-0.444700	2.384402	-1.163635
H	3.561988	4.000765	-0.799991
H	1.058644	4.553490	-1.738124
C	-1.156634	-0.522766	2.868429
H	-1.102393	-0.610706	3.961703
H	-1.929419	0.213309	2.632798
H	-1.495212	-1.487238	2.472711
H	3.252874	-1.193363	1.330575
W	0.614387	-0.264558	0.101246

W-N-3-B

C	-0.950651	-1.860519	-1.249212
C	-3.453230	-2.007125	-0.969290
C	-2.362091	-1.642914	-1.662372
H	-0.856945	-2.652629	-0.489578
H	-2.502642	-1.112677	-2.605742
H	-0.301713	-2.100857	-2.093250
H	-0.568402	0.269409	-1.833455
O	-1.228486	-0.540625	1.396415
Si	-2.435105	-0.663053	2.566128
H	-2.803649	-2.102606	2.717181
H	-1.893995	-0.146365	3.857168
H	-3.632346	0.127858	2.159434
H	-3.319509	-2.540747	-0.026226
C	-4.864592	-1.765805	-1.402961
H	-5.411537	-2.710249	-1.518558
H	-5.415998	-1.175760	-0.659971
H	-4.905904	-1.231808	-2.357037
N	1.437148	-0.373313	-0.246093
C	2.800047	-0.531725	-0.121120
C	3.655816	0.038024	-1.079508
C	3.344870	-1.261351	0.949526
C	5.031894	-0.122950	-0.961945
H	3.220669	0.599505	-1.900086
C	4.723098	-1.412330	1.055603
H	2.675900	-1.700013	1.683933
C	5.571054	-0.846116	0.102855
H	5.687521	0.320776	-1.706016
H	5.137432	-1.976628	1.886477
H	6.646786	-0.967903	0.189954
W	-0.282810	-0.103657	-0.193327
N	-0.560430	1.894290	-0.310859
C	-1.225137	2.719164	-1.202689
C	-0.146639	2.691292	0.755157
C	-1.252333	3.998133	-0.708468
H	-1.615854	2.313439	-2.124434
C	-0.562435	3.980905	0.542225
H	0.420722	2.274164	1.577518
H	-1.706090	4.856376	-1.186177
H	-0.386159	4.822016	1.199887

E = -801.130235256
G = -800.884393

W-N-3-TSC

C	-0.966871	-1.926790	-0.513970
C	-3.277605	-2.890147	-0.238358
C	-2.280131	-2.413191	-0.998038
H	-0.750803	-2.343285	0.486836
H	-2.421328	-2.413517	-2.081637
H	-0.168178	-2.266959	-1.177712
H	-1.033605	0.224595	-1.609681
O	-0.892485	0.142320	1.978576

Si	-0.272936	-0.091135	3.520537
H	-0.492658	1.152893	4.316872
H	-0.997087	-1.231070	4.159173
H	1.189873	-0.399251	3.468741
C	-2.539530	0.637491	-1.378550
H	-2.859514	-0.191084	-2.004235
H	-2.376547	1.584498	-1.885676
C	-2.838437	0.619352	-0.019804
H	-2.873415	1.551617	0.535599
H	-3.336254	-0.243856	0.409985
H	-3.139930	-2.919533	0.844787
C	-4.579292	-3.416207	-0.756710
H	-4.726754	-4.465635	-0.471210
H	-5.430597	-2.859773	-0.343975
H	-4.632388	-3.353986	-1.848119
N	1.216084	-0.319786	-0.066220
C	2.482163	-0.759770	-0.349301
C	2.864573	-0.999662	-1.683177
C	3.411503	-0.977774	0.685677
C	4.147650	-1.451833	-1.967810
H	2.142267	-0.818833	-2.473324
C	4.691874	-1.426111	0.385535
H	3.110063	-0.784792	1.710360
C	5.065122	-1.666402	-0.938222
H	4.435236	-1.634038	-2.999557
H	5.404408	-1.588925	1.189385
H	6.067578	-2.016719	-1.166209
W	-0.477451	0.136666	0.098501
N	-0.245031	2.102980	-0.470116
C	0.065945	2.704229	-1.669502
C	-0.194320	3.086423	0.507850
C	0.303459	4.045460	-1.465260
H	0.118313	2.117801	-2.576681
C	0.133694	4.290114	-0.074352
H	-0.420896	2.855640	1.539874
H	0.571606	4.767439	-2.225420
H	0.225717	5.238620	0.438416

E = -879.665969653
G = -879.369065

W-N-3-C

C	-0.962472	-1.952233	-0.995874
C	-3.388257	-2.493680	-0.564119
C	-2.414434	-1.946557	-1.308760
H	-0.734354	-2.661608	-0.186135
H	-2.703751	-1.441965	-2.232812
H	-0.356776	-2.217858	-1.866970
H	0.055000	2.585065	-2.267892
O	-1.151796	-0.555150	1.421928
Si	-2.324493	-0.793555	2.608808
H	-3.645318	-0.274341	2.150515
H	-2.425463	-2.254508	2.900523
H	-1.888657	-0.067620	3.837502
C	0.145023	1.659553	-2.842025
H	1.207568	1.396936	-2.881346
H	-0.177321	1.870720	-3.870314
C	-0.684978	0.521391	-2.240890
H	-1.748467	0.811243	-2.234139
H	-0.616457	-0.349781	-2.900216
H	-3.113170	-3.027086	0.347975
C	-4.846606	-2.464967	-0.902384
H	-5.249484	-3.479405	-1.018532
H	-5.435068	-1.986292	-0.109091
H	-5.032036	-1.920788	-1.833722
N	1.470267	-0.318797	-0.231589
C	2.797255	-0.618098	0.000016
C	3.714595	-0.571713	-1.063024
C	3.242455	-0.965720	1.287226
C	5.053851	-0.870197	-0.835656
H	3.358261	-0.301499	-2.051834
C	4.584796	-1.258509	1.500372
H	2.525677	-0.998883	2.102433
C	5.494519	-1.213080	0.442950
H	5.757705	-0.833013	-1.662383
H	4.922432	-1.524654	2.498131
H	6.541778	-1.443525	0.615113
W	-0.248733	-0.051362	-0.164210
N	-0.562315	1.944155	0.091571
C	-1.739896	2.664131	-0.007040
C	0.396052	2.796703	0.634887
C	-1.542138	3.931701	0.483240
H	-2.635565	2.211206	-0.410729
C	-0.175734	4.016773	0.890966
H	1.413095	2.458781	0.775764
H	-2.287843	4.713387	0.546057
H	0.324577	4.879344	1.310803

E = -879.725119504
G = -879.425987

W-N-3'-I

O	-0.235567	1.979257	-0.793045
Si	0.088701	3.618924	-0.973016
H	-0.860262	4.177570	-1.979968
H	-0.090624	4.317030	0.336801
H	1.492999	3.805304	-1.447834
C	-0.077749	0.630305	2.010266
C	2.442772	-1.454676	-0.462739
N	1.287851	-0.659585	-0.128727
W	-0.116370	0.322225	0.141752
N	-1.777521	-0.811620	-0.083027
C	-2.838482	-1.050662	0.778683
C	-2.110379	-1.391350	-1.304420
C	-3.817234	-1.748694	0.118131
H	-2.790504	-0.702300	1.800206
C	-3.352820	-1.965482	-1.214366
H	-1.427479	-1.345147	-2.143245
H	-4.760116	-2.075336	0.536661
H	-3.873078	-2.486779	-2.007128
C	0.701695	0.251480	3.228996
H	1.180787	1.123539	3.693695
H	0.044709	-0.192453	3.989131
H	1.476774	-0.480517	2.989597
H	-0.855909	1.402083	2.183460
C	3.706616	-0.696856	-0.027816
H	3.693154	-0.512526	1.050246
H	4.601300	-1.280900	-0.268164
H	3.772313	0.267246	-0.540840
C	2.344463	-2.801239	0.271443
H	1.434303	-3.332626	-0.020487
H	3.208548	-3.429995	0.031236
H	2.318450	-2.647688	1.354076
C	2.456273	-1.679380	-1.983439
H	2.502589	-0.723671	-2.514376
H	3.327835	-2.277062	-2.270211
H	1.555073	-2.211662	-2.302107

E = -648.797705587
G = -648.570604

W-N-3'-Ianti

O	-0.161669	1.974776	-0.678371
Si	0.467824	3.356212	-1.401418
H	-0.612506	3.997943	-2.205831
H	0.944649	4.299280	-0.345801
H	1.609676	2.990543	-2.293849
C	-0.279355	0.532040	2.089995
C	2.552412	-1.446657	-0.053855
N	1.362426	-0.649439	0.104067
W	-0.090668	0.289650	0.207312
N	-1.674010	-0.889220	-0.239656
C	-2.792186	-1.237033	0.502852
C	-1.863395	-1.401088	-1.520493
C	-3.668733	-1.935749	-0.288426
H	-2.854716	-0.960057	1.545041
C	-3.076234	-2.039114	-1.582978
H	-1.108671	-1.272007	-2.286193
H	-4.625739	-2.335944	0.019733
H	-3.494011	-2.530549	-2.451797
C	-1.298113	1.528113	2.602498
H	-1.990503	1.041676	3.302833
H	-0.811811	2.350029	3.144617
H	-1.910150	1.977175	1.810493
H	0.357732	0.091708	2.857605
C	3.752407	-0.515936	-0.285653
H	3.878208	0.165270	0.561154
H	4.672234	-1.098916	-0.401688
H	3.605732	0.081972	-1.190291
C	2.752313	-2.267689	1.229882
H	1.894754	-2.923995	1.402518
H	3.654219	-2.883608	1.148721
H	2.862305	-1.607691	2.095387
C	2.358388	-2.381565	-1.257757
H	2.209539	-1.803039	-2.174909
H	3.241520	-3.015285	-1.390978
H	1.486849	-3.025126	-1.108302

E = -648.794984520
G = -648.567586

W-N-3'-TSI

W	-0.058503	0.261988	0.283270
O	-0.825968	1.863800	-0.456745
N	1.236867	-0.772339	-0.262132
C	2.366952	2.472672	-0.429671
C	0.145045	0.291535	2.175086
C	2.035551	2.731563	0.838477
H	-0.573394	1.034315	2.572571
Si	-1.818531	2.809744	-1.421304
H	2.626947	2.358904	1.669877
H	1.174973	3.345793	1.086199
H	3.240430	1.876948	-0.677965
H	-1.879122	2.248253	-2.805732
H	-1.246712	4.190410	-1.483859
H	-3.192839	2.868377	-0.841634
C	1.016390	-0.330632	3.220273
H	1.548996	0.428567	3.809764
H	1.751079	-1.005019	2.775423
H	0.412684	-0.910346	3.932132
H	1.784237	2.858475	-1.260782
C	2.188127	-1.606444	-0.950120
N	-1.663277	-0.960489	0.147826
C	-2.501406	-1.463572	1.126924
C	-2.175941	-1.369031	-1.075922
C	-3.527576	-2.162363	0.538923
H	-2.281523	-1.280428	2.168578
C	-3.320931	-2.100862	-0.870464
H	-1.682856	-1.103414	-2.002413
H	-4.334960	-2.664696	1.055302
H	-3.940218	-2.544235	-1.639314
C	2.362851	-1.110852	-2.394637
H	1.410237	-1.154335	-2.931864
H	3.087336	-1.732591	-2.931327
H	2.719031	-0.076351	-2.408132
C	3.530059	-1.544078	-0.202955
H	4.270912	-2.178904	-0.700423
H	3.412413	-1.892905	0.826929
H	3.914496	-0.520245	-0.177327
C	1.650015	-3.047129	-0.945475
H	0.678484	-3.096731	-1.444975
H	1.520316	-3.402470	0.080568
H	2.345509	-3.716338	-1.463830

E = -727.351529039
G = -727.077382

W-N-3'-TBP

W	0.205285	-0.245581	-0.033367
O	2.163221	-0.501340	-0.121609
C	0.155957	-1.828337	1.293239
H	1.142842	-1.971880	1.740022
C	0.170417	-1.775354	-1.450171
C	0.103882	-2.620469	-0.113307
H	1.094268	-1.947899	-1.999275
H	0.962261	-3.292015	-0.109319
H	-0.835454	-3.172881	-0.109313
Si	3.710764	-1.039077	-0.379945
H	4.650630	0.114206	-0.539169
H	3.780802	-1.880781	-1.620442
H	4.167304	-1.875601	0.776702
C	-0.949691	-2.187162	2.261480
H	-0.903130	-1.541111	3.143862
H	-0.856358	-3.224618	2.609829
H	-1.936291	-2.064382	1.807798
H	-0.710489	-1.916053	-2.070598
N	-1.533789	-0.018551	-0.123047
C	-2.936430	0.163660	-0.386817
N	0.623703	1.752118	0.152330
C	1.839811	2.387339	-0.075270
C	-0.268655	2.743894	0.547718
C	1.713625	3.730758	0.169043
H	2.699541	1.817705	-0.388981
C	0.365294	3.959003	0.575224
H	-1.287164	2.487521	0.793895
H	2.498762	4.469490	0.072990
H	-0.080809	4.904722	0.854762
C	-3.535188	-1.164367	-0.882140
H	-4.600051	-1.035439	-1.101962
H	-3.437401	-1.948462	-0.125254
H	-3.038601	-1.498081	-1.797722
C	-3.648731	0.604146	0.903559
H	-3.249935	1.553752	1.270767
H	-3.525242	-0.143891	1.691858
H	-4.719647	0.734314	0.715730
C	-3.092911	1.239117	-1.477292
H	-4.153957	1.416548	-1.682836
H	-2.609119	0.916798	-2.404080
H	-2.633988	2.180483	-1.164613

E = -727.385844941
G = -727.098184

W-N-3'-TSIII

O	1.507650	-1.506438	0.340337
C	-1.126751	-2.462246	0.680410
C	-0.124046	-0.744814	-2.204445
C	-1.020065	-2.770217	-0.651534
H	0.685128	-1.314878	-2.676404
H	-0.898068	-0.417534	-2.895857
Si	3.060322	-1.405359	0.977091
H	-1.884588	-2.733961	-1.307972
H	-0.132742	-3.260858	-1.035489
H	3.269261	-0.128997	1.717519
H	3.234052	-2.552489	1.928499
H	4.070968	-1.559471	-0.114381
C	-2.430525	-2.191410	1.374167
H	-2.333124	-1.434018	2.155468
H	-3.205208	-1.874709	0.672658
H	-2.770348	-3.115393	1.860180
H	-0.278621	-2.712151	1.314380
W	0.002556	-0.430793	-0.315081
N	1.304478	1.173126	-0.160125
C	2.438226	1.376353	-0.916795
C	1.334581	2.094442	0.866551
C	3.172072	2.417813	-0.385376
H	2.626873	0.775022	-1.795789
C	2.467195	2.875182	0.758960
H	0.542581	2.128288	1.602221
H	4.097542	2.813303	-0.783301
H	2.747753	3.686487	1.418059
N	-1.436183	0.546083	-0.075552
C	-2.474665	1.503266	0.212869
C	-3.784340	1.029315	-0.439606
H	-4.568826	1.779521	-0.294566
H	-3.645551	0.880277	-1.514303
H	-4.128561	0.088793	-0.000244
C	-2.669323	1.666941	1.728376
H	-1.742969	1.997657	2.206963
H	-3.441834	2.415902	1.931756
H	-2.980993	0.725834	2.189899
C	-2.049110	2.846737	-0.409613
H	-1.930821	2.744587	-1.491856
H	-2.809869	3.609553	-0.210773
H	-1.094482	3.181824	0.003284

E = -727.352524541
G = -727.068248

W-N-3'-IV

W	-0.035466	-0.433989	-0.373960
O	1.121617	-1.665801	0.613380
N	-1.313613	0.720755	-0.073183
C	-1.675667	-2.336495	0.489956
C	-0.081818	-0.595078	-2.284164
C	-1.302797	-2.686764	-0.771815
H	0.656347	-1.247884	-2.768376
H	-0.769865	-0.122948	-2.984317
Si	2.688732	-1.995192	1.117497
H	2.895989	-1.534731	2.525169
H	3.706375	-1.377347	0.218990
H	2.855118	-3.484918	1.089587
C	-2.064022	1.840058	0.444863
N	1.513345	0.915629	-0.211059
C	2.084202	1.706099	-1.185909
C	2.048466	1.317467	0.999705
C	2.974414	2.586077	-0.609947
H	1.802901	1.574750	-2.221181
C	2.949270	2.340268	0.790538
H	1.746781	0.846240	1.926410
H	3.582534	3.312651	-1.132929
H	3.532353	2.841832	1.552158
H	-0.991107	-2.567798	1.304046
H	-1.994060	-2.606598	-1.605354
H	-0.375253	-3.220671	-0.950950
C	-3.062273	-1.908189	0.861435
H	-3.060200	-1.109349	1.606152
H	-3.588971	-2.763033	1.305704
H	-3.630727	-1.575838	-0.010432
C	-3.517673	1.748390	-0.044726
H	-3.551435	1.703608	-1.137295
H	-4.079714	2.629715	0.281750
H	-4.015513	0.860054	0.353284
C	-2.008612	1.849644	1.980425
H	-0.971400	1.925528	2.319984
H	-2.445818	0.937484	2.398430
H	-2.564761	2.705290	2.377800
C	-1.407672	3.119361	-0.105415
H	-1.924048	4.002836	0.286086
H	-1.464620	3.138485	-1.197381
H	-0.354604	3.167200	0.183729

E = -727.354757113
G = -727.073328

W-N-3'-TSIV

W	0.057881	-0.251048	-0.436374
O	0.321321	-1.937029	0.457782
N	-0.854086	1.162300	0.015838
C	-2.893614	-1.808342	0.128693
C	-0.015428	-0.244447	-2.341868
C	-2.404488	-2.066761	-1.093284
H	0.406033	-1.124819	-2.847600
H	-0.478098	0.469803	-3.021090
Si	1.119429	-2.997275	1.486685
H	1.233774	-2.400140	2.852798
H	2.478581	-3.311865	0.957147
H	0.316369	-4.255658	1.576010
N	1.948662	0.422388	-0.199005
C	2.921794	0.730214	-1.133449
C	2.508499	0.625643	1.055333
C	4.074829	1.105493	-0.488227
H	2.692181	0.660652	-2.186616
C	3.811825	1.037635	0.911606
H	1.933530	0.454207	1.956422
H	5.003565	1.396897	-0.960737
H	4.501104	1.261566	1.715356
H	-2.408961	-2.267701	0.989587
H	-2.859678	-1.648837	-1.987535
H	-1.578873	-2.755596	-1.236130
C	-4.103361	-0.976216	0.409655
H	-3.887717	-0.186006	1.136829
H	-4.895951	-1.595525	0.848377
H	-4.497026	-0.513806	-0.499715
C	-1.402563	2.364175	0.593144
C	-1.742100	2.130234	2.073260
H	-2.468110	1.319390	2.184264
H	-2.168398	3.035895	2.517582
H	-0.841883	1.864584	2.636074
C	-0.341728	3.471255	0.466726
H	-0.708662	4.400505	0.916169
H	-0.109076	3.659694	-0.584892
H	0.583148	3.178387	0.971219
C	-2.663853	2.754102	-0.192926
H	-3.076426	3.691138	0.195901

H	-3.430645	1.978961	-0.112113
H	-2.425450	2.893189	-1.251243

E = -727.351758612
G = -727.074249

W-N-3'-V

W	-0.090896	0.330492	-0.328422
O	-0.047244	2.042154	0.491646
N	1.245963	-0.732577	-0.046416
C	-0.098684	0.505613	-2.218264
H	-0.762114	1.310197	-2.570270
H	0.495777	0.041668	-3.001715
Si	0.583826	3.570179	0.809933
H	1.943974	3.436158	1.412942
H	-0.328322	4.258586	1.768633
H	0.672721	4.347600	-0.462079
C	2.355469	-1.604391	0.249907
N	-1.807920	-0.659440	0.057934
C	-2.928300	-0.867667	-0.734938
C	-2.116751	-1.135041	1.330299
C	-3.918845	-1.444880	0.017603
H	-2.905646	-0.591343	-1.778960
C	-3.401535	-1.614271	1.337608
H	-1.387694	-1.093689	2.129463
H	-4.903752	-1.724296	-0.332585
H	-3.915967	-2.044129	2.186968
C	3.655606	-0.910809	-0.185558
H	3.630965	-0.685804	-1.255639
H	4.515778	-1.558846	0.012976
H	3.794775	0.026853	0.360822
C	2.375251	-1.874621	1.762574
H	1.447158	-2.359552	2.079309
H	2.489596	-0.940508	2.321041
H	3.211856	-2.533666	2.016986
C	2.163573	-2.918198	-0.523870
H	2.993532	-3.602992	-0.319745
H	2.127647	-2.727959	-1.600240
H	1.229422	-3.404704	-0.229739

E = -609.491430470
G = -609.290354

W-N-3'-TSA

O	1.540418	-1.345416	-0.581692
C	-0.668238	-2.255495	0.895928
H	0.073120	-3.053069	0.978460
C	-0.027968	-0.203855	2.326756
C	-0.886993	-1.520301	2.257728
H	0.980683	-0.450737	2.695477
H	-0.586177	-2.171343	3.088093
H	-1.938238	-1.246673	2.378249
Si	1.907682	-2.613015	-1.602614
H	1.433499	-2.325128	-2.993059
H	3.391332	-2.794193	-1.622481
H	1.269987	-3.886611	-1.138568
N	1.344681	1.245026	-0.185209
C	2.724922	1.266241	-0.320050
C	0.926180	2.577850	-0.175680
C	3.166429	2.562554	-0.373478
H	3.271485	0.336516	-0.370295
C	2.011508	3.405567	-0.278725
H	-0.124467	2.814134	-0.087906
H	4.195102	2.883533	-0.476082
H	1.993054	4.487688	-0.298881
C	-0.623748	0.945571	3.115425
H	0.001625	1.839507	3.033364
H	-1.621717	1.198082	2.744807
H	-0.710012	0.691834	4.180855
H	-1.596932	-2.653165	0.487496
N	-1.425401	0.307308	-0.290551
C	-2.538586	0.664170	-1.141282
C	-3.486104	-0.541976	-1.228445
H	-3.857172	-0.817926	-0.236921
H	-4.345297	-0.299038	-1.862308
H	-2.971803	-1.406370	-1.657989
C	-2.007853	1.030707	-2.536144
H	-2.832693	1.343202	-3.184992
H	-1.285270	1.849193	-2.473173
H	-1.513021	0.171101	-2.998574
C	-3.265027	1.863503	-0.512179
H	-4.125840	2.147961	-1.126100
H	-3.622925	1.616007	0.491443
H	-2.598440	2.727369	-0.436942
W	0.090637	-0.341755	0.258478

E = -727.371172956
G = -727.087007

W-N-3'-SBP

O	-0.507356	1.897058	-0.788846
C	0.612439	1.508469	1.785158
C	-0.413844	-0.494280	2.157748
C	0.647589	0.383638	2.812400
H	-1.407120	-0.088953	2.421083
Si	-0.735620	3.558189	-0.952372
H	-1.458623	4.102487	0.236736
H	0.592153	4.230223	-1.080096
H	-1.543138	3.792790	-2.184117
H	0.454659	0.675257	3.857049
H	1.618088	-0.126260	2.785113
H	-0.186222	2.231039	2.006538
N	1.403182	-0.506672	-0.271985
C	2.670295	-0.942638	-0.812940
N	-1.656908	-0.926122	-0.327261
C	-2.961756	-0.884944	0.134746
C	-1.640164	-1.787776	-1.421112
C	-3.753484	-1.679792	-0.657400
H	-3.227878	-0.282959	0.992752
C	-2.908246	-2.258367	-1.650958
H	-0.713565	-2.002378	-1.934400
H	-4.818200	-1.834232	-0.541226
H	-3.200335	-2.948479	-2.431438
C	3.795285	-0.215233	-0.061217
H	4.770899	-0.541660	-0.436443
H	3.715848	0.867074	-0.199185
H	3.746163	-0.431359	1.009633
C	2.788953	-2.461011	-0.609040
H	1.979918	-2.986410	-1.124571
H	3.743948	-2.822204	-1.004876
H	2.737015	-2.711965	0.453952
C	2.721411	-0.597790	-2.309158
H	2.619504	0.481026	-2.460445
H	3.676090	-0.919174	-2.738462
H	1.915257	-1.100568	-2.852014
C	-0.387426	-1.987471	2.437483
H	-0.548782	-2.186561	3.507060
H	-1.160491	-2.522077	1.877674
H	0.582266	-2.419323	2.166229
H	1.538856	2.063589	1.599432
W	-0.085392	0.284090	0.122682

E = -727.389651622
G = -727.106782

W-N-3'-TSB

C	0.436236	-1.109509	-2.164712
C	-1.770708	-1.462036	-1.389346
C	-0.969454	-0.709648	-2.306724
H	-1.412234	-2.481509	-1.236880
H	-1.353207	-0.132924	-3.153777
H	-0.728749	0.563139	-1.653781
O	-0.033883	-1.766063	1.046056
Si	0.816957	-2.554342	2.260076
H	1.090391	-3.958010	1.827772
H	2.111911	-1.856317	2.532650
H	-0.016301	-2.565535	3.499092
H	0.605828	-2.185678	-2.090213
C	-3.255033	-1.265791	-1.225664
H	-3.826405	-1.773409	-2.016191
H	-3.595950	-1.671417	-0.267816
H	-3.533147	-0.208011	-1.238035
H	1.182730	-0.587154	-2.756570
N	-1.429468	1.093755	0.420207
C	-1.518162	1.335200	1.785215
C	-2.307355	1.961319	-0.199742
C	-2.450649	2.317651	2.016870
H	-0.912760	0.779506	2.489282
C	-2.951582	2.722305	0.745785
H	-2.393850	1.979382	-1.276934
H	-2.742643	2.700902	2.985755
H	-3.695736	3.483556	0.552165
N	1.452998	0.545758	-0.030402
C	2.715595	1.208447	-0.234379
C	3.784803	0.159225	-0.579794
H	4.760674	0.637957	-0.714075
H	3.869535	-0.579332	0.222938
H	3.528784	-0.366432	-1.504526
C	3.082827	1.928885	1.074175
H	4.036347	2.456015	0.962774
H	2.310889	2.656472	1.340514
H	3.176812	1.211065	1.894441
C	2.568009	2.227881	-1.374953
H	3.508982	2.765717	-1.531908
H	2.298446	1.726576	-2.309573
H	1.785611	2.954256	-1.137177
W	-0.075326	-0.311077	-0.203222

E = -727.337589379
G = -727.057439

W-N-3'-B

C	-0.852205	-1.894339	-1.055994
C	-3.336068	-1.575067	-0.744040
C	-2.214346	-1.472024	-1.476181
H	-0.878499	-2.636983	-0.243381
H	-2.282712	-1.008281	-2.461574
H	-0.264892	-2.292447	-1.884364
H	-0.152796	0.112378	-1.804851
O	-0.889108	-0.374716	1.508945
Si	-2.059844	-0.267622	2.712062
H	-2.613438	-1.632951	2.961543
H	-1.416640	0.243500	3.958576
H	-3.157368	0.652236	2.293538
H	-3.275630	-2.038909	0.242473
C	-4.692929	-1.124908	-1.184877
H	-5.401372	-1.962848	-1.207848
H	-5.111394	-0.382109	-0.493981
H	-4.663618	-0.678743	-2.183428
N	1.726158	-0.639485	-0.158205
C	3.127185	-0.953360	-0.018623
W	0.062268	-0.172990	-0.132521
C	3.414175	-2.213565	-0.849390
H	3.167210	-2.043590	-1.901079
H	4.474853	-2.476201	-0.778893
H	2.822669	-3.059373	-0.486529
C	3.946268	0.234163	-0.546881
H	3.722699	1.141801	0.020772
H	5.017165	0.022746	-0.457989
H	3.712706	0.423348	-1.598136
C	3.438508	-1.207059	1.463975
H	2.837457	-2.036403	1.849007
H	4.496647	-1.457899	1.591733
H	3.222530	-0.316476	2.062074
N	-0.001729	1.839803	-0.381387
C	-0.538519	2.665357	-1.353605
C	0.471871	2.662608	0.637229
C	-0.428773	3.973977	-0.955931
H	-0.948622	2.237745	-2.256752
C	0.217331	3.972975	0.317121
H	0.948184	2.245496	1.515356
H	-0.765488	4.839468	-1.511159
H	0.467220	4.835387	0.921343

E = -727.372762590
G = -727.095267

W-N-3'-TSC

W	0.137251	-0.090118	-0.005619
C	1.811249	1.009132	-0.934296
C	4.184412	0.362914	-0.393645
C	3.141679	0.426708	-1.235269
H	1.894390	1.735448	-0.106614
H	3.285350	0.046909	-2.249457
H	1.424272	1.555489	-1.797148
H	0.369460	-0.809255	-1.642879
O	0.623204	-0.018337	1.856739
Si	0.339530	0.789972	3.300637
H	1.638352	1.325893	3.808814
H	-0.621039	1.919891	3.103982
H	-0.223992	-0.176717	4.289767
C	1.236124	-2.058863	-1.280836
H	1.993103	-1.755568	-1.998938
H	0.461024	-2.718379	-1.661840
C	1.542360	-2.065565	0.078197
H	0.984946	-2.709484	0.750400
H	2.504332	-1.692938	0.414796
H	4.063142	0.755405	0.618314
C	5.530650	-0.196621	-0.731973
H	6.317662	0.559852	-0.617542
H	5.799424	-1.026675	-0.065952
H	5.565906	-0.565677	-1.761766
N	-0.933860	1.248059	-0.327908
C	-1.895880	2.254221	-0.690121
C	-1.966804	2.341830	-2.222852
H	-2.697263	3.099513	-2.524915
H	-0.993643	2.615315	-2.641566
H	-2.268287	1.379832	-2.646221
C	-1.453046	3.601193	-0.096161
H	-1.386316	3.539176	0.993764
H	-0.474844	3.896698	-0.487683
H	-2.176694	4.381299	-0.354300

C	-3.258284	1.831399	-0.113774
H	-3.549136	0.848908	-0.495166
H	-3.214036	1.777367	0.977770
H	-4.024477	2.561855	-0.394555
N	-1.353724	-1.524788	-0.217007
C	-2.194991	-1.816700	-1.264091
C	-1.825338	-2.204924	0.892214
C	-3.186271	-2.676001	-0.835345
H	-2.023223	-1.382276	-2.239662
C	-2.950333	-2.922971	0.543528
H	-1.316206	-2.137489	1.844541
H	-3.984015	-3.082874	-1.443169
H	-3.523925	-3.563105	1.201136

E = -805.906578838
G = -805.577597

W-N-3'-C

C	0.552330	-1.963862	1.075655
C	2.965282	-1.604543	0.389709
C	1.977752	-1.623800	1.309452
H	0.410395	-2.773937	0.354343
H	2.228507	-1.286236	2.316141
H	0.013064	-2.188072	1.993413
H	-1.390756	-0.406461	3.231514
O	0.540515	-1.044776	-1.499413
Si	0.246739	-2.118510	-2.748600
H	1.375001	-2.050348	-3.723913
H	0.150144	-3.509397	-2.202695
H	-1.034479	-1.781107	-3.442719
C	-0.356878	-0.081697	3.395054
H	0.220558	-0.970276	3.674584
H	-0.354511	0.576287	4.274234
C	0.216119	0.628547	2.171878
H	-0.292873	1.598218	2.060624
H	1.268158	0.887693	2.351569
H	2.742273	-1.913847	-0.629870
C	4.381664	-1.216825	0.675764
H	5.062607	-2.058823	0.496739
H	4.715215	-0.405603	0.016403
H	4.512470	-0.892776	1.712953
W	-0.010294	-0.103767	0.090527
N	-1.733949	-0.032830	0.099507
C	-3.174823	0.044979	0.060861
C	-3.748918	-1.270231	0.608809
H	-4.843382	-1.236718	0.600610
H	-3.423645	-2.117461	-0.001901
H	-3.414452	-1.437995	1.636351
C	-3.620102	1.229206	0.932850
H	-3.286257	1.095127	1.965314
H	-3.201658	2.166877	0.555760
H	-4.712049	1.310550	0.928309
C	-3.620781	0.254746	-1.394483
H	-3.207409	1.183559	-1.798757
H	-3.288844	-0.574537	-2.025552
H	-4.712893	0.313963	-1.447191
N	0.846987	1.692895	-0.341778
C	2.142974	2.135912	-0.131523
C	0.189530	2.690273	-1.059915
C	2.307783	3.366702	-0.714204
H	2.845963	1.526320	0.418384
C	1.056980	3.721217	-1.309497
H	-0.849109	2.573124	-1.335043
H	3.216995	3.953518	-0.718999
H	0.829498	4.630264	-1.850467

E = -805.966508496
G = -805.633342

W-O-3-I

W	-0.289228	0.261410	-0.320571
O	-1.416277	-1.231627	-0.064365
C	-0.660602	1.593635	0.974325
H	-0.791705	1.096467	1.952740
Si	-2.687484	-2.063036	0.674777
H	-2.270122	-3.483360	0.847874
H	-2.973516	-1.441799	2.003350
H	-3.893237	-1.979545	-0.198376
C	-0.911021	3.069295	0.971622
H	-0.183883	3.582641	1.614438
H	-0.826590	3.484952	-0.035186
H	-1.908089	3.305655	1.364709
N	1.616985	-0.201218	0.092164
C	2.416774	0.062633	1.197716
C	2.350484	-1.037521	-0.751916
C	3.610231	-0.594786	1.061485
H	2.055041	0.712666	1.981130
C	3.568326	-1.297027	-0.183220
H	1.942227	-1.364913	-1.699788
H	4.432251	-0.573982	1.764634
H	4.350872	-1.911353	-0.608100
O	-0.392425	1.074364	-1.807796

E = -511.477334911
G -511.365350

W-O-3-Ianti

W	-0.285668	0.277948	-0.409378
O	-1.520638	-0.731735	0.595841
C	-0.313876	2.087735	0.184447
H	-0.292694	2.905954	-0.539304
Si	-2.857883	-1.739835	0.835997
H	-2.491969	-2.740281	1.878189
H	-4.001872	-0.901790	1.297202
H	-3.204034	-2.425426	-0.443315
C	-0.501249	2.506038	1.621177
H	-1.429595	3.079063	1.742602
H	-0.535556	1.662693	2.318708
H	0.323224	3.159565	1.935250
N	1.590542	-0.263377	0.042568
C	2.567070	0.336509	0.826393
C	2.089683	-1.505802	-0.352600
C	3.642627	-0.504707	0.934066
H	2.403171	1.324941	1.229249
C	3.338133	-1.681316	0.181506
H	1.515818	-2.153319	-1.003779
H	4.555015	-0.304739	1.480138
H	3.973176	-2.546299	0.044141
O	-0.445990	0.374498	-2.097965

E = -511.474940102
G = -511.362580

W-O-3-TSrot1

W	0.308699	0.297141	0.157816
O	1.792755	-0.493284	-0.685325
C	0.230332	2.083933	-0.495052
H	1.263531	2.473763	-0.512856
Si	3.051933	-1.596382	-0.407796
H	3.669717	-1.893403	-1.730681

H	4.047612	-0.973794	0.510203
H	2.494847	-2.842422	0.196441
C	-0.836779	3.141006	-0.594824
H	-0.743971	3.690462	-1.541051
H	-1.841479	2.709244	-0.562882
H	-0.761706	3.877966	0.216505
N	-1.493804	-0.492570	0.012832
C	-2.122428	-0.736631	-1.216113
C	-2.321754	-1.006216	1.013508
C	-3.309715	-1.370829	-0.984427
H	-1.672149	-0.405021	-2.142565
C	-3.435739	-1.542774	0.433413
H	-2.019512	-0.936827	2.048377
H	-4.024212	-1.672702	-1.738417
H	-4.261383	-2.007167	0.955581
O	0.646120	0.290519	1.848229

E = -511.436722062
G = -511.325771

W-O-3-TSrot2

W	0.256764	0.220451	0.201871
O	1.404541	-0.968637	-0.667393
C	0.640063	1.961899	-0.367008
H	-0.455173	2.158339	-0.134394
Si	2.684303	-2.077911	-0.579463
H	2.243979	-3.332720	-1.252315
H	3.856440	-1.493952	-1.291988
H	3.007951	-2.327843	0.853837
C	1.508252	3.166605	-0.461226
H	1.524874	3.747851	0.470182
H	2.535633	2.865049	-0.687613
H	1.182504	3.834663	-1.268301
N	-1.697368	-0.132090	-0.021708
C	-2.532693	0.383891	-1.013622
C	-2.427941	-1.089384	0.679870
C	-3.747981	-0.241603	-0.940158
H	-2.174320	1.147367	-1.690261
C	-3.682379	-1.176506	0.139091
H	-1.984417	-1.606092	1.519493
H	-4.599386	-0.047965	-1.578730
H	-4.476679	-1.825783	0.482134
O	0.607392	0.037846	1.877670

E = -511.438840278
G = -511.329380

W-O-3-TSI

W	-0.205403	-0.257295	0.136379
O	-0.695842	1.407160	-0.645601
C	-3.332573	0.347808	0.919137
C	-0.438302	-1.702164	-1.080074
C	-3.384236	-0.610663	-0.011747
H	-0.432634	-1.330497	-2.118530
Si	-0.928174	3.071799	-0.725460
H	-3.562783	-0.380978	-1.058843
H	-3.284859	-1.659842	0.249984
H	-3.466963	1.395152	0.662547
H	-0.003144	3.642652	-1.745770
H	-2.344403	3.334384	-1.121927
H	-0.663783	3.688198	0.609373
C	-0.693830	-3.171152	-0.942445
H	0.105247	-3.744571	-1.430991
H	-0.736880	-3.478669	0.104860
H	-1.632640	-3.460546	-1.433784
H	-3.166631	0.113167	1.966266
N	1.792391	-0.114446	0.106834
C	2.726680	-0.580411	-0.806081
C	2.475086	0.681602	1.022541
C	3.962967	-0.082479	-0.485476
H	2.417466	-1.235977	-1.607089
C	3.802821	0.722817	0.683615
H	1.957781	1.129430	1.861252
H	4.885454	-0.277663	-1.016068
H	4.579518	1.254126	1.217605
O	-0.518521	-0.880251	1.693204

E = -590.035767422
G = -589.876351

W-O-3-II

W	0.524098	-0.083136	-0.198853
O	-0.019139	1.668496	0.431585
C	2.495010	1.430397	-0.802290
C	1.202016	-1.235497	1.184057
C	2.944590	0.788635	0.310188
H	1.026428	-0.837292	2.196095
Si	-1.388090	2.561997	0.847308
H	2.821072	1.224883	1.297372
H	3.581968	-0.086865	0.239459
H	1.996652	2.390333	-0.724794
H	-2.389098	1.721201	1.562795
H	-0.922569	3.662031	1.749327
H	-1.989228	3.171633	-0.377100
C	1.930720	-2.541016	1.162526
H	1.333471	-3.306320	1.676502
H	2.126082	-2.887280	0.145784
H	2.881047	-2.474782	1.710207
H	2.744269	1.066112	-1.793595
N	-1.432013	-0.653936	-0.180226
C	-2.114796	-1.432305	0.737736
C	-2.367135	-0.181722	-1.086825
C	-3.451767	-1.452776	0.421286
H	-1.580481	-1.918245	1.541880
C	-3.613655	-0.653823	-0.747356
H	-2.066745	0.434978	-1.924410
H	-4.226152	-1.986741	0.956057
H	-4.534935	-0.460352	-1.281075
O	0.984437	-0.816373	-1.673589

E = -590.039147061
G = -589.874968

W-O-3-TBP

O	0.355882	1.597260	0.122217
C	1.692122	-0.055340	-1.644279
H	1.812548	0.949532	-2.043173
C	1.877884	-0.549322	1.058204
C	2.600522	-0.323580	-0.373535
H	2.035529	0.332712	1.681625
H	3.247103	0.543619	-0.245982
H	3.168680	-1.233887	-0.560327
Si	0.719688	3.224868	0.240875
H	-0.529738	4.019691	0.437473
H	1.635835	3.449493	1.402748
H	1.403731	3.681102	-1.010002
W	0.238499	-0.332057	-0.186018
N	-1.771632	-0.190211	0.030385
C	-2.538515	0.945255	0.288014
C	-2.659187	-1.264491	-0.054524

C	-3.859315	0.593901	0.363484
H	-2.064161	1.907502	0.397504
C	-3.936492	-0.816520	0.144999
H	-2.280510	-2.256196	-0.254513
H	-4.683994	1.268081	0.554807
H	-4.831341	-1.424905	0.136487
C	2.263111	-1.832294	1.761923
H	1.686448	-1.938851	2.686022
H	2.061139	-2.704902	1.135505
H	3.325754	-1.830203	2.037183
H	1.797321	-0.829039	-2.400525
O	0.175581	-2.017737	-0.502242

E = -590.058904093
G = -589.889295

W-O-3-TSIII

O	-0.116158	1.580086	0.328686
C	-2.534506	0.382160	-0.531370
C	-0.881943	-0.968193	1.930671
C	-2.770057	0.059767	0.804504
H	-0.799654	-0.321071	2.807554
H	-1.222296	-1.980020	2.147014
Si	0.444209	3.009215	-0.365127
H	-3.309574	-0.847066	1.062419
H	-2.740014	0.832331	1.565616
H	1.242102	2.721655	-1.591134
H	-0.740546	3.849494	-0.732155
H	1.267330	3.746758	0.637443
C	-3.092172	-0.433756	-1.671127
H	-2.449422	-0.397269	-2.554166
H	-3.214278	-1.483009	-1.393254
H	-4.073724	-0.033120	-1.954603
H	-2.328760	1.429809	-0.741400
O	-0.616107	-1.687862	-0.828557
W	-0.363169	-0.333425	0.179225
N	1.670957	-0.423621	-0.078759
C	2.625176	0.385086	0.520165
C	2.356025	-1.372831	-0.823484
C	3.880593	-0.038553	0.154723
H	2.331332	1.188244	1.181068
C	3.707739	-1.159830	-0.708028
H	1.805846	-2.123044	-1.373146
H	4.817051	0.403315	0.469691
H	4.486439	-1.738135	-1.187867

E = -590.035990792
G = -589.868570

W-O-3-IV

W	0.335906	-0.348391	-0.125012
O	0.221243	1.570009	-0.166547
C	2.990854	0.591914	0.436246
C	0.472596	-1.282025	-1.784913
C	2.874947	0.384964	-0.895179
H	0.258581	-0.779086	-2.734342
H	0.818091	-2.310217	-1.899244
Si	-0.881729	2.848963	-0.215318
H	3.328191	-0.480475	-1.370340
H	2.449973	1.141873	-1.546882
H	-2.106645	2.469611	-0.975087
H	-1.230681	3.262184	1.176200
H	-0.192820	3.984460	-0.902430
C	3.726672	-0.300280	1.381507
H	3.087410	-0.600912	2.216423
H	4.091524	-1.203396	0.886225
H	4.585200	0.241290	1.797579
H	2.577826	1.512117	0.848622
N	-1.657392	-0.524524	0.146768
C	-2.303673	-0.040749	1.277335
C	-2.634808	-1.038442	-0.691783
C	-3.656119	-0.239476	1.147978
H	-1.742998	0.388515	2.097669
C	-3.867105	-0.876505	-0.111582
H	-2.352188	-1.489757	-1.631890
H	-4.411135	0.030733	1.874555
H	-4.815026	-1.185902	-0.531426
O	0.919190	-1.396297	1.088381

E = -590.039346153
G = -589.876158

W-O-3-TSIV

W	0.048918	-0.366023	-0.131060
O	0.437036	1.458248	-0.450253
C	3.430471	-0.005655	0.411775
C	0.157172	-1.440098	-1.695256
C	3.238806	-0.184925	-0.901731
H	0.424980	-2.495211	-1.741747
H	0.035748	-0.959330	-2.672495
Si	0.626024	3.099293	-0.108263
H	3.277204	0.990282	0.830563
H	3.397386	-1.154385	-1.367631
H	2.957080	0.634432	-1.555762
H	-0.488128	3.855431	-0.746988
H	0.611548	3.307783	1.370218
H	1.936723	3.541704	-0.667994
C	3.848377	-1.067292	1.376292
H	4.750855	-0.766280	1.921409
H	3.058791	-1.240778	2.116405
H	4.048759	-2.014787	0.868526
N	-1.930867	-0.324998	0.134433
C	-2.496955	0.200814	1.294426
C	-2.972287	-0.606070	-0.739514
C	-3.857428	0.260004	1.143802
H	-1.878933	0.461947	2.143670
C	-4.160331	-0.254560	-0.154943
H	-2.760218	-1.044346	-1.703566
H	-4.564062	0.614377	1.882504
H	-5.142626	-0.362961	-0.595205
O	0.605436	-1.309576	1.173011

E = -590.038069728
G = -589.878597

W-O-3-V

W	0.296965	-0.511946	0.104247
O	1.532305	0.838262	-0.317502
C	0.328082	-1.855171	-1.234085
H	0.468723	-1.530599	-2.271495
H	0.330890	-2.934198	-1.088629
Si	2.953634	1.756735	-0.270257
H	2.609468	3.141349	-0.699136
H	3.493366	1.759123	1.120055
H	3.938462	1.145754	-1.208230
N	-1.567072	0.194385	-0.032532
C	-2.066859	1.085873	0.920586
C	-2.527393	0.083990	-1.031725
C	-3.297939	1.528477	0.519454
H	-1.505840	1.310795	1.818764

C	-3.591288	0.889240	-0.725908
H	-2.358577	-0.576941	-1.869137
H	-3.930184	2.222409	1.057020
H	-4.490165	1.006528	-1.316418
O	0.470130	-1.339469	1.575537

E = -472.170003701
G = -472.084791

W-O-3-TSA

O	-0.456290	1.640727	-0.477068
C	-2.501115	-0.210931	-0.091054
H	-2.905312	0.433383	-0.872258
C	-0.664103	-1.785590	-1.033908
C	-2.185519	-1.649646	-0.608746
H	-0.552622	-1.444152	-2.072771
H	-2.792246	-1.858362	-1.497036
H	-2.398589	-2.395579	0.160689
Si	-1.163694	3.127276	-0.160471
H	-0.782562	3.613226	1.200668
H	-0.680173	4.092976	-1.191565
H	-2.655046	3.022856	-0.238724
W	-0.379269	-0.169847	0.223283
N	1.626151	0.199046	0.053252
C	2.326947	1.027046	-0.812319
C	2.574781	-0.586568	0.721891
C	3.665792	0.759139	-0.717514
H	1.791254	1.732763	-1.428998
C	3.824565	-0.274013	0.266222
H	2.261315	-1.281576	1.488135
H	4.454514	1.244055	-1.277961
H	4.755459	-0.709495	0.605268
C	-0.038800	-3.153907	-0.829876
H	1.025766	-3.133243	-1.080366
H	-0.134227	-3.484636	0.208678
H	-0.522111	-3.903878	-1.469574
H	-3.148708	-0.209668	0.785436
O	-0.388391	-0.775518	1.809954

E = -590.045680688
G = -589.877093

W-O-3-SBP

O	-1.386822	-1.359264	-0.165900
C	-1.870381	1.271690	0.675484
C	0.303561	1.886396	0.888287
C	-1.069501	2.553830	0.865892
H	0.473139	1.467131	1.893035
Si	-2.564038	-2.306443	0.595356
H	-3.906604	-1.927290	0.067656
H	-2.263525	-3.730782	0.278185
H	-2.518316	-2.089092	2.072573
H	-1.326893	3.160071	1.747057
H	-1.161037	3.195404	-0.018251
H	-2.060775	0.764072	1.630502
W	-0.310406	0.180233	-0.357606
N	1.519918	-0.508210	0.100363
C	2.151233	-0.781545	1.303670
C	2.317015	-1.046438	-0.915854
C	3.300262	-1.488812	1.060927
H	1.722070	-0.456987	2.240910
C	3.407237	-1.655204	-0.354995
H	2.042484	-0.925173	-1.955286
H	3.994115	-1.848998	1.808937
H	4.203716	-2.152460	-0.892033
C	1.514205	2.697666	0.452610
H	1.654489	3.561848	1.117206
H	2.433289	2.104912	0.476210
H	1.386652	3.082947	-0.564753
H	-2.805588	1.317278	0.105378
O	-0.358411	0.904516	-1.888862

E = -590.069942912
G = -589.901522

W-O-3-TSB

C	1.515233	-1.725006	-1.301843
C	2.156536	-0.951646	0.825380
C	1.602322	-2.044347	0.118660
H	2.909009	-0.383096	0.274303
H	1.384827	-3.017064	0.561850
H	0.058974	-1.791149	0.287491
O	0.737855	1.370011	0.695918
Si	0.684752	3.041812	0.454758
H	1.945507	3.476880	-0.218462
H	-0.491695	3.433666	-0.375588
H	0.592691	3.671270	1.804812
H	2.410231	-1.293755	-1.752236
W	0.288549	-0.142918	-0.384370
C	2.197260	-0.842929	2.321131
H	3.154486	-1.193709	2.726725
H	2.066395	0.199142	2.629736
H	1.400524	-1.432700	2.787442
H	0.978364	-2.406223	-1.960133
O	0.096906	0.562264	-1.943821
N	-1.658069	-0.414449	0.055194
C	-2.610026	0.525115	-0.345561
C	-2.305803	-1.308526	0.904171
C	-3.809400	0.231197	0.244723
H	-2.343799	1.304739	-1.044014
C	-3.615354	-0.937840	1.044476
H	-1.765776	-2.137674	1.338886
H	-4.734327	0.775480	0.106577
H	-4.360793	-1.448403	1.639457

E = -590.009287658
G = -589.844399

W-O-3-TSB$_{transX}$

O	-0.722564	-1.733676	-0.118594
C	-0.191081	0.860698	2.084604
C	-1.137809	2.081188	0.280439
C	-1.402309	1.301924	1.483970
H	-0.274197	2.748059	0.379602
Si	-2.003951	-2.798714	0.137480
H	-2.725872	-3.036407	-1.146860
H	-1.439331	-4.077971	0.654758
H	-2.948731	-2.210573	1.139335
H	-2.391783	1.197834	1.934243
H	-1.815618	0.074529	0.675550
H	0.631301	1.570009	2.099069
W	-0.247481	0.113163	-0.189273
N	1.756054	0.059425	0.064877
C	2.567027	-0.169118	1.173087
C	2.594070	-0.002220	-1.062646
C	3.856323	-0.370747	0.764847
H	2.146608	-0.194230	2.165894
C	3.874200	-0.257156	-0.662042
H	2.185011	0.164177	-2.047773
H	4.701119	-0.573820	1.409774

H	4.737325	-0.338695	-1.309309
C	-2.261983	2.609785	-0.569921
H	-2.700695	3.521742	-0.145108
H	-1.904831	2.838471	-1.577695
H	-3.065522	1.869602	-0.668693
H	-0.223555	0.150580	2.907730
O	-0.305603	0.528990	-1.856055

E = -590.007272729
G = -589.842167

W-O-3-B

C	1.744708	-1.381880	0.605836
C	3.336907	0.560699	0.784599
C	2.428971	-0.270802	1.318339
H	3.628269	0.417330	-0.257769
H	2.145874	-0.131592	2.362972
H	-0.145529	-0.770042	1.600541
O	0.500068	0.288463	-1.489207
Si	1.107560	1.724078	-2.156350
H	2.499666	1.458945	-2.620744
H	0.239294	2.085745	-3.312177
H	1.097737	2.810101	-1.135815
H	2.257691	-1.650682	-0.331659
W	-0.198304	-0.777050	-0.101500
C	4.022251	1.668164	1.521105
H	5.109102	1.518007	1.539332
H	3.850263	2.637608	1.036732
H	3.673214	1.739972	2.555493
H	1.654781	-2.277652	1.225629
O	-0.840491	-2.283360	-0.534267
N	-1.730391	0.345198	0.545542
C	-2.775295	0.613226	-0.342472
C	-1.971076	1.081470	1.696293
C	-3.633103	1.510600	0.235019
H	-2.827874	0.124806	-1.307116
C	-3.118574	1.810810	1.535575
H	-1.293057	1.010718	2.534111
H	-4.537748	1.901259	-0.211790
H	-3.555609	2.479189	2.265390

E = -590.050410074
G = -589.886684

W-O-3-TSC

C	1.889094	0.080839	-1.163895
C	4.071254	-0.318112	0.016580
C	3.032948	-0.745463	-0.716888
H	2.118782	1.154634	-1.061142
H	3.039690	-1.782283	-1.062019
H	1.683789	-0.098771	-2.223312
H	0.430849	-1.546001	-0.195213
O	-0.307459	1.684536	0.901065
Si	-0.800291	3.264932	0.525350
H	-0.785430	4.031422	1.806226
H	0.154862	3.875564	-0.444545
H	-2.181901	3.262699	-0.041057
C	0.936210	-1.703510	1.250737
H	1.827052	-2.191314	0.863517
H	0.123753	-2.361343	1.549574
C	1.045580	-0.441225	1.820816
H	0.298488	-0.094426	2.527217
H	1.997250	0.079982	1.806946
H	4.084806	0.724565	0.341603
C	5.247376	-1.152338	0.416630
H	6.183168	-0.731857	0.027253
H	5.356305	-1.194050	1.507957
H	5.159377	-2.178135	0.045474
W	-0.129906	0.166758	-0.258754
N	-1.750271	-1.001601	0.021614
C	-1.997432	-2.365401	-0.095668
C	-2.985748	-0.384430	0.226142
C	-3.337290	-2.601567	0.048088
H	-1.189622	-3.053022	-0.300421
C	-3.968635	-1.335824	0.260928
H	-3.057594	0.688737	0.335451
H	-3.820827	-3.568395	0.005393
H	-5.022391	-1.154488	0.425797
O	-0.558983	0.928057	-1.732803

E = -668.577024156
G = -668.361357

W-O-3-C

C	1.760179	-1.371008	-0.427992
C	3.463737	-0.122736	0.944399
C	2.469677	-1.016976	0.828515
H	3.821074	0.382468	0.045124
H	2.143646	-1.539473	1.729165
O	0.746350	1.111761	-1.088358
Si	1.675897	2.518239	-0.974915
H	1.887229	2.891190	0.453059
H	2.989141	2.277260	-1.641901
H	0.936196	3.599111	-1.687258
H	2.291968	-0.984887	-1.308520
W	-0.210166	-0.437956	-0.585958
C	4.166003	0.219095	2.221092
H	5.238381	-0.004845	2.156327
H	4.085256	1.289505	2.449151
H	3.755617	-0.339014	3.068240
H	1.642184	-2.452405	-0.541270
O	-0.917443	-1.231295	-1.903238
C	-0.529677	-1.913281	1.013718
H	0.122331	-2.780898	0.869904
H	-0.219735	-1.452359	1.962274
C	-1.980214	-2.400422	1.132497
H	-2.064135	-3.152289	1.927874
H	-2.670989	-1.587183	1.370382
H	-2.323107	-2.869176	0.204039
N	-1.581202	0.551370	0.506918
C	-2.774593	0.990221	-0.073968
C	-1.524009	1.085471	1.783553
C	-3.435648	1.793768	0.815366
H	-3.051378	0.673510	-1.070231
C	-2.636024	1.858035	2.000039
H	-0.683636	0.880149	2.432006
H	-4.389810	2.275582	0.649517
H	-2.859952	2.410809	2.902810

E = -668.646932056
G = -668.429402

W-O-4-I

O	-1.075882	0.047155	-0.631229
C	1.350980	-1.792448	-1.009800
H	1.134583	-1.519758	-2.056765
C	2.080719	-3.086869	-0.827196
H	3.076314	-3.032485	-1.287166
H	2.208947	-3.331656	0.229703
H	1.548731	-3.913522	-1.315563
N	1.883792	0.988010	0.065153

C	2.930595	1.255832	-0.807447
C	1.775186	2.084437	0.922689
C	3.458139	2.486208	-0.518604
H	3.205043	0.528015	-1.556980
C	2.720879	3.015378	0.586097
H	1.037439	2.098735	1.715135
H	4.285579	2.960014	-1.029892
H	2.879964	3.966433	1.076542
O	0.623928	-1.227533	1.689739
C	-2.401498	0.241569	-0.375433
C	-3.105931	1.128741	-1.192550
C	-3.045376	-0.434605	0.664063
C	-4.461790	1.340941	-0.958660
H	-2.580840	1.638844	-1.993818
C	-4.402993	-0.213334	0.883625
H	-2.483897	-1.125346	1.288203
C	-5.115764	0.672990	0.076808
H	-5.009436	2.032664	-1.592585
H	-4.903779	-0.739722	1.691284
H	-6.173827	0.841289	0.253125
W	0.560884	-0.514454	0.148555

E = -737.306657916
G = -737.132181

W-O-4-Ianti

W	-0.563482	-0.564388	-0.331012
O	1.023125	-0.028219	0.557661
C	-1.298575	-2.053474	0.601894
H	-1.729052	-2.887513	0.042122
C	-1.234187	-2.248486	2.095241
H	-0.656825	-3.148343	2.343935
H	-0.781172	-1.404428	2.625252
H	-2.243892	-2.391234	2.502153
N	-1.978332	0.826660	-0.053939
C	-3.078835	0.882414	0.790205
C	-1.885538	2.066916	-0.688338
C	-3.655910	2.121704	0.701535
H	-3.355158	0.017427	1.374862
C	-2.893771	2.878416	-0.241716
H	-1.112408	2.260321	-1.421560
H	-4.532453	2.455754	1.240718
H	-3.078286	3.896354	-0.558087
O	-0.559517	-1.034003	-1.964277
C	2.343223	0.261888	0.367777
C	3.015195	0.954450	1.377249
C	3.010498	-0.128710	-0.796027
C	4.363723	1.259253	1.213154
H	2.471667	1.244802	2.270660
C	4.360020	0.182042	-0.944452
H	2.473288	-0.670033	-1.570953
C	5.041092	0.875418	0.055746
H	4.886950	1.799395	1.997163
H	4.879623	-0.122122	-1.848649
H	6.093227	1.114477	-0.065837

E = -737.304744448
G = -737.129753

W-O-4-TSrot1

W	0.543278	-0.530201	0.167552
O	-1.170545	-0.576346	-0.621136
C	1.438233	-2.053621	-0.540953
H	0.690678	-2.868553	-0.537645
C	2.862968	-2.513705	-0.677838
H	3.003166	-3.043081	-1.629584
H	3.563392	-1.673616	-0.662579
H	3.149818	-3.207982	0.123739
N	1.747682	1.024095	-0.017105
C	2.133770	1.552589	-1.256516
C	2.272917	1.858156	0.972588
C	2.885356	2.672763	-1.042500
H	1.856561	1.058257	-2.178240
C	2.973229	2.867022	0.375185
H	2.083222	1.640837	2.013655
H	3.338317	3.287486	-1.808719
H	3.499747	3.662163	0.885599
O	0.317296	-0.688724	1.869275
C	-2.423325	-0.081523	-0.361967
C	-3.286344	0.095608	-1.444592
C	-2.832272	0.212895	0.939776
C	-4.573370	0.575158	-1.216156
H	-2.939171	-0.148122	-2.443657
C	-4.123546	0.693156	1.149657
H	-2.145237	0.061867	1.767773
C	-4.997010	0.876365	0.078351
H	-5.247473	0.713260	-2.056891
H	-4.445619	0.923788	2.161305
H	-6.001405	1.251256	0.250789

E = -737.267109610
G = -737.094271

W-O-4-TSrot2

W	-0.571298	0.469107	0.175827
O	1.043562	-0.042220	-0.619480
C	-1.101720	2.112048	-0.551200
H	-2.164033	1.777033	-0.341566
C	-0.907793	3.568638	-0.787626
H	-1.223670	4.178759	0.068879
H	0.149800	3.776161	-0.977016
H	-1.468114	3.910204	-1.667001
N	-2.072211	-0.840387	0.015149
C	-3.044483	-0.889185	-0.985467
C	-2.226799	-1.982420	0.799682
C	-3.778734	-2.034302	-0.835375
H	-3.115501	-0.100448	-1.721650
C	-3.260532	-2.728274	0.301815
H	-1.589211	-2.144928	1.657467
H	-4.605494	-2.342671	-1.461126
H	-3.621119	-3.663197	0.709254
O	-0.202820	0.635311	1.850122
C	2.356360	-0.339979	-0.379741
C	3.093464	-0.911978	-1.417720
C	2.939874	-0.074267	0.859990
C	4.434035	-1.222383	-1.205157
H	2.608328	-1.104803	-2.369197
C	4.281721	-0.393322	1.054780
H	2.342517	0.368711	1.651534
C	5.033002	-0.965240	0.028025
H	5.011735	-1.668025	-2.010064
H	4.740915	-0.189951	2.018144
H	6.079052	-1.208768	0.187939

E = -737.268558368
G = -737.096598

W-O-4-TSI

O	-0.916252	-0.252200	0.672522
C	-2.118616	2.611054	-1.050366

C	1.544046	1.600472	1.082448
C	-1.394920	3.240220	-0.122763
H	1.265314	1.352349	2.120180
H	-1.733738	3.323377	0.906907
H	-0.448558	3.714668	-0.366305
H	-3.073589	2.149732	-0.815060
C	2.417134	2.807856	0.934637
H	3.383539	2.642567	1.429367
H	2.612157	3.040884	-0.114704
H	1.964679	3.687316	1.411802
H	-1.776302	2.537885	-2.078950
N	1.945035	-1.147883	-0.044972
C	2.938580	-1.479440	0.865323
C	1.841597	-2.209015	-0.942749
C	3.438228	-2.718489	0.560976
H	3.198810	-0.787901	1.653233
C	2.738568	-3.184265	-0.594648
H	1.148784	-2.167595	-1.773319
H	4.223439	-3.237246	1.094746
H	2.890629	-4.122392	-1.111644
O	0.891911	1.072166	-1.674708
C	-2.194518	-0.654065	0.452194
C	-3.053474	-0.759092	1.549726
C	-2.648580	-0.971214	-0.832147
C	-4.366644	-1.178461	1.356064
H	-2.676875	-0.513167	2.537523
C	-3.964610	-1.390900	-1.011259
H	-1.972355	-0.889736	-1.679337
C	-4.828639	-1.495123	0.078369
H	-5.031768	-1.259856	2.211270
H	-4.313382	-1.638449	-2.009950
H	-5.853369	-1.823452	-0.066783
W	0.684907	0.407422	-0.121237

E = -815.866582148
G = -815.646258

W-O-4-TBP

O	0.995659	0.032518	0.282598
C	0.002260	-1.661531	-1.581112
H	1.050528	-1.505668	-1.829115
C	-0.802525	-2.042702	1.022179
C	-0.192489	-2.642129	-0.355698
H	-0.005288	-1.980548	1.766006
H	0.788677	-3.037071	-0.095611
H	-0.883515	-3.426566	-0.662007
N	-1.285274	1.588348	0.097322
C	-0.440736	2.600491	0.552588
C	-2.535490	2.171039	-0.114721
C	-1.140015	3.775148	0.626498
H	0.589228	2.385322	0.791127
C	-2.476420	3.501583	0.199910
H	-3.352801	1.565672	-0.478574
H	-0.743612	4.728394	0.951150
H	-3.294521	4.206789	0.133381
C	-2.023556	-2.771434	1.541252
H	-2.413725	-2.262180	2.427911
H	-2.817835	-2.797403	0.790860
H	-1.777744	-3.800399	1.833835
H	-0.602240	-1.943453	-2.439533
O	-2.417360	-0.725219	-0.800849
C	2.328300	0.163018	0.175840
C	2.899220	0.680876	-0.995805
C	3.152601	-0.216534	1.244605
C	4.282876	0.802262	-1.094235
H	2.248259	0.993110	-1.807083
C	4.533752	-0.088847	1.131112
H	2.695949	-0.598073	2.153000
C	5.106298	0.417355	-0.036383
H	4.718511	1.205858	-2.004256
H	5.166729	-0.383919	1.963677
H	6.184512	0.516514	-0.118178
W	-0.856014	-0.372632	-0.186595

E = -815.893505361
G = -815.661317

W-O-4-TSIII

O	0.898282	-0.045062	-0.701911
C	-0.385477	-2.826791	-0.712719
C	-1.822702	-1.046394	-1.740306
C	0.131745	-2.483251	0.528598
H	-1.360730	-0.935548	-2.724883
H	-2.822852	-1.477652	-1.755443
H	1.168043	-2.147764	0.552711
H	0.225886	-2.750710	-1.605530
C	-0.420189	-3.031197	1.819933
H	-0.325632	-2.318394	2.642569
H	-1.476007	-3.294792	1.727138
H	0.141357	-3.933560	2.093216
H	-1.272042	-3.449989	-0.787865
N	-1.140163	1.609020	0.068744
C	-2.121411	2.236129	0.826935
C	-0.452713	2.606770	-0.608899
C	-2.045698	3.593221	0.640701
H	-2.789286	1.644250	1.436062
C	-0.980704	3.830167	-0.279137
H	0.363687	2.356442	-1.270216
H	-2.674962	4.336321	1.113023
H	-0.639594	4.789118	-0.647165
O	-2.051648	-0.753546	1.083539
C	2.172796	0.164459	-0.305746
C	2.460232	0.627483	0.985091
C	3.214006	-0.084590	-1.208455
C	3.784739	0.830029	1.364674
H	1.643523	0.849193	1.666593
C	4.532782	0.123418	-0.814563
H	2.972263	-0.432668	-2.208204
C	4.825735	0.578045	0.471443
H	4.001210	1.193713	2.365396
H	5.336551	-0.070899	-1.519496
H	5.856250	0.739144	0.773262
W	-0.925655	-0.414533	-0.151226

E = -815.869471093
G = -815.641307

W-O-4-IV

O	0.881607	-0.073058	-0.765946
C	-0.270470	-2.906205	-0.675769
C	-1.972835	-0.928923	-1.688326
C	0.273083	-2.615167	0.544121
H	-1.587270	-0.763654	-2.698837
H	-2.986198	-1.326837	-1.648784
H	1.271412	-2.177659	0.565085
H	0.279644	-2.725321	-1.593133
C	-0.258785	-3.134851	1.847504
H	-0.238238	-2.375309	2.632569
H	-1.285351	-3.494201	1.750012
H	0.373742	-3.969450	2.176016
H	-1.175156	-3.501434	-0.758930

N	-1.160884	1.586603	0.068548
C	-2.047272	2.201022	0.943106
C	-0.589426	2.587181	-0.702915
C	-2.022234	3.557895	0.738450
H	-2.621594	1.602505	1.635459
C	-1.091841	3.804969	-0.314586
H	0.142914	2.345941	-1.459831
H	-2.598090	4.294098	1.283884
H	-0.817449	4.766485	-0.728689
O	-1.906027	-0.812477	1.172851
C	2.141878	0.195865	-0.347685
C	2.373969	0.838045	0.875547
C	3.218179	-0.172164	-1.163189
C	3.681873	1.100801	1.275433
H	1.529937	1.150285	1.484317
C	4.519984	0.097666	-0.749340
H	3.017756	-0.659073	-2.112814
C	4.759065	0.731587	0.469915
H	3.856605	1.604233	2.222303
H	5.352206	-0.189511	-1.386215
H	5.776126	0.940434	0.787759
W	-0.922439	-0.428240	-0.164849

E = -815.869824098
G = -815.643351

W-O-4-V

O	0.982626	0.067001	-0.629843
C	-1.273066	-1.890535	-1.353966
H	-1.118695	-1.602313	-2.399807
H	-1.709998	-2.877556	-1.209965
N	-2.039385	0.665798	0.099738
C	-2.027761	1.626569	1.114326
C	-3.074718	0.997424	-0.766082
C	-3.020499	2.538667	0.879442
H	-1.319633	1.564031	1.930853
C	-3.688080	2.137119	-0.319883
H	-3.278972	0.372302	-1.622750
H	-3.256949	3.393632	1.498633
H	-4.529463	2.631220	-0.787157
O	-0.629501	-1.636344	1.426875
C	2.286900	0.330755	-0.322018
C	2.956239	-0.392851	0.667565
C	2.937630	1.339486	-1.034863
C	4.288779	-0.095677	0.943067
H	2.435390	-1.178228	1.209460
C	4.269067	1.625906	-0.745723
H	2.392138	1.883226	-1.799452
C	4.949355	0.911987	0.240841
H	4.811162	-0.658456	1.711444
H	4.776552	2.411894	-1.297782
H	5.988247	1.138626	0.460386
W	-0.613002	-0.729153	-0.007899

E = -697.999394331
G = -697.850725

W-O-4-TSA

O	0.977156	0.660295	0.298478
C	0.743241	-2.075409	0.221024
H	1.498342	-1.913504	0.990722
C	-1.619346	-1.576378	1.131652
C	-0.568648	-2.705436	0.776283
H	-1.408711	-1.203941	2.143864
H	-0.344803	-3.252704	1.699335
H	-1.015088	-3.389359	0.050123
N	-1.446242	1.380073	-0.084963
C	-1.154191	2.502226	0.676275
C	-2.703093	1.598458	-0.671357
C	-2.194963	3.387143	0.599671
H	-0.214542	2.559467	1.203860
C	-3.186439	2.808558	-0.262477
H	-3.120865	0.872176	-1.354587
H	-2.250673	4.349011	1.092470
H	-4.128034	3.252366	-0.558105
C	-3.081876	-1.953643	0.974085
H	-3.726442	-1.090882	1.166558
H	-3.293972	-2.313473	-0.037378
H	-3.360658	-2.746875	1.680139
H	1.164560	-2.623140	-0.621164
O	-1.045068	-0.951506	-1.785368
C	2.318344	0.568820	0.165899
C	2.913979	0.257932	-1.063332
C	3.125745	0.827641	1.281560
C	4.301582	0.198279	-1.166428
H	2.284150	0.074408	-1.929861
C	4.511641	0.768228	1.163885
H	2.651381	1.077110	2.226164
C	5.107842	0.451985	-0.057063
H	4.753991	-0.043408	-2.124560
H	5.129298	0.970927	2.034893
H	6.189340	0.407147	-0.143795
W	-0.557070	-0.441440	-0.238471

E = -815.879507089
G = -815.647836

W-O-4-SBP

O	1.209000	0.072432	-0.816746
C	0.361567	-2.030761	0.792647
C	-1.696078	-1.232872	1.314534
C	-0.930403	-2.550822	1.410456
H	-1.391629	-0.591341	2.157423
H	-0.847876	-2.988950	2.416118
H	-1.389911	-3.301506	0.756903
H	1.009850	-1.536282	1.529122
N	-1.498490	1.251906	-0.000311
C	-1.558465	2.050590	1.131339
C	-2.062380	1.983185	-1.050077
C	-2.125347	3.256037	0.805738
H	-1.189368	1.693803	2.082499
C	-2.448723	3.211897	-0.585646
H	-2.153947	1.550293	-2.037450
H	-2.297578	4.080981	1.484353
H	-2.922586	3.991100	-1.167286
C	-3.213151	-1.267121	1.212039
H	-3.649361	-1.717014	2.115051
H	-3.636235	-0.264138	1.100609
H	-3.537388	-1.867015	0.355001
H	0.972965	-2.717818	0.196905
O	-1.281084	-1.366254	-1.653520
C	2.453765	0.272276	-0.307503
C	3.547478	-0.312133	-0.952203
C	2.640733	1.078168	0.820079
C	4.829270	-0.095438	-0.454632
H	3.375810	-0.924831	-1.831583
C	3.929426	1.290011	1.303715
H	1.781138	1.549237	1.288829
C	5.025980	0.703127	0.672636
H	5.679595	-0.551662	-0.953665
H	4.075383	1.920461	2.176346

H	6.028678	0.870607	1.054227
W	-0.558966	-0.483048	-0.400511

E = -815.901721880
G = -815.671000

W-O-4-TSB

C	-2.741121	-1.086951	-1.016406
C	-1.875885	-1.827976	1.039707
C	-2.888431	-1.048180	0.436783
H	-1.564375	-2.703300	0.465956
H	-3.723080	-0.598529	0.976379
H	-2.273635	0.391925	0.473666
O	0.634560	-1.047371	0.593914
H	-2.598306	-2.074658	-1.456728
W	-0.821456	-0.234938	-0.382795
C	-1.586209	-1.854620	2.510475
H	-2.100856	-2.686608	3.007340
H	-0.512157	-1.978030	2.680646
H	-1.902007	-0.926074	2.998533
H	-3.356157	-0.422758	-1.621991
O	-0.284413	-0.270196	-2.017309
C	1.973509	-0.832917	0.361064
C	2.722002	-0.183621	1.346077
C	2.591026	-1.314775	-0.795048
C	4.092941	-0.016118	1.166892
H	2.220286	0.180814	2.236976
C	3.963335	-1.139996	-0.960422
H	1.992401	-1.806095	-1.555403
C	4.719949	-0.492196	0.015656
H	4.671959	0.491507	1.933590
H	4.441779	-1.514702	-1.861243
H	5.789084	-0.358508	-0.120156
N	-0.576790	1.729837	-0.028117
C	0.487652	2.426483	-0.608225
C	-1.200116	2.608464	0.855917
C	0.530466	3.692457	-0.092178
H	1.107881	1.950828	-1.353559
C	-0.545339	3.809034	0.843361
H	-2.064394	2.291467	1.422035
H	1.240151	4.462937	-0.362979
H	-0.807144	4.682373	1.425797

E = -815.838921314
G = -815.611255

W-O-4-TSB$_{transX}$

O	-0.988228	-0.756218	-0.515912
C	0.567097	0.436119	2.203633
C	0.931696	2.309674	0.784325
C	0.015468	1.652307	1.715187
H	1.980599	2.238864	1.092467
H	-0.894331	2.122140	2.096265
H	-0.875531	1.186251	0.600261
H	1.628587	0.442987	2.432516
W	0.509666	0.387921	-0.201181
N	2.047271	-0.902688	0.034642
C	2.394229	-1.800014	1.040426
C	2.885368	-1.185291	-1.059559
C	3.400234	-2.615374	0.601359
H	1.869843	-1.795612	1.982923
C	3.718124	-2.217810	-0.736913
H	2.809303	-0.598688	-1.962803
H	3.865886	-3.410156	1.169145
H	4.482595	-2.640076	-1.375526
C	0.552104	3.597822	0.102063
H	0.700374	4.462791	0.761070
H	1.152031	3.746747	-0.799606
H	-0.500793	3.588684	-0.203828
H	-0.048063	-0.238100	2.794568
O	0.912063	1.084340	-1.722792
C	-2.331767	-0.787000	-0.305286
C	-3.156852	0.225084	-0.804235
C	-2.878606	-1.871635	0.386290
C	-4.532391	0.153737	-0.592074
H	-2.715729	1.044432	-1.364830
C	-4.254999	-1.929693	0.588361
H	-2.218140	-2.653193	0.748671
C	-5.086757	-0.919028	0.105006
H	-5.172971	0.939926	-0.982194
H	-4.678818	-2.772149	1.128058
H	-6.159397	-0.970518	0.265842

E = -815.841057352
G = -815.613638

W-O-4-B

C	-0.216181	-2.062656	-1.292222
C	0.638307	-3.364412	0.684786
C	-0.343974	-3.017081	-0.160155
H	1.628762	-2.928572	0.543784
H	-1.336294	-3.445790	-0.011541
H	-2.060869	-1.079352	-0.527052
O	0.872871	0.101098	0.324850
H	0.830308	-1.944644	-1.618586
W	-0.716243	-0.049836	-0.697259
C	0.490255	-4.327685	1.819418
H	1.167895	-5.183299	1.704980
H	0.744375	-3.856028	2.777196
H	-0.531532	-4.712097	1.891644
H	-0.820417	-2.356734	-2.154038
O	-0.826655	0.666882	-2.228439
C	2.148077	0.577469	0.333025
C	2.885614	0.457495	1.513670
C	2.711736	1.165936	-0.803436
C	4.193716	0.932423	1.552063
H	2.419780	0.000747	2.380804
C	4.022220	1.633478	-0.749874
H	2.124447	1.254589	-1.714194
C	4.767125	1.519469	0.424068
H	4.766933	0.842503	2.470451
H	4.461038	2.090211	-1.632423
H	5.788153	1.887151	0.459331
N	-2.051364	0.893616	0.466209
C	-1.911891	2.273811	0.633326
C	-3.073812	0.479670	1.305044
C	-2.813490	2.703580	1.569805
H	-1.191328	2.837860	0.054731
C	-3.554204	1.558046	1.999505
H	-3.364545	-0.560308	1.330018
H	-2.943757	3.724525	1.903344
H	-4.352128	1.540668	2.729854

E = -815.879833642
G = -815.655246

W-O-4-TSC

C	-1.782992	-1.252808	-1.195382
C	-3.252190	-2.841554	0.082606
C	-3.066651	-1.717870	-0.626356

H	-1.046168	-2.074121	-1.221951
H	-3.941871	-1.103560	-0.851813
H	-1.924088	-0.916272	-2.226154
H	-2.074143	0.853246	-0.073285
O	1.024857	-0.628844	0.628497
C	-2.373901	0.464472	1.359054
H	-3.334182	0.064295	1.043025
H	-2.380884	1.490878	1.717871
C	-1.388375	-0.413859	1.801493
H	-0.601899	-0.056334	2.458319
H	-1.561150	-1.484298	1.766485
H	-2.387407	-3.476349	0.287644
C	-4.568674	-3.323763	0.605419
H	-4.821296	-4.309810	0.195541
H	-4.549320	-3.437003	1.696927
H	-5.380357	-2.635286	0.350566
W	-0.390535	0.247785	-0.341268
N	-0.249024	2.202013	0.147823
C	-1.143260	3.265790	0.146482
C	1.023488	2.742474	0.336819
C	-0.461451	4.436147	0.344517
H	-2.196333	3.096860	-0.027701
C	0.922645	4.101270	0.472866
H	1.897408	2.106190	0.373042
H	-0.896443	5.425589	0.391809
H	1.742494	4.783154	0.655671
O	0.257817	0.275388	-1.926610
C	2.303266	-1.044220	0.372842
C	2.891994	-1.003552	-0.894524
C	3.022043	-1.534760	1.469671
C	4.200789	-1.456206	-1.051360
H	2.327002	-0.623521	-1.739504
C	4.329381	-1.978646	1.297331
H	2.539300	-1.557774	2.441690
C	4.925038	-1.942403	0.036465
H	4.656090	-1.424942	-2.037485
H	4.882703	-2.356070	2.152895
H	5.945033	-2.290466	-0.097249

E = -894.406916612
G = -894.129613

W-O-4-C

C	-0.060035	2.307602	-0.097640
C	-1.839333	1.961841	1.653960
C	-0.573929	2.237664	1.296680
H	-2.580599	1.789092	0.873594
H	0.152152	2.428229	2.087776
O	-0.844956	-0.168012	-1.090814
H	-0.878531	2.415284	-0.820833
W	0.898554	0.421091	-0.609677
C	-2.334463	1.896948	3.063902
H	-3.117894	2.644644	3.241851
H	-2.784284	0.919917	3.280034
H	-1.530369	2.071479	3.785471
H	0.643929	3.131547	-0.239267
O	1.780581	0.682259	-2.030710
C	2.354904	1.266814	0.796767
H	2.409321	2.353530	0.666548
H	2.008487	1.097355	1.824566
C	3.762680	0.676054	0.633545
H	4.459201	1.152454	1.335690
H	3.781978	-0.400016	0.828310
H	4.151690	0.839783	-0.376645
N	1.385061	-1.271191	0.375231
C	1.832485	-2.408430	-0.296465
C	1.193311	-1.625058	1.701770
C	1.905859	-3.452706	0.587070
H	2.066298	-2.369157	-1.351789
C	1.494606	-2.953896	1.862566
H	0.855014	-0.894878	2.423778
H	2.226482	-4.459714	0.356446
H	1.436083	-3.511826	2.787827
C	-2.123663	-0.490282	-0.786326
C	-2.409865	-1.291579	0.325267
C	-3.149682	-0.042134	-1.624873
C	-3.731594	-1.637144	0.591725
H	-1.595722	-1.646801	0.950016
C	-4.467767	-0.386652	-1.336454
H	-2.898600	0.564689	-2.489268
C	-4.764208	-1.183303	-0.230275
H	-3.955018	-2.267037	1.448368
H	-5.265598	-0.035478	-1.984873
H	-5.793250	-1.453903	-0.013249

E = -894.479858068
G = -894.198982

W-N-5-I

W	0.723972	0.000000	-0.096364
O	1.494961	-1.565615	-0.875989
N	-1.021249	-0.000002	-0.031532
C	1.173210	-0.000004	1.743939
H	2.279566	-0.000002	1.806742
Si	2.166951	-3.038651	-0.410578
H	2.983464	-3.554948	-1.548991
H	3.034703	-2.844279	0.791733
H	1.082328	-4.014968	-0.090361
C	0.472108	-0.000010	3.069055
H	0.743838	0.881697	3.664790
H	-0.613273	-0.000012	2.939965
H	0.743842	-0.881718	3.664785
C	-2.397147	-0.000001	-0.094383
C	-3.106735	-1.213491	-0.123634
C	-4.495973	-1.206866	-0.183019
C	-5.195943	0.000000	-0.213015
C	-4.495972	1.206865	-0.183024
C	-3.106734	1.213489	-0.123639
H	-2.551300	-2.146040	-0.099724
H	-5.035602	-2.149652	-0.206114
H	-6.281099	0.000000	-0.259594
H	-5.035599	2.149651	-0.206123
H	-2.551297	2.146038	-0.099733
O	1.494959	1.565619	-0.875982
Si	2.166944	3.038658	-0.410570
H	3.034690	2.844289	0.791747
H	2.983463	3.554954	-1.548979
H	1.082318	4.014973	-0.090361

E = -594.004243836
G = -593.850550

W-N-5-Ianti

O	1.415202	-1.560824	-0.846335
N	-1.076875	0.000047	0.085876
C	1.161942	0.000002	1.793610
H	0.458225	0.000025	2.627326
Si	1.863048	-3.162913	-0.590250
H	2.806726	-3.557541	-1.677670
H	2.529320	-3.310215	0.738935
H	0.652408	-4.037528	-0.637752
C	2.624786	-0.000012	2.186480

H	2.869321	-0.884442	2.789118
H	3.308455	0.000030	1.327668
H	2.869315	0.884369	2.789190
C	-2.453102	0.000074	0.070384
C	-3.163451	-1.213521	0.066231
C	-4.553808	-1.206766	0.055272
C	-5.254378	0.000125	0.049114
C	-4.553763	1.206991	0.055184
C	-3.163405	1.213695	0.066142
H	-2.607519	-2.146006	0.071598
H	-5.093935	-2.149534	0.051362
H	-6.340489	0.000145	0.039935
H	-5.093855	2.149778	0.051205
H	-2.607438	2.146159	0.071439
O	1.415281	1.560739	-0.846412
Si	1.863458	3.162723	-0.590246
H	2.530061	3.309758	0.738801
H	2.806953	3.557312	-1.677839
H	0.652957	4.037551	-0.637372
W	0.663699	-0.000005	-0.043955

E = -594.001106702
G = -593.848859

W-N-5-TSrot

W	-0.889040	0.029051	0.237115
O	-1.418220	1.844733	0.374320
N	0.750700	0.097981	-0.474051
C	-0.826588	-0.616640	2.028263
Si	-0.904125	3.341335	-0.220882
H	-1.986765	4.327210	0.063833
H	0.354682	3.750051	0.468399
H	-0.672830	3.252670	-1.694313
C	2.119441	-0.049549	-0.307487
C	2.663755	-0.795713	0.753737
C	4.041598	-0.931907	0.882301
C	4.901439	-0.328176	-0.037065
C	4.369287	0.413043	-1.092613
C	2.992029	0.549923	-1.233244
H	1.983666	-1.257286	1.464498
H	4.448706	-1.513099	1.705798
H	5.977188	-0.436847	0.067481
H	5.031334	0.885061	-1.813807
H	2.566463	1.118543	-2.054911
O	-1.868958	-1.193942	-0.786117
Si	-1.763261	-2.066108	-2.244173
H	-2.831172	-3.104760	-2.203914
H	-1.999086	-1.127986	-3.379717
H	-0.417223	-2.694907	-2.353499
C	-1.030118	-1.959291	2.678710
H	-1.453997	-2.690448	1.983902
H	-0.091918	-2.375167	3.071255
H	-1.721351	-1.873068	3.527415
H	-0.397873	0.154782	2.688956

E = -593.979631822
G = -593.825837

W-N-5-TSI

W	0.672364	0.113090	-0.019099
O	1.871829	-1.207505	-0.728207
O	1.251715	1.614480	-1.049993
N	-1.083693	0.204616	-0.012639
C	-0.496224	-2.955832	0.569299
C	1.128685	0.566776	1.769786
C	0.049919	-2.559106	1.723093
H	2.232656	0.557876	1.842358
H	1.094643	-2.745444	1.955624
H	-0.537065	-2.060398	2.488607
H	0.088353	-3.467554	-0.189780
C	0.431264	0.923666	3.046257
H	0.702164	1.934602	3.379177
H	-0.654514	0.887372	2.928626
H	0.712593	0.240251	3.859597
H	-1.546160	-2.784455	0.349446
C	-2.436021	0.059559	-0.211870
C	-2.936472	-0.733236	-1.262242
C	-4.308712	-0.866481	-1.447293
C	-5.204826	-0.223448	-0.593138
C	-4.714709	0.564717	0.448981
C	-3.345487	0.712574	0.640698
H	-2.234968	-1.227893	-1.927924
H	-4.679865	-1.477842	-2.265534
H	-6.275274	-0.332170	-0.740558
H	-5.404841	1.073945	1.116356
H	-2.956850	1.333436	1.441808
Si	3.345224	-1.986870	-0.892298
H	3.935203	-1.663918	-2.225307
H	4.284808	-1.552421	0.188875
H	3.132147	-3.463127	-0.788931
Si	1.464633	3.242636	-0.681513
H	2.394741	3.387611	0.481670
H	2.056032	3.903834	-1.883841
H	0.156246	3.883656	-0.350903

E = -672.557403529
G = -672.356016

W-N-5-TBP

W	0.706530	-0.145562	-0.068957
C	0.646903	-1.490505	-1.652953
N	-1.064307	-0.012552	-0.033123
O	2.662087	-0.349121	-0.222352
H	1.551822	-1.553842	-2.253741
C	0.673671	-2.490805	-0.427369
C	0.751286	-1.877158	1.062935
H	1.755758	-2.044791	1.457379
H	-0.245014	-3.076079	-0.456962
H	1.560976	-3.112745	-0.538957
Si	4.066503	0.552798	-0.231017
H	5.227286	-0.367582	-0.457061
H	4.055919	1.568134	-1.331021
H	4.274532	1.252222	1.075830
C	-0.321477	-2.380350	2.004253
H	-1.323721	-2.215183	1.600196
H	-0.202226	-3.452921	2.207288
H	-0.253474	-1.859453	2.964902
H	-0.261005	-1.586212	-2.243568
C	-2.432468	0.056023	-0.115244
C	-3.222858	0.081801	1.049973
C	-4.608668	0.137919	0.952963
C	-5.230601	0.171308	-0.295889
C	-4.453056	0.152572	-1.454731
C	-3.066416	0.097282	-1.372606
H	-2.730893	0.062818	2.017465
H	-5.207631	0.158330	1.859358
H	-6.313477	0.216156	-0.365676
H	-4.930286	0.185249	-2.430412
H	-2.453482	0.093435	-2.268871
O	1.099797	1.716545	0.235855
Si	0.120994	3.054621	0.520768

H	-0.662905	2.880434	1.782823
H	1.010843	4.246237	0.659842
H	-0.823985	3.273445	-0.616630

E = -672.597261446
G = -672.385207

W-N-5-TSIV

W	-0.787026	-0.175978	-0.262074
O	-2.033326	1.063280	0.502707
N	0.957807	-0.321653	-0.148848
C	0.380773	3.026862	-0.555218
C	-1.121637	-0.508163	-2.106448
C	-0.312258	2.655897	-1.641619
H	-0.427163	-0.738038	-2.911280
H	-2.173160	-0.449171	-2.416989
Si	-3.020694	1.748922	1.672149
H	-0.169005	3.271465	0.353979
H	0.186753	2.420042	-2.578174
H	-1.396385	2.624396	-1.642066
H	-2.217829	2.684522	2.519240
H	-4.111637	2.513624	0.996831
H	-3.609581	0.680004	2.532590
C	1.866808	3.181360	-0.491873
H	2.132023	4.222560	-0.268714
H	2.300452	2.565910	0.303559
H	2.342225	2.901682	-1.435873
C	2.293650	-0.380847	0.172060
C	2.737633	-0.135474	1.484701
C	4.092251	-0.214555	1.790842
C	5.024843	-0.531935	0.802791
C	4.589066	-0.776627	-0.500062
C	3.237341	-0.705918	-0.818992
H	2.007125	0.107453	2.250992
H	4.421105	-0.026871	2.809482
H	6.081471	-0.590912	1.046700
H	5.307627	-1.028511	-1.275442
H	2.888838	-0.901829	-1.828174
O	-1.436565	-1.737318	0.619233
Si	-1.675134	-3.314496	0.071305
H	-2.307934	-4.080337	1.187954
H	-2.579369	-3.311360	-1.119042
H	-0.370371	-3.943965	-0.291091

E = -672.559217718
G = -672.357722

W-N-5-V

W	0.750629	0.000002	0.062880
O	1.526461	1.559326	-0.706745
N	-0.992990	0.000024	0.097336
C	1.163907	0.000011	1.914233
H	0.513847	0.000024	2.786920
H	2.238971	0.000003	2.146144
Si	2.149770	3.060679	-0.252866
H	2.957192	3.583025	-1.394516
H	1.029822	4.003054	0.043763
H	3.012153	2.904701	0.957347
C	-2.367080	0.000008	0.016039
C	-3.075510	1.213945	-0.021551
C	-4.463818	1.207054	-0.097536
C	-5.163047	-0.000020	-0.136208
C	-4.463790	-1.207080	-0.097598
C	-3.075482	-1.213944	-0.021612
H	-2.520398	2.146374	0.010398
H	-5.003326	2.149695	-0.126364
H	-6.247563	-0.000031	-0.195644
H	-5.003276	-2.149733	-0.126475
H	-2.520349	-2.146362	0.010289
O	1.526435	-1.559345	-0.706724
Si	2.149790	-3.060677	-0.252839
H	1.029870	-4.003076	0.043821
H	2.957205	-3.583016	-1.394497
H	3.012190	-2.904663	0.957357

E = -554.698913983
G = -554.571659

W-N-5-TSA

W	-0.568159	-0.256021	0.060602
C	-0.638351	-0.250208	2.211150
N	1.180590	-0.244129	-0.018235
O	-1.925633	1.175724	0.179483
H	-1.574309	0.059373	2.682953
C	-0.570752	-1.799935	2.043174
C	-1.002649	-2.214840	0.587107
H	-2.100017	-2.308863	0.552027
H	0.445999	-2.160720	2.216102
H	-1.252218	-2.282671	2.754094
Si	-2.420921	2.351326	1.260476
H	-3.101974	3.438401	0.493055
H	-3.392393	1.793994	2.255706
H	-1.261586	2.937965	2.004521
C	-0.333337	-3.453502	0.022279
H	0.755861	-3.359940	0.056844
H	-0.616458	-4.347835	0.593765
H	-0.623688	-3.617322	-1.019852
H	0.207083	0.145685	2.774269
C	2.491852	0.168784	-0.098102
C	3.418247	-0.594549	-0.830535
C	4.746402	-0.189897	-0.906207
C	5.170211	0.969866	-0.256133
C	4.253827	1.729575	0.472651
C	2.922417	1.338033	0.555050
H	3.074877	-1.492941	-1.333776
H	5.455120	-0.783879	-1.476580
H	6.209132	1.280502	-0.317218
H	4.578103	2.634065	0.979845
H	2.200966	1.921224	1.119473
O	-1.076651	-0.144964	-1.788297
Si	-2.295388	0.633943	-2.669739
H	-3.655187	0.331280	-2.131758
H	-2.062163	2.106640	-2.699156
H	-2.208082	0.099653	-4.063634

E = -672.581021708
G = -672.369028

W-N-5-SBP

O	-1.329973	1.682874	-0.828552
C	-0.996466	1.118652	1.859450
C	-1.006944	-1.163428	1.718669
C	-0.665764	-0.080801	2.739960
H	-2.101207	-1.307658	1.711654
Si	-1.999046	3.223006	-0.705194
H	-1.005693	4.165217	-0.108018
H	-2.353301	3.670435	-2.083917
H	-3.231427	3.197527	0.140553
H	-1.206365	-0.142801	3.697224
H	0.407858	-0.103849	2.961618

H	-2.067686	1.364522	1.901629
W	-0.625710	0.100978	-0.031010
C	-0.310352	-2.510020	1.844569
H	-0.587824	-3.007956	2.784942
H	-0.566992	-3.196027	1.029254
H	0.778345	-2.389531	1.843586
H	-0.425997	2.040510	2.020109
O	-1.476083	-1.247495	-1.063638
Si	-2.433055	-2.591335	-1.393650
H	-3.357083	-2.865754	-0.251908
H	-3.227209	-2.299241	-2.622837
H	-1.558993	-3.779073	-1.627912
N	1.116382	0.050776	0.013142
C	2.483409	0.029183	-0.159546
C	3.119039	-1.113620	-0.675477
C	3.255728	1.150537	0.189457
C	4.499737	-1.126442	-0.840381
H	2.515027	-1.975748	-0.941337
C	4.636170	1.123217	0.023353
H	2.755612	2.027925	0.587608
C	5.263552	-0.011705	-0.491918
H	4.982640	-2.012949	-1.242204
H	5.225506	1.994265	0.296334
H	6.341839	-0.027506	-0.621155

E = -672.600870764
G = -672.391206

W-N-5-TSB

C	-0.415414	0.562783	2.147347
C	-2.430627	-0.464384	1.438398
C	-1.193912	-0.678375	2.126311
H	-2.863621	0.524209	1.600673
H	-0.966898	-1.561605	2.729602
H	-0.329497	-1.317141	1.083366
O	-1.449594	1.762425	-0.501149
Si	-1.264560	3.400338	-0.828568
H	-1.493511	4.184336	0.422950
H	0.113382	3.670870	-1.340961
H	-2.273768	3.791817	-1.855958
H	-0.985356	1.450877	2.423546
W	-0.665708	0.098285	0.013186
C	-3.396467	-1.583062	1.155497
H	-4.034643	-1.802653	2.022794
H	-4.055304	-1.334981	0.317692
H	-2.869299	-2.505499	0.890543
H	0.589268	0.531492	2.563415
O	-1.305117	-1.302727	-1.138841
Si	-0.819447	-2.739218	-1.856894
H	-1.856572	-3.126719	-2.858510
H	0.501160	-2.565762	-2.535164
H	-0.701577	-3.814000	-0.821711
N	1.081051	0.195989	-0.305269
C	2.431529	0.040155	-0.077683
C	3.329350	1.039914	-0.493819
C	2.934798	-1.112162	0.553614
C	4.694007	0.888224	-0.274629
H	2.934782	1.923818	-0.985516
C	4.301706	-1.252742	0.766714
H	2.237167	-1.886139	0.861400
C	5.187022	-0.255485	0.355288
H	5.378131	1.667669	-0.599005
H	4.678866	-2.147688	1.254397
H	6.254161	-0.370348	0.521727

E = -672.547624536
G = -672.343005

W-N-5-B

C	-1.138510	0.784441	1.792930
C	-3.559464	0.587729	1.081268
C	-2.494558	0.170287	1.792324
H	-3.466915	1.490055	0.476928
H	-2.603700	-0.743354	2.378384
H	-0.537853	-1.330209	1.186373
O	-1.077575	1.407941	-0.928372
Si	-1.253002	3.005445	-1.404072
H	-1.332258	3.884250	-0.196135
H	-0.085258	3.419568	-2.239361
H	-2.510312	3.139625	-2.197899
H	-1.162102	1.872024	1.658669
W	-0.342049	-0.108777	-0.016979
C	-4.897074	-0.081898	1.073752
H	-5.678067	0.590927	1.450830
H	-5.196460	-0.365171	0.056724
H	-4.899886	-0.984087	1.692797
H	-0.570872	0.534458	2.689776
O	-0.822135	-1.565563	-1.142377
Si	-1.378368	-3.153775	-0.993856
H	-2.524498	-3.221419	-0.039307
H	-1.824356	-3.595896	-2.348695
H	-0.271214	-4.035218	-0.517554
N	1.379721	-0.000723	0.187790
C	2.757143	0.022654	0.232009
C	3.441814	1.248718	0.273532
C	3.484965	-1.179146	0.241527
C	4.831700	1.266059	0.317467
H	2.870082	2.171547	0.270503
C	4.874153	-1.147480	0.290588
H	2.944396	-2.119947	0.214297
C	5.552593	0.071517	0.326687
H	5.354598	2.217934	0.347285
H	5.430623	-2.080560	0.299687
H	6.637934	0.090352	0.363119

E = -672.579190393
G = -672.377156

W-N-5-TSC

W	-0.397672	0.468546	0.060228
C	-0.982612	-1.589714	-0.606606
C	-3.367506	-2.417995	-0.627841
C	-2.262546	-1.976201	-1.247655
H	-0.905418	-2.062384	0.385745
H	-2.288781	-1.921259	-2.339552
H	-0.144788	-1.965196	-1.201836
H	-0.587508	0.536290	-1.721767
O	-1.130328	0.277697	1.825385
Si	-0.931576	-0.239719	3.404923
H	-1.749064	-1.471056	3.628516
H	0.506009	-0.549233	3.685594
H	-1.395599	0.840472	4.325474
C	-2.097406	1.106971	-1.760636
H	-2.337653	0.327827	-2.478381
H	-1.757518	2.049269	-2.180721
C	-2.661468	1.068963	-0.491154
H	-2.725142	1.981062	0.095668
H	-3.287700	0.230857	-0.205213
H	-3.355626	-2.505495	0.460686
C	-4.632517	-2.831054	-1.314682
H	-4.875983	-3.881456	-1.108151

H	-5.491772	-2.240700	-0.970589
H	-4.556539	-2.712498	-2.400393
N	1.259801	-0.123391	0.096419
C	2.480358	-0.724275	-0.096971
C	2.982273	-0.909482	-1.398142
C	3.236707	-1.163580	1.004792
C	4.214669	-1.524704	-1.586669
H	2.391120	-0.561461	-2.239963
C	4.468825	-1.774244	0.801441
H	2.841543	-1.015263	2.004932
C	4.962665	-1.958113	-0.491096
H	4.594849	-1.664770	-2.594833
H	5.047583	-2.109605	1.657622
H	5.926003	-2.435998	-0.643469
O	-0.109201	2.359826	-0.214385
Si	1.095613	3.342734	-0.846116
H	0.787634	4.751387	-0.456539
H	2.436450	2.952045	-0.314682
H	1.108082	3.236647	-2.339902

E = -751.116823089
G = -750.862147

W-N-5-C

C	-1.148297	-1.137298	-1.660398
C	-3.558558	-1.146243	-0.878003
C	-2.575078	-0.705024	-1.682983
H	-3.330037	-1.918936	-0.144393
H	-2.826589	0.078728	-2.398943
O	-0.952062	-1.433836	1.017439
Si	-0.715528	-2.994350	1.582529
H	-0.770774	-3.961335	0.441672
H	0.612456	-3.108146	2.258825
H	-1.802636	-3.318176	2.553998
H	-1.041452	-2.192942	-1.390759
W	-0.315984	0.055009	-0.026822
C	-4.976022	-0.668193	-0.924354
H	-5.663030	-1.488657	-1.169194
H	-5.299463	-0.274237	0.047575
H	-5.111748	0.119162	-1.672400
H	-0.654133	-0.962275	-2.616820
C	-0.550434	1.581544	-1.602014
H	-0.352110	1.169550	-2.596454
H	-1.599484	1.909550	-1.606196
C	0.359874	2.798551	-1.381609
H	0.173636	3.570067	-2.140969
H	0.206667	3.266858	-0.403220
H	1.417959	2.524341	-1.445921
Si	-1.996669	2.594557	1.679137
H	-1.226284	3.736636	2.253953
H	-2.835230	3.073526	0.539626
H	-2.869559	1.995075	2.731391
O	-0.911575	1.420024	1.151425
N	1.407656	-0.101544	-0.192888
C	2.784959	-0.122317	-0.143064
C	3.500680	-0.969154	-1.006088
C	3.483473	0.697297	0.760220
C	4.890543	-0.991112	-0.961877
H	2.950169	-1.596895	-1.699806
C	4.873134	0.662292	0.796136
H	2.922648	1.349259	1.423035
C	5.582078	-0.178900	-0.062494
H	5.436663	-1.648175	-1.633058
H	5.405831	1.297253	1.498673
H	6.667454	-0.201181	-0.030603

E = -751.177401409
G = -750.920396

W-O-5-I

W	0.000008	0.096612	-0.366183
O	-1.547873	-0.985275	-0.166422
C	0.000523	1.362079	1.045205
H	0.000207	0.824029	2.009745
Si	-3.001703	-1.050075	0.693463
H	-3.477128	-2.463718	0.677991
H	-2.766615	-0.600665	2.099768
H	-4.007308	-0.163009	0.039511
C	0.001114	2.857804	1.148606
H	0.883184	3.215606	1.695467
H	0.001411	3.321917	0.159147
H	-0.880794	3.216308	1.695273
O	0.000368	1.074645	-1.751551
O	1.547242	-0.986272	-0.166594
Si	3.000982	-1.050924	0.693455
H	2.765739	-0.601081	2.099588
H	3.476281	-2.464611	0.678417
H	4.006785	-0.164142	0.039423

E = -382.926020299
G = -382.855849

W-O-5-Ianti

W	-0.000867	-0.429835	0.191053
O	1.542150	-0.120920	-0.866060
C	-0.003318	0.837558	1.612541
H	-0.010205	0.510871	2.653877
Si	3.072452	0.586845	-0.966172
H	3.390802	0.770434	-2.411630
H	3.066068	1.909324	-0.272219
H	4.075597	-0.315014	-0.329389
C	0.003982	2.333418	1.403347
H	0.886477	2.786951	1.872069
H	0.011613	2.626391	0.346804
H	-0.880471	2.794089	1.861302
O	-0.010757	-1.913087	1.011140
O	-1.533098	-0.108868	-0.878727
Si	-3.068285	0.589953	-0.967820
H	-3.055896	1.927058	-0.302502
H	-3.411305	0.741234	-2.411341
H	-4.057166	-0.301607	-0.295116

E = -382.923011740
G = -382.854083

W-O-5-TSrot

W	0.029532	0.204626	0.058949
O	1.768470	-0.099308	-0.575856
C	-0.328024	2.043353	-0.286900
H	0.608557	2.609739	-0.151903
Si	3.231790	-0.869626	-0.195519
H	4.146706	-0.660466	-1.352643
H	3.797681	-0.262957	1.042256
H	2.979591	-2.327152	0.005813
C	-1.576638	2.882480	-0.277851
H	-1.542640	3.630291	-1.080934
H	-2.475523	2.278264	-0.434961
H	-1.700126	3.427358	0.668635
O	0.108310	-0.059738	1.766557
O	-1.447904	-0.757044	-0.546069

Si	-2.605517	-1.936464	-0.140291
H	-3.726754	-1.793268	-1.109934
H	-1.973003	-3.280791	-0.270985
H	-3.070678	-1.704344	1.255265

E = -382.891593040
G = -382.824341

W-O-5-TSI

W	0.106868	0.107125	-0.192024
O	-1.182735	-1.089678	0.557345
C	-2.831298	1.347061	-0.751241
C	0.698994	1.324800	1.145280
C	-2.372061	2.002005	0.321362
H	0.656384	0.848296	2.138397
Si	-2.353511	-2.291174	0.509476
H	-2.625328	1.693424	1.331834
H	-1.758935	2.892333	0.220691
H	-3.479607	0.480214	-0.654289
H	-1.769610	-3.561522	1.030720
H	-3.504583	-1.876155	1.366649
H	-2.831667	-2.494962	-0.892572
C	1.184665	2.743092	1.147519
H	2.208325	2.806945	1.539478
H	1.181357	3.171432	0.141998
H	0.561050	3.373741	1.796223
H	-2.585765	1.665814	-1.759469
O	0.111963	1.024722	-1.628015
O	1.540214	-1.126024	-0.402981
Si	3.160706	-1.162040	0.060591
H	3.283528	-0.831215	1.514214
H	3.668855	-2.543375	-0.190389
H	3.949736	-0.181134	-0.742938

E = -461.481105418
G = -461.363622

W-O-5-TBP

O	1.125846	1.286036	0.168466
C	1.152917	-0.686842	-1.730218
H	1.778677	0.110565	-2.123897
C	1.216759	-1.365112	0.933973
C	1.849559	-1.478855	-0.548708
H	1.873300	-0.754222	1.555296
H	2.869357	-1.106091	-0.465735
H	1.814594	-2.538295	-0.799426
Si	1.972513	2.710924	0.349578
H	1.036425	3.859934	0.540842
H	2.878655	2.614554	1.537745
H	2.810676	2.960818	-0.866708
W	-0.109513	-0.201124	-0.152523
C	0.874792	-2.691186	1.577348
H	0.393462	-2.523919	2.546243
H	0.187322	-3.268101	0.953600
H	1.777753	-3.288192	1.759931
H	0.763894	-1.347976	-2.500111
O	-1.073498	-1.587230	-0.496953
O	-1.544503	0.993305	0.222868
Si	-3.226530	0.829037	0.217319
H	-3.647089	-0.224005	1.188974
H	-3.797331	2.146262	0.626245
H	-3.706394	0.477485	-1.152301

E = -461.509283177
G = -461.383465

W-O-5-TSIII

W	-0.177752	-0.227041	0.140215
O	0.030303	1.713855	0.060469
C	-2.529332	0.292191	0.843261
C	-0.654934	-0.697467	1.955416
C	-2.354122	0.468519	-0.530955
H	-0.520383	0.008575	2.778473
H	-1.027443	-1.675012	2.258380
Si	1.310765	2.767509	-0.229595
H	0.760300	4.157731	-0.160152
H	2.384297	2.630295	0.799857
H	1.880508	2.545058	-1.592445
H	-2.115445	1.478743	-0.855093
H	-2.435323	1.139455	1.514313
C	-3.008081	-0.433059	-1.548263
H	-2.417208	-0.510018	-2.464232
H	-3.149975	-1.444188	-1.160006
H	-3.989869	-0.021860	-1.815720
H	-3.094466	-0.556954	1.217119
O	-0.534507	-1.663292	-0.719433
O	1.734445	-0.244025	-0.140167
Si	2.877147	-1.462891	-0.320670
H	4.199082	-0.815348	-0.575567
H	2.964736	-2.283681	0.928142
H	2.520950	-2.349826	-1.468947

E = -461.484247128
G = -461.360296

W-O-5-IV

W	-0.101760	-0.278100	0.061547
O	-0.124250	1.659508	0.153974
C	-2.736353	0.425583	-0.199236
C	-0.010857	-1.187516	1.741694
C	-2.501512	0.209375	1.121019
H	0.333124	-0.667908	2.641729
H	-0.288081	-2.228591	1.905438
Si	1.000316	2.884864	-0.117736
H	-2.859420	-0.689272	1.614782
H	-2.104636	0.996323	1.753987
H	2.189575	2.738226	0.774782
H	1.433987	2.889368	-1.546374
H	0.320912	4.180117	0.193772
C	-3.506660	-0.496369	-1.089946
H	-2.989677	-0.665175	-2.037779
H	-3.680265	-1.465801	-0.617140
H	-4.478802	-0.040025	-1.316459
H	-2.452473	1.392144	-0.613388
O	-0.704771	-1.441708	-1.031528
O	1.733966	-0.156746	-0.488683
Si	3.070205	-1.152388	-0.257028
H	2.887075	-2.451521	-0.972112
H	4.266251	-0.444872	-0.804990
H	3.258138	-1.413186	1.204652

E = -461.486354815
G = -461.365318

W-O-5-TSIV

O	-0.484418	1.507382	0.275607
C	-3.064458	-0.505925	-0.083680
C	0.512660	-1.150571	1.661788
C	-2.679258	-0.577353	1.199831

H	0.428371	-2.222128	1.835333
H	0.765704	-0.560561	2.549011
Si	-0.934361	3.075393	-0.130263
H	-3.117249	0.474314	-0.559268
H	-2.636245	-1.529476	1.722549
H	-2.450381	0.310684	1.779597
H	0.263373	3.824993	-0.609882
H	-1.972101	3.041182	-1.205606
H	-1.497824	3.731879	1.085695
C	-3.451999	-1.672660	-0.932181
H	-4.463916	-1.539560	-1.333191
H	-2.769250	-1.769892	-1.783459
H	-3.421665	-2.607833	-0.366644
O	-0.286362	-1.451200	-1.076259
O	1.945928	0.246656	-0.583431
Si	3.498983	-0.272537	-0.163366
H	3.689734	-1.695248	-0.571674
H	4.467843	0.599592	-0.891580
H	3.695037	-0.137139	1.311731
W	0.213662	-0.245195	0.015491

E = -461.484615617
G = -461.366726

W-O-5-V

W	0.000068	-0.396756	-0.063076
O	-1.537025	0.591839	-0.545226
C	0.000350	-0.598321	1.822987
H	-0.000545	0.316830	2.426670
H	0.001253	-1.524311	2.394141
Si	-3.015297	1.164408	0.050986
H	-3.437214	2.301203	-0.816750
H	-4.025260	0.068845	-0.004857
H	-2.832690	1.625297	1.459920
O	0.001624	-1.991566	-0.633915
O	1.535412	0.594691	-0.545067
Si	3.014776	1.164733	0.050899
H	3.440645	2.297846	-0.819709
H	2.832112	1.630205	1.458321
H	4.021780	0.066243	-0.000766

E = -343.620167365
G = -343.576392

W-O-5-TSA

O	1.430813	0.635428	-0.393357
C	-0.954712	1.966982	0.044982
H	-0.444176	2.619259	-0.663847
C	-1.880167	-0.237596	-1.045961
C	-2.190855	1.261949	-0.596757
H	-1.493612	-0.224276	-2.074591
H	-2.478669	1.806363	-1.500830
H	-3.027578	1.234525	0.104064
Si	2.310409	2.058646	-0.305166
H	2.110136	2.744928	1.008760
H	3.756892	1.723774	-0.470539
H	1.911960	2.997980	-1.402522
W	-0.303714	-0.059785	0.263050
C	-3.036040	-1.210127	-0.892971
H	-2.729989	-2.221467	-1.175979
H	-3.391797	-1.244435	0.140651
H	-3.878111	-0.921350	-1.535319
H	-1.203272	2.504081	0.958851
O	-0.966764	-0.223473	1.819220
O	0.705447	-1.669117	0.155225
Si	2.275336	-2.090821	-0.346080
H	2.340623	-3.578663	-0.225205
H	2.518745	-1.713023	-1.767846
H	3.297937	-1.483120	0.551618

E = -461.497848991
G = -461.369453

W-O-5-SBP

O	1.781374	0.725431	-0.189237
C	0.913926	-1.639769	0.935067
C	-1.326455	-1.247842	0.843574
C	-0.384230	-2.428441	1.069155
H	-1.410146	-0.679765	1.784503
Si	3.276597	0.868018	0.585165
H	4.143221	-0.289560	0.218903
H	3.892490	2.142020	0.116182
H	3.090441	0.912921	2.067049
H	-0.524801	-2.977908	2.011618
H	-0.479050	-3.146370	0.245954
H	1.201171	-1.171039	1.886209
W	0.091581	-0.111728	-0.377311
C	-2.708347	-1.519454	0.267236
H	-3.295397	-2.147827	0.951816
H	-3.281513	-0.601378	0.097577
H	-2.639259	-2.046499	-0.690199
H	1.788222	-2.155357	0.521225
O	-0.055746	-0.981901	-1.823805
O	-1.085512	1.353558	-0.206868
Si	-2.249586	2.332338	0.527558
H	-2.525423	1.845944	1.912399
H	-1.707000	3.720510	0.574905
H	-3.498362	2.293530	-0.286125

E = -461.522989579
G = -461.397282

W-O-5-TSB

C	0.767666	0.983600	1.929197
C	0.035598	2.027040	-0.071355
C	-0.305399	1.758547	1.292521
H	1.096519	2.230633	-0.221758
H	-1.105503	2.256593	1.849575
H	-1.210619	0.624588	1.220419
O	1.656857	-0.586695	-0.610447
Si	3.123314	-0.205176	-1.355244
H	4.159356	-1.171448	-0.891486
H	2.941569	-0.307326	-2.831682
H	3.520790	1.185982	-0.983907
H	1.774427	1.351136	1.725544
C	-0.918491	2.705562	-1.018018
H	-0.892790	3.800504	-0.922342
H	-0.686461	2.465850	-2.060944
H	-1.951814	2.389817	-0.836849
H	0.617320	0.635360	2.947993
O	-0.114886	-1.662658	1.432718
O	-1.418260	-0.486489	-0.861469
Si	-3.089821	-0.616341	-1.034810
H	-3.407359	-0.466793	-2.484419
H	-3.539238	-1.951651	-0.543260
H	-3.766948	0.461218	-0.250460
W	0.047512	-0.337365	0.341403

E = -461.453346929
G = -461.332784

W-O-5-B

C	-1.066568	0.104579	-1.668201
C	-3.059798	1.077272	-0.463706
C	-1.878063	1.207725	-1.085773
H	-3.505921	0.083683	-0.388668
H	-1.451534	2.208922	-1.176568
H	0.806558	1.210670	-1.050268
O	-0.543189	-1.336885	0.717818
Si	-1.812756	-1.668411	1.784567
H	-2.169799	-0.443295	2.556000
H	-2.986907	-2.146285	0.998612
H	-1.345283	-2.740637	2.708734
H	-1.639784	-0.831090	-1.740660
W	0.626283	-0.364437	-0.393631
C	-3.854308	2.206891	0.113625
H	-4.838042	2.286593	-0.366261
H	-4.042021	2.059282	1.184768
H	-3.339789	3.164651	-0.010199
H	-0.692384	0.364481	-2.663290
O	1.563517	-1.292628	-1.450808
O	1.745046	0.450332	0.901826
Si	2.394396	1.981163	1.237614
H	1.312102	3.009558	1.208179
H	2.992101	1.908091	2.602183
H	3.442255	2.309859	0.229245

E = -461.499048688
G = -461.378250

W-O-5-TSC

C	1.586290	0.072369	-1.235400
C	3.820408	-0.092012	-0.082070
C	2.820029	-0.622941	-0.800777
H	1.727778	1.165462	-1.200759
H	2.929401	-1.657623	-1.136176
H	1.355362	-0.183465	-2.273536
H	0.213581	-1.656833	-0.260180
O	-0.273788	1.667926	0.809089
C	0.778843	-1.862526	1.114607
H	1.672666	-2.302757	0.679673
H	0.004711	-2.569219	1.406008
C	0.878753	-0.634464	1.767788
H	0.147421	-0.358524	2.522019
H	1.816933	-0.091196	1.755256
H	3.738501	0.949515	0.236328
C	5.073770	-0.810218	0.310644
H	5.963619	-0.310677	-0.093309
H	5.199422	-0.833686	1.400854
H	5.075292	-1.843233	-0.051371
W	-0.386654	0.057316	-0.211285
O	-0.996867	0.636154	-1.703399
O	-1.881847	-0.922634	0.444705
Si	-2.938197	-2.187144	0.085152
H	-2.167290	-3.463136	-0.042563
H	-3.909112	-2.292620	1.211916
H	-3.649049	-1.899405	-1.194223
Si	-0.849383	3.235863	0.519594
H	-2.303823	3.209939	0.185525
H	-0.633021	4.017718	1.772187
H	-0.072399	3.843482	-0.600909

E = -540.026232678
G = -539.855430

W-O-5-C

C	1.198408	-1.110714	-1.170898
C	3.140707	-1.330789	0.427044
C	1.927824	-1.697196	-0.013725
H	3.683837	-0.553884	-0.114109
H	1.417195	-2.501524	0.519061
O	0.858005	1.452756	-0.322708
Si	2.275540	2.277925	0.065084
H	3.344880	1.914927	-0.911185
H	1.978296	3.736449	-0.033208
H	2.711113	1.940469	1.451366
H	1.853294	-0.450061	-1.754191
W	-0.491923	0.150832	-0.566889
C	3.845002	-1.936910	1.601250
H	4.798963	-2.390417	1.303183
H	4.083786	-1.181620	2.360899
H	3.237349	-2.712895	2.077120
H	0.819839	-1.889623	-1.840681
O	-1.306794	0.367109	-2.033977
C	-1.211831	-1.844775	-0.022262
H	-0.773575	-2.623841	-0.651782
H	-0.872271	-2.048573	1.003676
C	-2.742263	-1.949774	-0.095762
H	-3.075652	-2.943207	0.230865
H	-3.247848	-1.211838	0.534754
H	-3.102118	-1.800477	-1.118829
Si	-1.952613	0.640640	2.564854
H	-3.433250	0.782751	2.662253
H	-1.517568	-0.648410	3.181109
H	-1.279007	1.782074	3.250272
O	-1.512837	0.680030	0.934959

E = -540.099043818
G = -539.924720

Mo-N-1-I

Mo	.411546	.672143	.493051
O	.403950	.412210	2.384242
C	2.409745	1.096127	-.121107
N	-.121373	-.427803	-.733964
C	-.416589	2.276122	-.010101
H	-.206183	2.992053	.808182
Si	-.186879	.129207	3.925741
H	2.963753	.174385	.126255
H	2.465021	1.216401	-1.207025
C	3.028564	2.300197	.590555
H	4.101396	2.387246	.371065
H	.964421	.025491	4.872346
H	-1.078063	1.253243	4.349419
H	-.964945	-1.147951	3.954947
H	2.934191	2.233493	1.681227
H	2.549667	3.233350	.275018
C	-1.278424	2.809294	-1.108215
H	-.778396	3.640398	-1.625053
H	-1.502708	2.037269	-1.848189
H	-2.226974	3.204523	-.719999
C	-.641541	-1.435843	-1.514724
C	-1.360006	-2.501253	-.941590
C	-1.878104	-3.506963	-1.749279
C	-1.688764	-3.470463	-3.131751
C	-.975217	-2.417217	-3.705267
C	-.453568	-1.403990	-2.908550
H	-1.500242	-2.520747	.135155
H	-2.432538	-4.324977	-1.297545
H	-2.094939	-4.259056	-3.758532
H	-.824299	-2.384355	-4.780810

H	.103643	-.578810	-3.340980

E = -593.311673435
G = -593.122571

Mo-N-1-Ianti

H	2.359896	2.951628	2.395231
O	2.025645	1.187477	-1.238345
Si	3.105614	1.344780	-2.510209
H	4.381515	1.945017	-2.014498
H	3.397142	0.008480	-3.117070
H	2.507540	2.236004	-3.549628
C	-1.013427	0.775143	-0.223179
H	-1.224416	0.267423	-1.179962
H	-1.010806	1.857017	-0.437071
C	-2.094293	0.443662	0.798355
H	-2.121356	-0.629973	1.008004
H	-1.907349	0.957638	1.746498
H	-3.092074	0.738004	0.444949
C	1.419052	2.709783	1.882561
H	1.450508	3.187393	0.896867
H	0.609151	3.186070	2.452415
C	1.205244	1.218552	1.816724
H	1.199543	0.706319	2.781149
C	1.120694	-2.689136	0.765920
C	0.277760	-3.384988	1.651759
C	2.101839	-3.400011	0.050025
C	0.416637	-4.759310	1.811381
H	-0.474818	-2.828209	2.201064
C	2.231901	-4.773396	0.220283
H	2.751020	-2.857742	-0.631220
C	1.391544	-5.458906	1.099055
H	-0.239924	-5.287668	2.497261
H	2.993263	-5.312740	-0.336587
H	1.496380	-6.532251	1.228039
N	0.978666	-1.327588	0.618766
Mo	1.032625	0.340951	0.155477

E = -593.309438193
G = -593.118471

Mo-N-1-TSrot1

Mo	-0.980653	-0.420663	-0.168150
O	-2.135481	1.089671	-0.075122
C	-1.427399	-1.670076	-1.827006
N	0.637604	0.152993	-0.557322
C	-0.914564	-1.375561	1.400278
H	-0.987652	-2.253116	0.668646
Si	-2.129933	2.752260	0.151382
H	-1.345958	-0.989985	-2.686494
H	-0.654194	-2.436244	-1.961959
C	-2.824530	-2.288586	-1.735224
H	-3.094050	-2.788310	-2.674705
H	-3.419185	3.297444	-0.370786
H	-2.010180	3.081903	1.605462
H	-0.986164	3.371596	-0.587289
H	-3.597709	-1.536113	-1.541270
H	-2.889531	-3.037513	-0.938319
C	-0.610444	-1.688846	2.819998
H	0.323935	-2.251616	2.940544
H	-0.514548	-0.757394	3.386557
H	-1.416288	-2.271640	3.284507
C	1.968122	0.311239	-0.219752
C	2.598333	1.551612	-0.429292
C	3.940841	1.717596	-0.106896
C	4.681164	0.653822	0.410752
C	4.065279	-0.583295	0.608211
C	2.721184	-0.758511	0.299283
H	2.014864	2.368844	-0.842221
H	4.414313	2.682630	-0.266685
H	5.731528	0.786000	0.653719
H	4.637410	-1.417814	1.005211
H	2.232581	-1.717153	0.448149

E = -593.284495742
G = -593.094656

Mo-N-1-TSrot2

Mo	-0.939730	-0.476428	-0.109421
O	-2.024402	1.006223	0.381469
C	-1.592654	-1.441240	-1.845176
N	0.617342	0.223018	-0.565892
C	-0.751705	-1.587878	1.405283
H	-0.400015	-1.121851	2.334037
Si	-1.859192	2.678818	0.384035
H	-1.408258	-0.833747	-2.738048
H	-0.896863	-2.299351	-1.901787
C	-3.049505	-1.898632	-1.743044
H	-3.319678	-2.554149	-2.580684
H	-3.228961	3.267166	0.480885
H	-1.046151	3.117866	1.559625
H	-1.200337	3.150569	-0.873491
H	-3.735700	-1.045862	-1.760020
H	-3.248311	-2.461516	-0.822693
C	-0.854818	-3.095225	1.439067
H	-1.580109	-3.409086	2.202178
H	-1.188488	-3.526448	0.487831
H	0.105006	-3.567567	1.690742
C	1.925245	0.488914	-0.193814
C	2.597692	1.570016	-0.793956
C	3.914829	1.854326	-0.450612
C	4.585855	1.064129	0.483930
C	3.928667	-0.015887	1.077085
C	2.610070	-0.304248	0.745381
H	2.063981	2.170922	-1.524122
H	4.422610	2.694174	-0.917145
H	5.616330	1.286046	0.746521
H	4.449081	-0.636439	1.801988
H	2.084976	-1.140759	1.198022

E = -593.277509149
G = -593.086133

Mo-N-1-TSI

Mo	-.851786	-.386283	-.019435
O	-2.267798	.889993	-.233402
C	-1.262421	-1.607373	-1.721800
N	.883877	-.385463	-.137040
C	.143934	2.375398	1.929092
C	-1.213233	-1.661179	1.310804
C	-.361792	1.456905	2.754689
H	-2.309536	-1.645205	1.457694
Si	-3.009676	2.309565	-.708620
H	-1.401356	1.482725	3.070479
H	.249987	.653863	3.155218
H	-.464431	3.188043	1.540150
H	-1.086324	-.937982	-2.580785
H	-.517347	-2.405859	-1.786292
C	-2.676507	-2.183106	-1.775015
H	-2.864589	-2.695392	-2.728608
H	-4.185703	1.995263	-1.576062
H	-3.478442	3.061123	.497035
H	-2.059380	3.177181	-1.474805
H	-3.442401	-1.406869	-1.669087

H	-2.835100	-2.912911	-.973120
C	-.480240	-2.626212	2.183821
H	-.782446	-3.658503	1.957562
H	.600713	-2.553320	2.044726
H	-.707787	-2.460360	3.246076
H	1.185090	2.350923	1.619287
C	2.212542	-.076299	-.313506
C	2.609556	1.158591	-.862760
C	3.958698	1.449447	-1.031799
C	4.933699	.523512	-.658071
C	4.548194	-.703466	-.116119
C	3.202255	-1.007222	.055035
H	1.845524	1.873260	-1.154749
H	4.251199	2.405055	-1.458635
H	5.986389	.755406	-.791093
H	5.301937	-1.430813	.173159
H	2.891635	-1.961342	.469052

E = -671.871132541
G = -671.633993

Mo-N-1-II

Mo	.747051	.287079	.040268
O	2.345384	-.781071	.350723
C	1.125315	.120127	-2.073262
N	-.992102	.237670	-.106309
C	.275539	-.712844	2.493303
C	1.104299	2.130877	.260196
C	.795267	.500959	2.777579
H	2.199743	2.253808	.331787
Si	3.357707	-2.064852	.038757
H	1.864904	.642989	2.900289
H	.160248	1.357634	2.979768
H	.913651	-1.584857	2.390088
H	1.058366	-.960044	-2.288118
H	.300331	.595716	-2.614384
C	2.460221	.668662	-2.574105
H	2.619828	.449465	-3.638911
H	3.078481	-2.671745	-1.301371
H	4.783844	-1.613701	.081109
H	3.168797	-3.126923	1.081446
H	3.311847	.248573	-2.027385
H	2.507353	1.757623	-2.453511
C	.336091	3.408236	.327378
H	.602188	4.056575	-.519213
H	-.741394	3.235270	.298411
H	.579808	3.974260	1.237676
H	-.798283	-.871974	2.459630
C	-2.306372	-.156731	-.181289
C	-2.658068	-1.518709	-.264398
C	-3.994822	-1.894724	-.332692
C	-5.002662	-.929441	-.319502
C	-4.662808	.422053	-.241114
C	-3.329994	.810818	-.173722
H	-1.868680	-2.264768	-.281195
H	-4.251862	-2.948533	-.398183
H	-6.045498	-1.228220	-.372737
H	-5.442329	1.179108	-.234136
H	-3.055768	1.859511	-.116758

E = -671.873241605
G = -671.631329

Mo-N-1-TSII

Mo	-.716505	.223180	.043062
N	1.026091	.144111	.143452
C	-.998162	-.707825	1.980899
H	-.095809	-.551929	2.583683
H	-1.043331	-1.789623	1.765624
C	-2.234016	-.287266	2.777108
H	-2.167609	.762641	3.086790
H	-3.152719	-.393442	2.191455
H	-2.356287	-.885830	3.690500
O	-2.518877	-.473993	-.338504
Si	-3.605751	-1.711644	-.534403
H	-5.002564	-1.186577	-.413459
H	-3.456950	-2.328974	-1.896534
H	-3.409592	-2.796330	.480555
C	-1.015983	2.122495	.087523
H	-2.097810	2.320715	.108454
C	-.160148	3.340766	.192168
H	-.269479	3.766230	1.198988
H	-.469779	4.124970	-.511805
H	.895972	3.111350	.036031
C	-.892734	1.385361	-2.166185
H	-1.918460	1.706599	-2.318607
H	-.128969	2.146854	-2.285516
C	-.562816	.034001	-2.276926
H	-1.333210	-.680595	-2.546854
H	.464886	-.245776	-2.489285
C	2.346261	-.228380	.089542
C	2.726863	-1.485371	-.421290
C	4.069917	-1.839147	-.480873
C	5.054233	-.956597	-.033886
C	4.684752	.287612	.479685
C	3.345549	.654146	.544282
H	1.955196	-2.170497	-.760052
H	4.350242	-2.811602	-.876482
H	6.102117	-1.238038	-.081689
H	5.446104	.976999	.834458
H	3.047844	1.616699	.948392

E = -671.870614572
G = -671.624954

Mo-N-1-TBP

Mo	.748648	-.002164	.039444
C	.961765	.731135	1.963356
C	.939703	-2.977369	.133853
N	-1.000877	-.027064	.052872
C	.785340	-1.908765	-.947570
O	2.711984	-.112946	-.061582
H	1.850372	-2.831693	.726685
H	1.002645	-3.983319	-.303095
H	.088030	-2.984286	.824681
H	-.130200	-2.067868	-1.526745
H	1.643187	-1.915732	-1.630695
H	1.894876	.453851	2.452712
C	1.056147	2.094918	1.181671
C	.919002	2.010929	-.407899
H	1.890700	2.197892	-.871346
H	.245189	2.738932	1.528240
H	2.027610	2.542990	1.398386
Si	4.290756	-.505873	-.376470
H	5.001649	.654614	-1.006381
H	5.007923	-.861103	.890970
H	4.388246	-1.673688	-1.312586
C	-.168178	2.881056	-1.000366
H	-1.142055	2.674884	-.547406
H	.056059	3.947840	-.858581
H	-.254397	2.710476	-2.078536
H	.107876	.681094	2.634974
C	-2.365361	-.144849	.001226

C	-3.063819	.153393	-1.185241
C	-4.448144	.034888	-1.227975
C	-5.157763	-.378849	-.099535
C	-4.471522	-.678217	1.078728
C	-3.087407	-.565617	1.135559
H	-2.501216	.474178	-2.056411
H	-4.977324	.266406	-2.148307
H	-6.239342	-.469582	-.138532
H	-5.019045	-1.004187	1.958847
H	-2.542892	-.801519	2.044741

E = -671.893456112
G = -671.645977

Mo-N-1-TSIII

Mo	-.796145	.157517	-.444127
O	-2.636908	-.058376	.224489
C	-.944759	-1.942364	-.937237
N	.946312	.084445	-.373927
C	-1.241315	2.594761	.014316
C	-1.042736	1.309816	-1.958417
C	-.850074	1.902453	1.162918
H	-2.064355	1.462364	-2.318844
H	-.276092	1.824628	-2.534429
Si	-4.011957	-.887426	.648039
H	-5.199293	.012411	.482761
H	-4.230335	-2.105997	-.196539
H	-3.950152	-1.318045	2.083176
H	-1.653161	1.510763	1.783659
H	-2.295088	2.719099	-.208145
H	-.207754	-2.181138	-1.712988
H	-1.940656	-2.113446	-1.365746
C	-.733453	-2.842346	.283009
H	-.904414	-3.901347	.046296
H	.288887	-2.763125	.670455
H	-1.416467	-2.592684	1.105692
C	.459348	2.187247	1.855654
H	.838314	1.319725	2.402279
H	1.231396	2.500456	1.147766
H	.321682	2.996272	2.585231
H	-.561289	3.305087	-.448203
C	2.281151	-.128438	-.131208
C	3.233113	.267292	-1.090506
C	4.587861	.059095	-.858486
C	5.018208	-.544456	.324179
C	4.080261	-.942790	1.277825
C	2.722729	-.739334	1.058435
H	2.886444	.729998	-2.009373
H	5.312994	.367820	-1.606546
H	6.077672	-.706002	.500351
H	4.408701	-1.417089	2.198628
H	1.987507	-1.051228	1.793995

E = -671.864737441
G = -671.618826

Mo-N-1-IV

Mo	-.842953	-.212150	-.513070
O	-2.369987	.369910	.517312
C	-1.188926	-2.238213	.100371
N	.887885	-.318271	-.379778
C	-.323947	2.757365	-.095191
C	-1.152385	-.442925	-2.356524
C	-1.008660	2.590243	-1.241082
H	-2.206314	-.403421	-2.663745
H	-.449456	-.609827	-3.171061
Si	-3.315808	.426315	1.891931
H	-.521858	2.676560	-2.209031
H	-2.082790	2.435795	-1.240631
H	-.373629	-2.866184	-.271022
H	-1.094597	-2.210848	1.198947
C	-2.536799	-2.835582	-.297873
H	-2.687921	-3.826177	.152791
H	-3.023339	-.731007	2.795121
H	-3.040757	1.694242	2.642136
H	-4.761640	.400274	1.511887
H	-2.606440	-2.954028	-1.385209
H	-3.378175	-2.207042	.014589
C	1.129271	3.100083	-.005239
H	1.670505	2.400391	.639913
H	1.606113	3.097398	-.989042
H	1.252010	4.098279	.433573
H	-.870734	2.701537	.846311
C	2.196827	-.382933	.035408
C	2.534338	-.400622	1.402775
C	3.866615	-.480039	1.793333
C	4.881480	-.537497	.837104
C	4.554090	-.520377	-.519755
C	3.225972	-.446625	-.923250
H	1.738989	-.360744	2.141467
H	4.114376	-.497501	2.851238
H	5.920559	-.597953	1.147424
H	5.339613	-.568408	-1.269051
H	2.958289	-.438067	-1.975213

E = -671.871901643
G = -671.631415

Mo-N-1-TSIV

Mo	-.920055	-.433066	-.415937
O	-2.325754	.493694	.497452
C	-1.371987	-2.373698	.349330
N	.804475	-.552231	-.261665
C	.013712	2.988729	-.531901
C	-1.235304	-.781491	-2.236395
C	-.744900	2.624349	-1.572703
H	-.549529	-1.029498	-3.044582
H	-2.287863	-.692181	-2.539570
Si	-3.173103	1.151099	1.781725
H	-.465758	3.142517	.435854
H	-.315936	2.469525	-2.559835
H	-1.818699	2.497759	-1.478686
H	-.608481	-3.081340	.014273
H	-1.249058	-2.262883	1.439882
C	-2.768987	-2.895533	.019608
H	-2.978953	-3.834441	.550199
H	-3.627971	.067096	2.705745
H	-2.304312	2.103425	2.543547
H	-4.363142	1.890499	1.261726
H	-2.870452	-3.092670	-1.053241
H	-3.554521	-2.185062	.299831
C	1.488198	3.236614	-.586340
H	1.716621	4.272841	-.307101
H	2.026774	2.592609	.118059
H	1.888654	3.055515	-1.587710
C	2.125352	-.520764	.120808
C	2.505845	-.109426	1.412629
C	3.848076	-.097758	1.775990
C	4.830215	-.488664	.864620
C	4.459520	-.898196	-.417104
C	3.120619	-.919220	-.790969
H	1.735830	.191405	2.117170
H	4.129314	.218418	2.776870
H	5.877423	-.476521	1.152447

H	5.219279	-1.206672	-1.130115
H	2.819096	-1.240552	-1.782957

E = -671.871393002
G = -671.632858

Mo-N-1-V

Mo	.272493	-.876437	.427264
O	.352062	-.599126	2.306845
C	2.206070	-1.460333	-.246683
N	-.207745	.270169	-.772618
C	-.719676	-2.396706	-.046559
H	-1.400617	-2.586607	-.874788
H	-.645526	-3.213710	.685836
Si	-.127146	-.122100	3.842874
H	2.227678	-1.546944	-1.336721
H	2.842386	-.598297	.018577
C	2.727947	-2.738377	.411141
H	3.787894	-2.903705	.175143
H	1.073666	-.093604	4.730553
H	-.737381	1.242037	3.790763
H	-1.128415	-1.089676	4.385849
H	2.168868	-3.613276	.063752
H	2.649610	-2.708707	1.504791
C	-.665845	1.304823	-1.555903
C	-1.254916	2.446133	-.981635
C	-1.713917	3.475560	-1.795014
C	-1.592133	3.386876	-3.182770
C	-1.007499	2.257108	-3.756736
C	-.546245	1.219216	-2.954886
H	-1.344422	2.504344	.099024
H	-2.169324	4.352764	-1.343794
H	-1.951748	4.194513	-3.813706
H	-.911126	2.183436	-4.836445
H	-.091181	.333237	-3.386330

E = -554.004159387
G = -553.840961

Mo-N-1-TSA

Mo	-0.896991	0.296867	0.075501
C	-1.580347	0.103746	-1.925897
C	-0.376345	-1.017687	2.944869
N	0.822179	0.430895	-0.052048
C	-1.058778	0.151247	2.248152
O	-1.821606	-1.453272	0.384949
H	-0.730078	-1.964959	2.528080
H	-0.588470	-1.028587	4.022928
H	0.712312	-0.977049	2.825823
H	-0.651326	1.111736	2.600217
H	-2.138632	0.141121	2.449934
H	-2.537615	-0.371162	-2.143211
C	-1.689791	1.631390	-1.685306
C	-1.741561	2.129389	-0.130296
H	-2.786325	2.062606	0.205291
H	-0.882585	2.178903	-2.173592
H	-2.658220	1.957183	-2.071635
Si	-2.235171	-2.734249	-0.585881
H	-2.363520	-3.965462	0.257546
H	-3.554707	-2.513401	-1.271849
H	-1.218434	-3.013383	-1.656927
C	-1.157300	3.504103	0.094659
H	-0.117473	3.552842	-0.240341
H	-1.724947	4.284476	-0.430345
H	-1.176969	3.744120	1.162578
H	-0.825867	-0.158534	-2.666447
C	2.156966	0.097707	-0.150429
C	3.132426	1.021874	0.263867
C	4.481226	0.698501	0.165563
C	4.875135	-0.538555	-0.346010
C	3.909148	-1.457698	-0.759578
C	2.557247	-1.149153	-0.665060
H	2.811358	1.979649	0.661243
H	5.229201	1.416607	0.490013
H	5.929974	-0.785780	-0.422008
H	4.211123	-2.422509	-1.157463
H	1.796679	-1.856604	-0.981008

E = -671.861864241
G = -671.613829

Mo-N-1-SBP

Mo	-.755452	.008965	-.069471
C	-1.050846	-.172267	2.054085
H	-2.100883	.081745	2.249810
C	-.788610	-1.660170	2.160928
C	-1.230825	-2.008626	.747624
H	-2.332868	-2.004520	.713994
H	.285612	-1.849684	2.272547
H	-1.308215	-2.195161	2.973874
C	-1.313310	-1.029622	-1.832754
O	-1.855201	1.554191	-.208582
Si	-2.812204	2.865737	.215014
H	-3.625931	2.542314	1.427039
H	-1.947758	4.050792	.502722
H	-3.724082	3.182425	-.925072
N	.972355	-.091063	-.099962
H	-.638957	-1.844446	-2.102998
H	-1.047638	-.168784	-2.483907
C	-2.775493	-1.407657	-2.028976
H	-3.454124	-.601567	-1.728124
H	-2.987493	-1.630949	-3.082974
H	-3.041613	-2.298382	-1.451448
C	2.322872	.179191	-.129201
C	2.797735	1.503789	-.147466
C	4.164910	1.753331	-.174837
C	5.076010	.695931	-.184070
C	4.609990	-.619310	-.166107
C	3.245085	-.883051	-.139352
H	2.080345	2.319270	-.139730
H	4.521968	2.779439	-.188388
H	6.143309	.896045	-.204789
H	5.314693	-1.446306	-.172994
H	2.870076	-1.901375	-.124947
H	-.399206	.513634	2.608982
C	-.694184	-3.308234	.175243
H	-.945582	-4.144671	.844419
H	-1.104088	-3.552156	-.809153
H	.397378	-3.280464	.086417

E = -671.897468922
G = -671.650347

Mo-N-1-TSB

C	0.213310	-0.431500	-2.132800
C	2.355070	-0.988371	-1.252820
C	1.081560	-1.494612	-1.677415
H	2.713433	-0.145089	-1.845880
H	0.865075	-2.555681	-1.827291
H	0.380011	-1.672412	-0.367875
O	1.693784	1.581646	0.333901
Si	3.233962	2.232461	0.343189
H	3.827993	2.206678	-1.031621

H	3.168909	3.651490	0.810187
H	4.126181	1.460625	1.265100
C	0.987132	-1.275872	1.677389
H	2.052698	-1.532390	1.618263
H	0.428813	-2.214724	1.706492
C	0.693448	-0.448793	2.928890
H	1.212296	0.515446	2.924937
H	-0.377145	-0.245618	3.028020
H	1.018595	-0.988193	3.829943
H	0.676585	0.365951	-2.716092
C	-2.456639	0.147933	0.073922
C	-3.283061	1.284839	0.158190
C	-3.041238	-1.108646	-0.176345
C	-4.656422	1.163105	-0.017063
H	-2.823622	2.248022	0.358258
C	-4.417243	-1.218939	-0.342051
H	-2.396957	-1.981937	-0.224760
C	-5.228898	-0.085918	-0.266205
H	-5.285973	2.046546	0.044566
H	-4.859800	-2.193208	-0.531323
H	-6.303370	-0.176219	-0.397432
N	-1.097909	0.277114	0.249726
Mo	0.620785	0.013922	-0.033129
C	3.425380	-1.898251	-0.705385
H	4.025190	-2.352851	-1.506553
H	4.120563	-1.360622	-0.051415
H	2.995444	-2.717607	-0.118540
H	-0.812668	-0.660195	-2.409344

E = -671.861576346
G = -671.616999

Mo-N-1-TSB*TransX*

O	1.237948	-1.506715	-1.203045
C	2.044493	0.893780	1.827411
C	0.056747	-0.318142	2.102923
C	1.480824	-0.319187	2.317366
H	-0.437911	0.629577	2.315462
Si	2.011208	-2.987333	-1.065569
H	1.310194	-3.855432	-0.065028
H	1.987995	-3.664964	-2.399255
H	3.436518	-2.823928	-0.633286
H	2.027537	-1.078418	2.877549
H	1.762512	-1.306926	1.084860
H	1.468096	1.801493	1.993046
N	-0.579382	0.666866	-0.406561
C	-1.932358	0.911619	-0.352984
C	-2.410986	2.154724	0.104502
C	-2.858915	-0.057765	-0.786692
C	-3.777355	2.412936	0.132831
H	-1.693289	2.905544	0.421886
C	-4.222252	0.211363	-0.749639
H	-2.484687	-1.008434	-1.154882
C	-4.688744	1.444653	-0.290257
H	-4.133251	3.377020	0.486410
H	-4.926698	-0.544829	-1.085872
H	-5.754904	1.650774	-0.266621
Mo	0.947943	-0.070394	0.066540
C	-0.773398	-1.553904	2.321069
H	-0.950454	-1.733830	3.390632
H	-1.749965	-1.461375	1.837544
H	-0.275454	-2.444474	1.918140
H	3.121223	1.030810	1.787223
C	2.250461	1.404728	-0.813848
H	2.241021	2.371138	-0.304255
H	3.257546	0.979922	-0.682254
C	1.912449	1.565344	-2.294628
H	2.678667	2.175520	-2.794315
H	1.864528	0.604182	-2.814856
H	0.946528	2.060593	-2.426880

E = -671.853717402
G = -671.608033

Mo-N-1-B

C	1.834628	-0.706446	-1.048607
C	4.100932	-0.076457	-0.148861
C	3.116202	-0.966885	-0.350671
H	1.888198	0.183527	-1.699363
H	3.239446	-1.973576	0.053697
H	1.500057	-1.560630	-1.640276
H	0.813171	-1.623994	0.671719
O	1.029199	1.640999	0.859688
Si	1.635472	3.051000	1.527806
H	2.828098	3.496913	0.744846
H	0.592007	4.121044	1.482078
H	2.035353	2.815712	2.949010
C	-0.300229	-0.685634	2.282764
H	-0.950939	0.170248	2.539990
H	0.598685	-0.611605	2.913668
C	-1.025758	-1.997400	2.532138
H	-1.909642	-2.086731	1.893145
H	-0.376771	-2.852561	2.317425
H	-1.357481	-2.081795	3.575759
H	3.980283	0.934214	-0.543329
C	5.379385	-0.361824	0.574657
H	6.250422	-0.202090	-0.073991
H	5.509259	0.304413	1.437495
H	5.413578	-1.393859	0.937228
N	-1.105921	-0.405894	-0.530788
C	-2.300992	-0.426639	-1.216554
C	-2.832548	-1.657570	-1.640209
C	-2.996105	0.762662	-1.500059
C	-4.038036	-1.691078	-2.332189
H	-2.284996	-2.567267	-1.415083
C	-4.199735	0.714319	-2.193901
H	-2.578244	1.709196	-1.170112
C	-4.725471	-0.509242	-2.611871
H	-4.443274	-2.645866	-2.655596
H	-4.731118	1.637163	-2.409445
H	-5.666525	-0.541139	-3.153202
Mo	0.337811	-0.062354	0.347935

E = -671.887036521
G = -671.647921

Mo-N-1-TSC

C	-1.808270	0.364823	0.617733
C	-4.116304	0.850674	-0.256473
C	-3.229367	0.055107	0.362667
H	-1.627197	1.452405	0.556379
H	-3.587643	-0.904798	0.744061
H	-1.520547	0.033496	1.618080
H	-0.973879	-1.603364	-0.480908
O	0.252243	1.442866	-1.841929
Si	1.274577	2.749660	-1.994989
H	2.303637	2.468502	-3.045763
H	0.486220	3.954549	-2.402778
H	1.983926	3.061448	-0.709941
C	1.078844	-1.668795	-1.624361
H	2.002568	-1.092308	-1.791886
H	0.656850	-1.880721	-2.615053
C	1.395331	-2.958775	-0.886019
H	1.859657	-2.758126	0.084115

H	0.489548	-3.547950	-0.699379
H	2.084920	-3.593461	-1.459266
C	-1.866285	-1.629802	-1.797385
H	-2.758808	-1.756079	-1.191779
H	-1.395639	-2.551548	-2.129277
C	-1.701496	-0.456546	-2.513088
H	-1.030507	-0.404156	-3.363750
H	-2.404320	0.360024	-2.382416
H	-3.777863	1.822646	-0.622200
C	-5.560768	0.524716	-0.473883
H	-6.214339	1.263542	0.007625
H	-5.818722	0.531671	-1.540910
H	-5.815042	-0.461164	-0.071853
N	0.938547	-0.080228	0.693663
C	1.641220	-0.164578	1.869810
C	1.372276	-1.202402	2.782745
C	2.627283	0.791916	2.177799
C	2.078748	-1.276147	3.977447
H	0.611323	-1.934303	2.529719
C	3.327078	0.704519	3.375154
H	2.823442	1.588643	1.467152
C	3.056881	-0.326393	4.277329
H	1.866935	-2.078964	4.678146
H	4.087406	1.444877	3.607655
H	3.607324	-0.389185	5.211600
Mo	-0.098622	-0.098860	-0.702966

E = -750.423595583
G = -750.129853

Mo-N-1-C

C	1.523438	-1.347639	-0.575549
C	3.968697	-0.934644	-0.158627
C	2.831909	-1.612573	0.065373
H	1.638657	-0.666751	-1.437936
H	2.871581	-2.442746	0.773184
H	1.033478	-2.260571	-0.919069
H	-2.070652	-2.569806	0.765526
O	1.432819	1.317921	0.921837
Si	2.496261	2.578632	1.223071
H	3.796371	2.044325	1.725237
H	2.726102	3.348785	-0.037229
H	1.897360	3.481604	2.252924
C	-1.000949	0.325778	2.290434
H	-1.055977	1.417063	2.105659
H	-0.358713	0.179017	3.170222
C	-2.398920	-0.216074	2.530241
H	-3.050828	-0.024086	1.672552
H	-2.393476	-1.295138	2.710700
H	-2.858847	0.252084	3.410834
C	-1.060600	-2.990946	0.764953
H	-0.785208	-3.169622	-0.280074
H	-1.110833	-3.971896	1.258435
C	-0.067520	-2.070545	1.477098
H	-0.372345	-1.966943	2.522992
H	0.914718	-2.553794	1.497962
H	3.954685	-0.112225	-0.876928
C	5.285068	-1.227622	0.490268
H	6.052097	-1.477623	-0.254278
H	5.661864	-0.357949	1.044060
H	5.209842	-2.065418	1.190464
Mo	0.182704	-0.052395	0.544813
N	-1.097483	0.013477	-0.610547
C	-2.011141	0.371341	-1.577751
C	-2.819677	-0.616916	-2.167889
C	-2.151646	1.711842	-1.982015
C	-3.746431	-0.264746	-3.142954
H	-2.702875	-1.646742	-1.847482
C	-3.085535	2.050208	-2.954401
H	-1.523714	2.468996	-1.522179
C	-3.884655	1.066184	-3.538773
H	-4.365873	-1.033976	-3.595264
H	-3.189646	3.087601	-3.259481
H	-4.611397	1.335944	-4.299253

E = -750.469001681
G = -750.172806

Mo-N-1'-I

O	2.133185	-0.614691	-0.305665
Si	3.505857	-1.522248	-0.009313
H	4.219532	-1.006954	1.201012
H	3.139898	-2.955155	0.216729
H	4.415902	-1.431628	-1.191844
C	0.355933	1.807540	-1.567078
H	0.278279	1.234227	-2.506249
H	1.363378	2.256328	-1.559331
C	-0.702957	2.902979	-1.530048
H	-1.711272	2.477399	-1.527304
H	-0.605052	3.512730	-0.626503
H	-0.627702	3.572992	-2.397826
C	0.480422	1.418398	1.472476
C	-2.273731	-1.196202	-0.067621
N	-1.098587	-0.357841	-0.040821
Mo	0.479884	0.316973	-0.048594
C	-0.434128	1.847693	2.573497
H	-0.052924	1.539120	3.556951
H	-0.526837	2.942172	2.602404
H	-1.434784	1.428351	2.444262
H	1.517786	1.796019	1.562622
C	-2.333540	-1.911243	-1.427262
H	-1.450041	-2.540633	-1.571567
H	-3.223911	-2.546607	-1.482752
H	-2.376944	-1.183611	-2.243053
C	-2.177938	-2.223414	1.071617
H	-2.100125	-1.718609	2.038921
H	-3.068297	-2.861177	1.083680
H	-1.297660	-2.860646	0.943744
C	-3.514084	-0.307865	0.118421
H	-3.572436	0.441107	-0.676232
H	-4.425150	-0.915284	0.091773
H	-3.473993	0.213548	1.078935

E = -519.552555292
G = -519.332698

Mo-N-1'-Ianti

O	1.970175	-0.849323	-0.215187
Si	2.831444	-2.272900	-0.393378
H	3.368531	-2.712522	0.931221
H	1.956250	-3.355452	-0.944245
H	3.969390	-2.042466	-1.334808
C	0.438196	1.699114	-1.558458
H	0.271819	1.105041	-2.472940
H	1.489540	2.031967	-1.591285
C	-0.491450	2.906528	-1.538085
H	-1.539856	2.595077	-1.499296
H	-0.305237	3.526429	-0.655465
H	-0.363779	3.537252	-2.428850
C	0.597764	1.474623	1.476123
C	-2.508449	-0.821760	0.169610
N	-1.216819	-0.181517	0.112855

Mo	0.434662	0.274048	0.025624
C	1.957446	2.025097	1.832045
H	1.953676	3.122557	1.773035
H	2.238034	1.758309	2.860160
H	2.757274	1.667105	1.173196
H	-0.215195	1.789468	2.132421
C	-3.177306	-0.684351	-1.207385
H	-2.577003	-1.174934	-1.979514
H	-4.168930	-1.148995	-1.192765
H	-3.291160	0.369380	-1.476539
C	-2.329441	-2.304487	0.530823
H	-1.835974	-2.405506	1.502268
H	-3.301310	-2.806915	0.582480
H	-1.717892	-2.812155	-0.221523
C	-3.346757	-0.107432	1.241789
H	-3.460729	0.952219	0.996392
H	-4.342117	-0.559450	1.308936
H	-2.865060	-0.184614	2.220924

E = -519.550619728
G = -519.328269

Mo-N-1'-TSI

Mo	-0.339291	-0.335143	0.153346
N	1.310355	-0.105518	-0.286359
C	-0.708410	-2.085610	-1.025815
H	-0.819797	-1.704290	-2.054971
H	0.173119	-2.732455	-1.021393
C	-1.951099	-2.874984	-0.616520
H	-2.845329	-2.243650	-0.567598
H	-1.819195	-3.331108	0.371085
H	-2.166028	-3.684308	-1.328148
O	-2.017532	0.554193	-0.211450
Si	-3.167644	1.310876	-1.152499
H	-4.519827	1.144699	-0.534807
H	-3.188527	0.732409	-2.533182
H	-2.869443	2.775941	-1.257100
C	-0.238234	-1.181369	1.830935
H	-1.280555	-1.300526	2.183833
C	0.796265	-1.700275	2.775934
H	0.700403	-1.243301	3.771066
H	0.681408	-2.784158	2.919233
H	1.806384	-1.514268	2.404409
C	-0.384045	2.248675	2.248631
H	0.341939	1.949643	2.999348
H	-1.413986	1.948903	2.418883
C	-0.032758	2.962374	1.176733
H	0.995053	3.275147	1.013509
H	-0.760869	3.264644	0.429535
C	2.571639	0.289632	-0.862902
C	3.499861	0.756351	0.270337
H	3.064755	1.609540	0.798396
H	4.472099	1.057128	-0.134661
H	3.659756	-0.049021	0.992736
C	3.176377	-0.935041	-1.569101
H	3.321225	-1.754613	-0.859528
H	4.146197	-0.679002	-2.009424
H	2.515424	-1.285267	-2.367249
C	2.351033	1.427331	-1.872528
H	3.303085	1.742197	-2.313507
H	1.894014	2.292673	-1.383318
H	1.689914	1.099384	-2.680798

E = -598.110352461
G = -597.840140

Mo-N-1'-II

Mo	0.291238	0.210601	0.167918
N	-1.370681	-0.098648	-0.190707
C	0.770802	0.966547	-1.800728
H	0.949104	0.068806	-2.416571
H	-0.108939	1.463773	-2.221542
C	1.976311	1.901743	-1.888530
H	2.874674	1.465433	-1.437892
H	1.780631	2.844911	-1.364379
H	2.226382	2.151945	-2.929067
O	2.090236	-0.574680	0.198370
Si	3.366029	-1.370750	-0.507298
H	4.649727	-0.656790	-0.215518
H	3.205426	-1.479885	-1.993177
H	3.471851	-2.761405	0.048172
C	0.208627	1.859996	1.095392
H	1.241251	2.170197	1.336944
C	-0.838612	2.824984	1.542911
H	-0.763076	3.028423	2.620832
H	-0.706008	3.792360	1.038052
H	-1.844122	2.460365	1.323251
C	0.320748	-0.587757	2.781427
H	-0.489468	-0.033482	3.243938
H	1.331173	-0.265311	3.014286
C	0.092070	-1.699457	2.047783
H	-0.914862	-2.076833	1.900670
H	0.911615	-2.303134	1.672605
C	-2.627003	-0.629844	-0.657904
C	-3.622851	-0.644835	0.513709
H	-4.596246	-1.021068	0.181234
H	-3.760402	0.363382	0.914864
H	-3.265587	-1.289577	1.322484
C	-3.145296	0.291720	-1.775074
H	-3.276756	1.311280	-1.401862
H	-4.109218	-0.070578	-2.148702
H	-2.438628	0.320773	-2.608968
C	-2.423647	-2.053165	-1.202595
H	-1.703877	-2.047538	-2.026711
H	-3.369369	-2.463238	-1.573241
H	-2.045709	-2.719180	-0.420462

E = -598.111833191
G = -597.837939

Mo-N-1'-TSII

Mo	0.321455	0.205625	-0.117703
O	2.256509	0.064894	0.322289
N	-1.370818	-0.133019	0.017345
C	0.440920	2.350899	1.165093
C	0.291384	1.815600	-1.172257
C	0.361716	1.225251	1.983256
H	1.320034	2.115350	-1.419947
Si	3.763826	-0.618710	0.341321
H	4.801706	0.461083	0.431658
H	4.052670	-1.427752	-0.888667
H	3.933343	-1.518112	1.531002
H	1.264778	0.830684	2.435611
H	1.403967	2.812814	0.972986
H	-0.432260	2.972563	0.996025
C	-2.696400	-0.622566	0.297694
H	-0.580769	0.979167	2.461725
C	-0.759706	2.684326	-1.778439
H	-0.580710	3.750064	-1.579731
H	-1.760544	2.416251	-1.434708
H	-0.732373	2.565667	-2.870483

C	0.716505	-1.521122	-1.374881
H	-0.055260	-1.600828	-2.149413
H	1.671371	-1.341683	-1.885311
C	0.794553	-2.825602	-0.576094
H	1.091372	-3.677464	-1.203570
H	-0.170079	-3.084367	-0.122442
H	1.527094	-2.768695	0.239287
C	-3.630667	0.579497	0.519015
H	-4.646863	0.234778	0.738663
H	-3.669218	1.209672	-0.374329
H	-3.287596	1.191049	1.359294
C	-3.171781	-1.442988	-0.912893
H	-4.186509	-1.818341	-0.741674
H	-2.509447	-2.295892	-1.083034
H	-3.175977	-0.826922	-1.816632
C	-2.669119	-1.504044	1.557632
H	-3.670939	-1.889929	1.774566
H	-2.328233	-0.932867	2.426548
H	-1.995024	-2.354131	1.419101

E = -598.110169884
G = -597.832206

Mo-N-1'-TBP

Mo	-0.332815	-0.020946	-0.083528
C	-0.561240	-2.146042	0.174610
O	-2.319766	-0.025817	-0.096912
C	-0.421274	1.637242	1.146836
H	-1.399728	1.647648	1.634056
C	-0.480221	1.446704	-1.541688
C	-0.515718	2.373412	-0.264187
H	-1.419029	1.453855	-2.093443
H	-1.456373	2.926877	-0.278213
H	0.336046	3.054589	-0.317784
Si	-3.882608	-0.368268	-0.515561
H	-4.295519	0.412136	-1.730336
H	-4.817448	-0.010825	0.600882
H	-4.067943	-1.825448	-0.825256
H	0.292660	-2.707635	-0.214906
H	-1.463236	-2.459497	-0.362977
C	-0.721435	-2.369307	1.678981
H	0.162151	-2.039334	2.239763
H	-0.865787	-3.432865	1.913987
H	-1.590608	-1.835368	2.080121
C	0.672434	2.133522	2.065673
H	0.739379	1.505298	2.959878
H	0.476206	3.161345	2.402970
H	1.647720	2.118122	1.571470
H	0.378432	1.640369	-2.179910
N	1.393766	-0.150396	-0.174561
C	2.800333	-0.377748	-0.369165
C	3.424264	-0.800993	0.971306
H	2.960159	-1.721383	1.337200
H	3.284478	-0.021981	1.726240
H	4.498364	-0.979041	0.851678
C	3.449897	0.922506	-0.873090
H	2.997155	1.240806	-1.816743
H	4.520876	0.767803	-1.041871
H	3.331572	1.728268	-0.142796
C	2.984418	-1.490426	-1.415831
H	4.050198	-1.676052	-1.587165
H	2.524834	-1.203713	-2.366295
H	2.523215	-2.422398	-1.077954

E = -598.131659530
G = -597.850955

Mo-N-1'-TSIII

O	2.276527	-0.130991	0.073199
C	0.463813	-2.127207	0.825176
C	0.340247	-0.850712	-2.126873
C	0.620491	-2.579388	-0.484141
H	1.312019	-0.987713	-2.611144
H	-0.512241	-1.169782	-2.723748
Si	3.780614	0.482589	0.398246
H	-0.184591	-3.118004	-0.976769
H	1.614805	-2.713760	-0.893859
H	4.027410	1.802237	-0.270752
H	3.974662	0.671795	1.874296
H	4.828808	-0.476985	-0.082726
C	-0.739230	-2.477727	1.663550
H	-0.942260	-1.719569	2.424417
H	-1.636581	-2.600644	1.051738
H	-0.558685	-3.424844	2.189510
H	1.380685	-1.912235	1.369363
C	0.664408	2.071185	-0.429570
H	1.624381	2.239342	-0.933350
H	-0.108265	2.561091	-1.031798
C	0.700641	2.675954	0.976714
H	1.442935	2.185019	1.619153
H	0.959361	3.743703	0.959766
H	-0.268981	2.589776	1.482619
Mo	0.335870	-0.072164	-0.373674
N	-1.371002	0.117915	-0.161674
C	-2.751728	0.453515	0.081144
C	-3.636849	-0.624340	-0.567711
H	-4.694969	-0.373251	-0.437795
H	-3.429315	-0.698017	-1.639252
H	-3.459830	-1.603419	-0.113084
C	-3.030735	0.535019	1.590196
H	-2.379540	1.275321	2.063969
H	-4.070589	0.830752	1.765848
H	-2.865104	-0.431264	2.073173
C	-3.030576	1.817106	-0.575306
H	-2.814949	1.779779	-1.646794
H	-4.082631	2.090214	-0.439919
H	-2.409755	2.597194	-0.126981

E = -598.102193298
G = -597.823277

Mo-N-1'-V

Mo	0.421294	-0.338228	0.213223
O	1.834997	0.877593	-0.194016
C	0.700077	-2.120342	-0.927987
N	-1.252254	-0.035754	0.021927
C	0.508799	-1.039025	1.954995
H	-0.251114	-1.258542	2.702314
H	1.543933	-1.187450	2.297167
Si	2.734277	2.291330	-0.202180
H	0.663861	-1.771900	-1.974663
H	-0.139083	-2.808339	-0.793803
C	2.028918	-2.822034	-0.642582
H	2.223251	-3.622536	-1.369424
H	3.808047	2.172672	-1.234598
H	3.357139	2.510503	1.139326
H	1.861989	3.460508	-0.533250
H	2.883974	-2.136618	-0.693630
H	2.026858	-3.271944	0.355602
C	-2.601144	0.444516	-0.156816
C	-3.424236	0.011890	1.066715

H	-3.419365	-1.076999	1.167412
H	-4.461058	0.348813	0.962252
H	-3.009824	0.444916	1.981712
C	-2.590968	1.975489	-0.282020
H	-3.609421	2.353872	-0.420326
H	-1.987726	2.288347	-1.139776
H	-2.172982	2.432177	0.620203
C	-3.167435	-0.194603	-1.434783
H	-4.200480	0.132537	-1.592816
H	-3.155355	-1.285381	-1.357578
H	-2.575151	0.096521	-2.307472

E = -480.245778570
G = -480.050540

Mo-N-1'-TSA

O	-1.754495	-1.095081	0.325726
C	-0.897974	0.106255	-2.043992
H	-1.931751	-0.129120	-2.298013
C	-0.602752	2.257821	-0.400777
C	-0.627520	1.624119	-1.915198
H	-1.638675	2.513595	-0.136766
H	-1.461787	2.154332	-2.379363
H	0.314220	1.908523	-2.385547
Si	-2.456213	-2.290553	-0.580732
H	-2.971433	-3.364005	0.329664
H	-3.625071	-1.780439	-1.379657
H	-1.506968	-2.933804	-1.553180
Mo	-0.326798	0.289480	-0.000624
C	0.328669	3.438582	-0.255691
H	0.327602	3.785482	0.782474
H	1.355912	3.168491	-0.516102
H	0.024678	4.284550	-0.887613
H	-0.197700	-0.399837	-2.705847
C	-0.607237	0.290489	2.172406
H	-0.403903	-0.721893	2.540300
H	0.182868	0.952709	2.558080
C	-1.984948	0.750683	2.637285
H	-2.765978	0.112992	2.213271
H	-2.079498	0.706403	3.731292
H	-2.194852	1.787563	2.343963
N	1.348973	-0.062212	0.009185
C	2.586622	-0.807789	0.097875
C	2.272788	-2.280109	0.400376
H	1.656434	-2.713196	-0.392828
H	3.199334	-2.858905	0.476629
H	1.728694	-2.369982	1.344805
C	3.316699	-0.677946	-1.247746
H	3.522207	0.371664	-1.478193
H	4.269766	-1.215895	-1.210241
H	2.714476	-1.101187	-2.057034
C	3.427604	-0.191143	1.226325
H	4.377437	-0.727356	1.323830
H	3.642343	0.860923	1.017528
H	2.895583	-0.251670	2.179715

E = -598.103554512
G = -597.823286

Mo-N-1'-SBP

O	1.906766	-1.087654	-0.137966
C	0.653636	1.228318	-1.796768
C	0.519713	0.319679	2.089131
C	0.146030	2.118010	0.771253
C	-0.206597	1.646197	2.173362
H	1.190455	2.471123	0.775869
Si	3.148486	-2.148575	0.232516
H	3.761152	-1.789294	1.548654
H	2.623693	-3.547457	0.302554
H	4.190856	-2.068552	-0.835587
H	0.086413	2.318416	2.998201
H	-1.288719	1.483719	2.248184
H	0.698937	0.340029	-2.462759
H	-0.223561	1.801513	-2.101175
C	1.935550	2.042433	-1.921859
H	2.120660	2.332216	-2.964902
H	1.884360	2.965685	-1.336248
H	2.815721	1.483845	-1.583427
N	-1.274495	-0.388376	-0.153882
C	-2.543807	-1.070027	-0.261466
Mo	0.378122	0.052531	-0.045262
C	-2.710496	-1.997383	0.951969
H	-2.672983	-1.424207	1.882762
H	-3.673911	-2.515947	0.903258
H	-1.914243	-2.747597	0.975579
C	-2.558262	-1.884419	-1.564618
H	-3.518768	-2.397878	-1.679291
H	-2.411416	-1.230552	-2.429376
H	-1.763181	-2.636352	-1.559201
C	-3.658278	-0.011904	-0.282597
H	-3.532681	0.662491	-1.134447
H	-4.638210	-0.494384	-0.363319
H	-3.639465	0.584237	0.634017
H	1.590927	0.418802	2.309699
H	0.114101	-0.534713	2.644017
C	-0.758682	3.179128	0.170444
H	-1.778501	2.801617	0.039032
H	-0.816036	4.049877	0.841094
H	-0.411037	3.546805	-0.799626

E = -598.138645810
G = -597.860130

Mo-N-1'-TSB

C	0.010196	-1.624651	-1.605572
C	1.996822	-1.608818	-0.296059
C	0.733732	-2.260124	-0.516401
H	2.461909	-1.239219	-1.211603
H	0.473164	-3.245865	-0.118393
H	-0.095004	-1.716324	0.532849
O	1.302607	1.409566	-0.594805
Si	2.804535	2.073846	-0.896480
H	3.496813	2.391604	0.392679
H	3.664003	1.131498	-1.682112
H	2.642221	3.337790	-1.679873
H	0.603990	-1.308687	-2.464646
Mo	0.204461	-0.090847	-0.067027
C	2.959800	-2.086550	0.761112
H	3.615584	-2.885666	0.386562
H	3.610557	-1.279560	1.116274
H	2.435882	-2.489089	1.635224
H	-0.983870	-1.982027	-1.856864
C	0.369656	-0.263735	2.099655
H	-0.470963	-0.794709	2.553216
H	1.281398	-0.814185	2.349882
C	0.439238	1.166645	2.641639
H	0.505003	1.155539	3.738943
H	1.312885	1.710791	2.269799
H	-0.449210	1.747967	2.373588
N	-1.489580	0.313889	-0.083857
C	-2.928462	0.239976	-0.162160

C	-3.345459	0.558582	-1.607823
H	-2.925493	-0.174560	-2.302623
H	-4.436632	0.537836	-1.700697
H	-2.989212	1.550635	-1.899665
C	-3.503036	1.296322	0.797431
H	-4.597482	1.291226	0.754425
H	-3.197540	1.088912	1.827275
H	-3.148130	2.294822	0.526988
C	-3.409526	-1.161485	0.243627
H	-4.502848	-1.218084	0.208914
H	-3.006295	-1.921383	-0.432244
H	-3.083119	-1.398269	1.260679

E = -598.099920567
G = -597.824099

Mo-N-1'-B

C	0.896109	-1.724607	-0.692093
C	3.395457	-1.433595	-0.535658
C	2.230527	-1.920374	-0.076565
H	0.967990	-1.426336	-1.752323
H	2.242533	-2.492982	0.853093
H	0.268222	-2.613471	-0.612929
H	0.148263	-1.163024	1.308293
O	1.060087	1.415825	-0.581461
Si	2.302317	2.520448	-0.769387
H	3.233670	2.048887	-1.840094
H	1.736884	3.846709	-1.166948
H	3.063942	2.679883	0.508326
C	-0.195654	0.828056	2.118826
H	-0.568322	1.840924	1.881466
H	0.852141	0.939114	2.440014
C	-1.026535	0.203457	3.227146
H	-2.067223	0.072248	2.914396
H	-0.641589	-0.784794	3.498215
H	-1.026479	0.824661	4.133176
H	3.391828	-0.855312	-1.461534
C	4.726141	-1.636816	0.118874
H	5.424646	-2.158212	-0.548442
H	5.198847	-0.679840	0.375403
H	4.635405	-2.224944	1.037376
N	-1.685546	-0.262964	-0.196484
C	-3.056127	-0.276759	-0.653320
Mo	-0.036350	0.020517	0.150321
C	-3.063237	-0.390689	-2.186043
H	-2.555238	-1.304604	-2.507540
H	-4.093221	-0.419722	-2.556766
H	-2.556814	0.466399	-2.640283
C	-3.754958	-1.491620	-0.023382
H	-3.733766	-1.423814	1.067699
H	-4.798904	-1.539298	-0.350860
H	-3.254402	-2.418013	-0.318512
C	-3.738684	1.026320	-0.210096
H	-3.236167	1.894187	-0.647801
H	-4.784967	1.032969	-0.533484
H	-3.713138	1.124329	0.878933

E = -598.128817621
G = -597.857163

Mo-N-1'-TSC

Mo	0.026666	0.171646	0.380157
C	1.258278	-1.005512	-1.039737
C	3.724195	-0.574619	-1.296490
C	2.691964	-1.324394	-0.878015
H	1.111122	-0.284731	-1.862142
H	2.921900	-2.277609	-0.394676
H	0.694197	-1.908275	-1.279790
H	0.724428	-1.159546	1.304396
O	0.168950	2.059091	-0.092996
Si	-0.662395	3.268481	-0.879449
H	0.228475	3.907678	-1.898734
H	-1.885728	2.751903	-1.578984
H	-1.091139	4.310982	0.106201
C	-0.880544	0.200018	2.353713
H	-1.682539	0.929493	2.161406
H	-0.174038	0.686085	3.037980
C	-1.456232	-1.055048	2.988854
H	-2.197609	-1.526902	2.336951
H	-0.678298	-1.802813	3.182944
H	-1.946728	-0.837253	3.947694
C	1.956987	-0.484650	1.973396
H	2.616413	-1.246938	1.568740
H	1.571774	-0.691572	2.969030
C	2.094249	0.823149	1.531796
H	1.724959	1.657788	2.117846
H	2.768320	1.050888	0.712811
H	3.510801	0.371259	-1.799344
C	5.168554	-0.936779	-1.145287
H	5.667967	-1.008723	-2.120152
H	5.715579	-0.176828	-0.572223
H	5.290402	-1.896688	-0.633432
N	-1.396547	-0.479665	-0.342106
C	-2.549770	-1.064999	-0.978154
C	-2.541212	-2.584148	-0.744710
H	-3.412668	-3.045269	-1.221427
H	-1.639055	-3.035820	-1.167102
H	-2.568804	-2.812548	0.324173
C	-2.475781	-0.755586	-2.483421
H	-2.473982	0.324347	-2.655099
H	-1.566917	-1.177857	-2.921752
H	-3.340031	-1.188707	-2.997968
C	-3.811809	-0.431857	-0.368957
H	-3.869857	-0.633893	0.704251
H	-3.808850	0.651582	-0.518090
H	-4.705576	-0.846438	-0.847024

E = -676.662670067
G = -676.336511

Mo-N-1'-C

C	-0.987508	0.266804	-1.614242
C	-3.454848	-0.229051	-1.541281
C	-2.420469	0.627140	-1.501098
H	-0.876278	-0.790915	-1.908391
H	-2.651226	1.688743	-1.387782
H	-0.461444	0.887240	-2.343087
H	2.182351	2.620526	-0.676079
O	-1.199016	-0.984607	1.127372
Si	-2.642924	-1.443763	1.853526
H	-3.543207	-0.268560	2.053138
H	-3.327389	-2.463905	1.004482
H	-2.324239	-2.047033	3.184080
C	0.715217	1.096738	2.102565
H	0.822487	0.144627	2.659548
H	-0.159611	1.616139	2.520092
C	1.974970	1.926863	2.275217
H	2.857107	1.387289	1.918891
H	1.920416	2.871127	1.724983
H	2.143020	2.181490	3.330349
C	1.203445	2.777911	-1.139600

H	1.207623	2.237316	-2.092218
H	1.116041	3.848484	-1.374148
C	0.068020	2.321788	-0.221794
H	0.092386	2.924015	0.691706
H	-0.889494	2.548915	-0.701905
H	-3.248994	-1.292815	-1.675889
C	-4.896800	0.162501	-1.444694
H	-5.451124	-0.127066	-2.346987
H	-5.395025	-0.334480	-0.602190
H	-5.010861	1.243021	-1.312425
Mo	0.077090	0.144135	0.289416
N	1.588600	-0.379378	-0.319778
C	2.694996	-1.208952	-0.746621
C	2.864308	-1.019882	-2.262592
H	3.704066	-1.622520	-2.624481
H	1.960868	-1.331395	-2.794868
H	3.059789	0.029384	-2.499369
C	3.960725	-0.744699	-0.009756
H	4.165157	0.308481	-0.220680
H	3.846250	-0.867041	1.071225
H	4.821947	-1.338178	-0.334404
C	2.395950	-2.679688	-0.418901
H	2.251641	-2.813801	0.657558
H	1.488775	-3.013347	-0.931988
H	3.226011	-3.319047	-0.737758

E = -676.710023281
G = -676.382200

Mo-O-1-I

Mo	0.219775	-0.165160	0.317915
O	-1.512804	0.067025	-0.408604
C	1.430161	-0.775020	-0.987383
H	1.112590	-0.408830	-1.977945
Si	-3.173136	-0.225741	-0.367840
H	-3.877540	1.053941	-0.672909
H	-3.509683	-1.250293	-1.400151
H	-3.581081	-0.718947	0.982357
C	2.625872	-1.672119	-0.992982
H	3.506217	-1.132567	-1.368491
H	2.856664	-2.045997	0.007303
H	2.473436	-2.530531	-1.660776
O	0.620630	-1.000719	1.712801
C	1.015556	1.791713	0.608719
H	0.313790	2.261151	1.319490
H	1.972980	1.696480	1.133383
C	1.167429	2.654188	-0.642804
H	0.236672	2.716999	-1.218654
H	1.453761	3.682808	-0.386646
H	1.938843	2.249856	-1.306514

E = -382.232207176
G = -382.124728

Mo-O-1-Ianti

Mo	-0.231183	0.028572	0.549753
O	1.358750	0.014492	-0.472059
C	-1.404359	1.409807	0.009392
H	-2.050474	1.873934	0.760117
Si	3.044721	-0.056317	-0.539080
H	3.426431	-1.043403	-1.590883
H	3.567206	1.295697	-0.894777
H	3.598832	-0.481663	0.781394
C	-1.476970	2.025871	-1.359963
H	-1.205115	3.089284	-1.321149
H	-0.822524	1.538488	-2.089064
H	-2.503942	1.974458	-1.745566
O	-0.350000	-0.035459	2.218735
C	-1.369149	-1.652556	-0.108339
H	-0.709200	-2.511489	0.103422
H	-2.237462	-1.756204	0.551633
C	-1.799871	-1.656467	-1.573594
H	-0.956980	-1.491336	-2.254920
H	-2.251353	-2.617553	-1.853051
H	-2.539717	-0.874011	-1.768034

E = -382.229983487
G = -382.121933

Mo-O-1-TSrot1

Mo	0.207182	-0.100962	0.256085
O	-1.421850	0.363483	-0.548362
C	1.022602	-1.509743	-0.703852
H	0.422356	-2.394051	-0.944179
Si	-3.066488	-0.002670	-0.411346
H	-3.790732	0.881294	-1.370164
H	-3.306243	-1.434820	-0.763463
H	-3.519491	0.260089	0.985898
C	2.519668	-1.721118	-0.735692
H	2.845238	-1.937893	-1.762524
H	3.093022	-0.844876	-0.409497
H	2.827020	-2.568317	-0.107073
O	-0.215338	-0.649852	1.809253
C	1.427383	1.574723	0.572999
H	0.969233	2.248090	1.306417
H	2.351389	1.184987	1.032475
C	1.709214	2.281659	-0.756985
H	0.801447	2.731292	-1.172148
H	2.441703	3.087495	-0.623905
H	2.118532	1.602341	-1.514514

E = -382.186342943
G = -382.080724

Mo-O-1-TSrot2

Mo	-0.310337	0.000371	0.316498
O	1.359402	-0.539885	-0.359399
C	-0.976117	1.496979	-0.528444
H	-1.955737	0.949559	-0.279977
Si	3.020516	-0.242848	-0.368502
H	3.670089	-1.343342	-1.138827
H	3.300326	1.067550	-1.029730
H	3.534561	-0.221875	1.032677
C	-1.089702	2.951608	-0.798966
H	-1.514903	3.507204	0.047981
H	-0.097849	3.363059	-1.010514
H	-1.714115	3.148201	-1.680084
O	-0.147766	0.332876	1.974128
C	-1.695897	-1.605835	0.236642
H	-1.227013	-2.408301	0.821903
H	-2.630811	-1.343255	0.746801
C	-1.947811	-2.040990	-1.209250
H	-1.017193	-2.277774	-1.737233
H	-2.570777	-2.943917	-1.238501
H	-2.465588	-1.267331	-1.786106

E = -382.194603053
G = -382.089227

Mo-O-1-II

Mo	0.330748	0.037474	0.290644
O	-1.423931	-0.050066	-0.483375
C	-0.258462	-2.855428	0.381468
C	1.715385	0.237931	-0.984380
C	0.530853	-2.732440	-0.696489
H	1.306836	0.481184	-1.978928
H	0.119045	-2.571651	-1.689141
H	1.608629	-2.844544	-0.626030
H	-1.339933	-2.792801	0.302619
C	3.205479	0.126739	-0.936403
H	3.664065	1.091661	-1.193731
H	3.563985	-0.167060	0.052660
H	3.573769	-0.598059	-1.675647
H	0.154947	-3.050847	1.366333
O	1.065062	-0.441492	1.724504
C	0.101651	2.114060	0.764082
H	-0.744178	2.140497	1.471091
H	0.988998	2.425264	1.325993
C	-0.152281	3.062777	-0.403819
H	-1.008433	2.746604	-1.009915
H	-0.360134	4.083913	-0.056800
H	0.717791	3.112056	-1.068612
Si	-3.094253	-0.080955	-0.364482
H	-3.680776	0.103255	-1.725752
H	-3.549323	-1.398146	0.185497
H	-3.571985	1.008782	0.540304

E = -460.792792127
G = -460.637465

Mo-O-1-TSII

Mo	-0.340844	0.140048	-0.342257
O	1.318319	-0.505865	0.480047
C	-0.605264	-2.090860	-0.688627
C	-1.613764	0.153409	1.127526
C	-1.460122	-1.911984	0.427769
H	-1.125105	0.019149	2.100524
H	-1.124788	-2.260436	1.400261
H	-2.534283	-1.919697	0.271120
H	0.353490	-2.574813	-0.539170
C	-3.072610	0.480012	1.199942
H	-3.180797	1.473915	1.652948
H	-3.534522	0.511135	0.210561
H	-3.625548	-0.220340	1.839308
H	-1.053226	-2.192290	-1.672642
O	-1.295042	0.424406	-1.700824
C	0.783734	1.968901	-0.614280
H	1.552144	1.717792	-1.364162
H	0.103074	2.682457	-1.094719
C	1.430304	2.596072	0.618478
H	2.092177	1.892875	1.133332
H	2.028991	3.479002	0.356406
H	0.675943	2.923665	1.343841
Si	2.897417	-1.024676	0.362959
H	3.474372	-1.155569	1.736538
H	2.958247	-2.366176	-0.308281
H	3.731553	-0.068855	-0.431143

E = -460.784613965
G = -460.622005

Mo-O-1-TBP

O	1.328773	-0.712180	-0.061698
C	-1.058309	-1.181024	-1.611301
H	-0.307641	-1.807486	-2.091088
C	-1.207225	-0.907831	1.061304
C	-1.562427	-1.765583	-0.226752
H	-0.442735	-1.408831	1.656732
H	-1.115705	-2.752953	-0.098595
H	-2.651174	-1.832903	-0.273405
Si	2.837368	-1.280718	0.358568
H	3.876227	-0.217687	0.174292
H	2.849064	-1.714321	1.792751
H	3.195202	-2.454624	-0.498622
Mo	-0.319663	0.300403	-0.384989
C	-2.387030	-0.451081	1.889078
H	-2.056094	0.201568	2.703211
H	-3.107112	0.105698	1.283351
H	-2.901374	-1.308079	2.345783
H	-1.871263	-0.910078	-2.281056
O	-1.668589	1.323675	-0.460343
C	0.972274	2.002838	-0.507860
H	1.942651	1.669642	-0.890363
H	0.524136	2.711940	-1.212293
C	1.092233	2.606345	0.887702
H	1.506378	1.893041	1.610818
H	1.761979	3.476777	0.887039
H	0.121584	2.947458	1.264337

E = -460.801150538
G = -460.638054

Mo-O-1-TSIII

Mo	0.284724	-0.448102	-0.277126
O	-0.999587	1.025513	-0.271074
C	2.052775	1.287914	-0.635360
C	1.227323	-0.307450	-1.958555
C	1.598203	1.225708	0.698514
H	0.855379	0.338507	-2.756123
H	2.115014	-0.882490	-2.218393
Si	-2.444803	1.769356	0.099233
H	-2.499199	3.084028	-0.614273
H	-3.617055	0.942945	-0.328678
H	-2.550117	2.020526	1.572686
H	0.833807	1.947402	0.974022
H	1.653475	2.054899	-1.290563
C	2.483515	0.730730	1.815403
H	1.899850	0.316870	2.641906
H	3.171140	-0.046401	1.472764
H	3.076461	1.565104	2.212397
H	3.054312	0.935885	-0.868312
O	1.161395	-1.581012	0.604575
C	-1.466275	-1.704109	-0.311486
H	-2.201494	-1.265039	-0.996524
H	-1.155446	-2.670453	-0.728739
C	-2.061701	-1.898465	1.083041
H	-2.337273	-0.946152	1.554887
H	-2.974819	-2.507778	1.055088
H	-1.352690	-2.400526	1.750510

E = -460.780339075
G = -460.618153

Mo-O-1-IV

Mo	-0.363571	-0.576970	-0.229926
O	-0.472470	1.294033	-0.514493
C	2.856110	0.390262	0.385025
C	-0.169377	-1.592008	-1.805879

C	2.714838	0.215149	-0.934997
H	-0.391758	-1.134950	-2.776329
H	0.213673	-2.611368	-1.862269
Si	-0.449661	2.902498	-0.022688
H	3.036530	-0.703015	-1.420698
H	2.306956	0.991668	-1.574952
H	-1.842780	3.437798	-0.048708
H	0.104434	3.019863	1.361209
H	0.407241	3.677746	-0.968388
C	3.434081	-0.610752	1.332499
H	2.680664	-0.923347	2.064529
H	3.785574	-1.503629	0.808160
H	4.274963	-0.180624	1.889593
H	2.534698	1.336044	0.824924
O	0.267186	-1.481111	1.032963
C	-2.443219	-0.941261	0.094109
H	-2.978306	-0.503743	-0.759436
H	-2.633048	-2.018341	0.065209
C	-2.916585	-0.336449	1.417049
H	-2.752908	0.746715	1.461625
H	-3.992810	-0.499614	1.563198
H	-2.400717	-0.786457	2.272257

E = -460.793974863
G = -460.641355

Mo-O-1-V

Mo	-0.270034	-0.320933	0.074858
O	1.461726	0.268408	-0.373190
C	-1.029555	-1.393257	-1.272077
H	-0.699180	-1.255230	-2.307345
H	-1.726624	-2.217176	-1.119325
Si	3.100822	0.466916	-0.009601
H	3.487131	1.860266	-0.375798
H	3.334367	0.237714	1.447457
H	3.888323	-0.513384	-0.812314
O	-0.737058	-0.994331	1.532686
C	-1.518758	1.387751	-0.115672
H	-1.172855	2.056433	0.690423
H	-1.223377	1.854671	-1.066884
C	-3.032138	1.211179	-0.051511
H	-3.336404	0.712199	0.873662
H	-3.548707	2.179135	-0.092350
H	-3.387400	0.601083	-0.887545

E = -342.924420572
G = -342.842699

Mo-O-1-TSA

O	-1.561214	0.099890	-0.469881
C	0.060858	-2.033228	-0.332447
H	-0.651947	-2.253574	-1.121921
C	1.885525	-0.032834	-0.821918
C	1.470522	-1.647052	-0.818760
H	1.642239	0.358856	-1.815841
H	1.545464	-1.899638	-1.876951
H	2.248269	-2.142809	-0.237326
Si	-3.053250	-0.588614	-0.251964
H	-3.713552	-0.099652	1.002899
H	-3.918682	-0.223203	-1.418351
H	-2.994644	-2.089681	-0.164845
Mo	0.254928	-0.049991	0.371741
C	3.325896	0.212331	-0.432267
H	3.528019	1.287838	-0.445739
H	3.542777	-0.155083	0.574813
H	4.026022	-0.264943	-1.130480
H	0.060822	-2.775902	0.463918
O	0.587147	-0.252218	1.997586
C	-0.215864	2.070172	0.468146
H	-1.094062	2.156233	1.119422
H	0.649609	2.478460	1.013867
C	-0.445536	2.798357	-0.847018
H	-1.254418	2.324877	-1.410087
H	-0.725955	3.846697	-0.678290
H	0.452712	2.803879	-1.476761

E = -460.779657617
G = -460.615024

Mo-O-1-SBP

O	-1.829232	0.103295	0.239722
C	0.129972	-1.831410	-0.764834
C	1.762679	-0.283068	-0.857568
C	1.624081	-1.792370	-1.012255
H	1.415488	0.197528	-1.783942
Si	-3.313172	-0.047838	-0.544891
H	-4.087553	-1.160717	0.078333
H	-4.050985	1.239750	-0.388415
H	-3.101351	-0.333183	-1.996908
H	1.975749	-2.215030	-1.967100
H	2.159499	-2.305905	-0.205007
H	-0.446089	-1.590484	-1.666665
Mo	0.023577	-0.119995	0.527880
C	3.138323	0.232906	-0.469934
H	3.887295	-0.128033	-1.190024
H	3.203691	1.324858	-0.460428
H	3.436593	-0.131653	0.519040
H	-0.304698	-2.707899	-0.269427
O	0.689093	-0.736126	1.932139
C	0.668838	1.898111	0.436503
H	1.644148	2.023777	0.913353
H	-0.087386	2.241940	1.173572
C	0.556503	2.701537	-0.850582
H	0.645062	3.776896	-0.649623
H	1.348157	2.439430	-1.558692
H	-0.404728	2.546688	-1.353423

E = -460.817951704
G = -460.654646

Mo-O-1-TSB

C	2.106854	-0.334063	-1.357680
C	1.719010	1.330020	0.253472
C	2.447927	0.136755	-0.024580
H	1.562655	1.987821	-0.601425
H	3.278372	-0.238391	0.579819
H	1.638547	-0.905022	0.637435
O	-1.047504	0.958351	0.280933
Si	-2.443838	1.646254	-0.351812
H	-2.083509	2.711297	-1.339367
H	-3.300287	0.622610	-1.023431
H	-3.193752	2.266239	0.782892
H	2.048740	0.412487	-2.148762
Mo	0.208997	-0.385147	-0.251994
C	1.655958	1.967724	1.611669
H	2.411948	2.755451	1.729105
H	0.674104	2.424349	1.775482
H	1.818725	1.234454	2.410060
H	2.459087	-1.310156	-1.686046
O	-0.474292	-1.161036	-1.599119

C	-0.217349	-1.867745	1.250944
H	0.403005	-2.759992	1.102452
H	0.079317	-1.442651	2.221317
C	-1.701119	-2.234335	1.244549
H	-1.925224	-2.945439	2.051333
H	-2.336575	-1.356493	1.396179
H	-1.992617	-2.696575	0.297318

E = -460.769502348
G = -460.610335

Mo-O-1-TSB$_{transX}$

Mo	0.170297	-0.084286	-0.221983
O	-1.455751	-1.106738	-0.310697
C	1.307766	0.482737	1.658392
C	0.640893	2.080222	0.076240
C	0.411324	1.565063	1.397800
H	1.685082	2.105406	-0.240487
Si	-3.006835	-0.881465	0.292517
H	-3.862992	-2.010431	-0.180816
H	-2.995394	-0.867488	1.790519
H	-3.576308	0.415651	-0.191283
H	-0.278590	1.992164	2.125043
H	-0.920978	0.785855	0.884898
H	2.335700	0.619456	1.329625
C	-0.278821	3.059790	-0.586016
H	-0.095081	4.085755	-0.239275
H	-0.142573	3.042130	-1.671111
H	-1.328528	2.824129	-0.369784
H	1.191899	-0.129084	2.549478
O	0.672488	0.148808	-1.825583
C	1.333509	-1.863119	0.167996
H	1.056108	-2.254453	1.153124
H	0.870225	-2.511258	-0.588182
C	2.843099	-1.832365	-0.018816
H	3.259323	-2.846753	0.039337
H	3.115581	-1.422056	-0.996187
H	3.349224	-1.239019	0.749805

E = -460.769216425
G = -460.607750

Mo-O-1-B

C	1.302247	-1.146181	-1.051133
C	3.224322	0.000405	0.088358
C	2.406137	-1.051082	-0.067294
H	3.088930	0.867650	-0.560540
H	2.535375	-1.914235	0.588227
H	0.028917	-1.841212	0.574495
O	-0.257607	1.270438	0.064096
Si	-0.419609	2.913139	-0.280692
H	0.918990	3.451596	-0.662649
H	-1.383298	3.115483	-1.404451
H	-0.917443	3.606649	0.943210
H	1.408692	-0.410152	-1.865987
Mo	-0.613473	-0.557296	-0.267742
C	4.333045	0.084186	1.089114
H	5.303819	0.231506	0.598665
H	4.194633	0.936711	1.766568
H	4.395924	-0.823637	1.696791
H	1.214860	-2.144798	-1.486393
O	-1.606745	-1.205557	-1.441228
C	-1.748986	-1.044569	1.479323
H	-1.984303	-2.109128	1.547814
H	-1.128035	-0.796557	2.350154
C	-3.022429	-0.196742	1.430608
H	-3.629399	-0.372638	2.329302
H	-2.812255	0.877967	1.396788
H	-3.646204	-0.447871	0.566045

E = -460.806459737
G = -460.648909

Mo-O-1-TSC

C	-1.232589	1.243643	0.762911
C	-3.615150	0.530646	0.457684
C	-2.430465	0.443897	1.085853
H	-1.471111	2.081257	0.104247
H	-2.317643	-0.287316	1.887034
H	-0.740589	1.628786	1.668225
H	-0.761042	0.166086	-1.282242
O	2.289451	0.430185	0.018261
Si	3.503572	-0.146460	1.039361
H	3.480613	-1.639643	1.120973
H	4.810740	0.293839	0.463426
H	3.344518	0.431172	2.408235
C	0.413971	-1.699282	-1.319916
H	1.231259	-2.300917	-0.896381
H	0.743498	-1.346598	-2.307509
C	-0.858087	-2.528773	-1.428622
H	-1.192791	-2.860915	-0.441216
H	-1.676763	-1.956832	-1.878441
H	-0.694936	-3.422920	-2.044327
C	-0.267064	1.488157	-2.106678
H	-1.303534	1.815182	-2.082349
H	0.007809	0.897924	-2.978810
C	0.708275	2.151060	-1.394617
H	1.755631	2.024085	-1.636868
H	0.456981	2.950631	-0.705181
H	-3.731308	1.262284	-0.345081
C	-4.819467	-0.296156	0.780307
H	-5.668393	0.333090	1.077940
H	-5.153166	-0.875479	-0.090457
H	-4.616614	-0.997860	1.594859
Mo	0.414016	-0.007603	-0.011232
O	0.168253	-0.908340	1.389625

E = -539.337166691
G = -539.128099

Mo-O-1-C

C	0.799720	-1.533365	-0.755385
C	3.177473	-0.836471	-0.349243
C	2.028498	-1.399041	0.060914
H	3.232517	-0.438452	-1.364290
H	1.996218	-1.811836	1.070916
O	0.390044	1.478529	-0.396959
Si	1.582398	2.400938	0.367914
H	2.814884	2.382552	-0.470276
H	1.065265	3.796853	0.481081
H	1.875843	1.865932	1.730696
H	0.988636	-1.247576	-1.804353
Mo	-0.723311	-0.037057	-0.368512
C	4.426007	-0.742661	0.470702
H	5.253427	-1.284299	-0.005341
H	4.758817	0.297330	0.579843
H	4.282456	-1.159137	1.472374
H	0.385952	-2.544371	-0.735826
O	-1.749663	-0.434542	-1.622212
C	-2.183946	0.743738	0.999082

H	-2.934415	0.019207	1.320745
H	-1.634920	1.070508	1.892577
C	-2.829914	1.924332	0.269880
H	-3.467618	2.489385	0.963819
H	-2.095900	2.631873	-0.131522
H	-3.459644	1.589065	-0.559738
C	-0.987532	-1.578407	1.221372
H	-0.048993	-2.099495	1.428138
H	-1.292781	-1.109058	2.162542
C	-2.041089	-2.611103	0.806744
H	-2.173723	-3.367928	1.591374
H	-3.018674	-2.152808	0.624254
H	-1.760220	-3.138521	-0.111347

E = -539.393896253
G = -539.179493

Mo-O-2-I

Mo	-1.100624	-0.246217	-0.227882
O	0.578631	0.368276	0.423052
C	-2.295891	-0.469501	1.208535
H	-2.023001	0.217663	2.026471
C	-3.446300	-1.379107	1.496636
H	-4.361524	-0.795519	1.666985
H	-3.632378	-2.072291	0.672991
H	-3.268897	-1.961348	2.410781
O	-1.427365	-1.509841	-1.278958
C	1.912792	0.158728	0.268410
C	2.797014	1.088254	0.825115
C	2.404750	-0.956317	-0.419455
C	4.169297	0.900675	0.685959
H	2.393394	1.943566	1.357805
C	3.780024	-1.132156	-0.549168
H	1.710414	-1.678179	-0.843398
C	4.667596	-0.207241	0.000428
H	4.852861	1.625897	1.118809
H	4.157476	-2.000229	-1.082444
H	5.738980	-0.350109	-0.103195
C	-2.001765	1.454313	-1.143160
H	-1.311487	1.706153	-1.966873
H	-2.941096	1.135299	-1.608740
C	-2.226604	2.666273	-0.241734
H	-1.312262	2.966838	0.282856
H	-2.563872	3.536794	-0.819855
H	-2.987991	2.455557	0.516698

E = -608.064062834
G = -607.893620

Mo-O-2-Ianti

Mo	-1.144418	-0.542924	-0.040984
O	0.473198	0.429091	0.174597
C	-2.359733	-0.131721	1.346942
H	-3.074377	-0.897571	1.661859
C	-2.395691	1.141354	2.144738
H	-2.192770	0.938091	3.204804
H	-1.671652	1.886808	1.801896
H	-3.394345	1.595184	2.092774
O	-1.349702	-2.176060	-0.353079
C	1.822877	0.278284	0.100656
C	2.617341	1.428867	0.099022
C	2.415063	-0.987796	0.034618
C	4.002117	1.307586	0.025278
H	2.135890	2.400124	0.154477
C	3.801556	-1.094003	-0.037202
H	1.789270	-1.877209	0.042671
C	4.600416	0.049378	-0.042990
H	4.616419	2.203756	0.022871
H	4.258027	-2.078596	-0.087598
H	5.681138	-0.039933	-0.098534
C	-2.146742	0.409348	-1.665618
H	-1.448590	0.274648	-2.509969
H	-3.042603	-0.174505	-1.903714
C	-2.493415	1.885904	-1.488074
H	-1.625571	2.482120	-1.182779
H	-2.865637	2.321818	-2.424636
H	-3.270345	2.020610	-0.729180

E = -608.062083856
G = -607.891053

Mo-O-2-TSrot1

Mo	-1.131241	-0.267087	-0.128752
O	0.505286	-0.012166	0.770935
C	-2.404139	-0.786308	1.171752
H	-2.070055	-1.601065	1.826971
C	-3.899560	-0.602919	1.090313
H	-4.287460	-0.287806	2.068754
H	-4.203303	0.166620	0.371380
H	-4.414848	-1.535084	0.820383
O	-0.845936	-1.537231	-1.222616
C	1.827829	-0.017355	0.433107
C	2.713280	0.648181	1.286742
C	2.298203	-0.678728	-0.704685
C	4.073824	0.651569	0.993592
H	2.321289	1.146373	2.167950
C	3.664196	-0.666352	-0.981072
H	1.597639	-1.199792	-1.350535
C	4.556677	-0.003498	-0.139689
H	4.760143	1.168881	1.658547
H	4.029904	-1.182762	-1.864519
H	5.619218	0.001497	-0.363676
C	-1.719243	1.368302	-1.301073
H	-1.074769	1.476851	-2.180924
H	-2.720071	1.088297	-1.676165
C	-1.771323	2.652002	-0.465748
H	-0.769154	2.974245	-0.165866
H	-2.221401	3.473280	-1.037217
H	-2.368294	2.533942	0.446489

E = -608.018009559
G = -607.849696

Mo-O-2-TSrot2

Mo	1.202044	0.080001	-0.293294
O	-0.476822	-0.633620	0.181753
C	1.831681	1.318932	0.918132
H	2.827990	0.858865	0.582185
C	1.903829	2.650178	1.568818
H	2.358952	3.411706	0.920974
H	0.895282	2.985347	1.829910
H	2.482364	2.610673	2.500969
O	1.066984	0.823664	-1.816326
C	-1.808917	-0.367839	0.124507
C	-2.651417	-0.999182	1.044209
C	-2.333135	0.494941	-0.843359
C	-4.022368	-0.762374	0.991044
H	-2.219783	-1.666728	1.783432
C	-3.706857	0.720012	-0.883206
H	-1.662552	0.973635	-1.551508

C	-4.556749	0.096319	0.030376
H	-4.675872	-1.253704	1.706798
H	-4.113471	1.390269	-1.635671
H	-5.626676	0.278406	-0.005754
C	2.596287	-1.491670	-0.583876
H	2.155721	-2.114583	-1.373777
H	3.548127	-1.107794	-0.971014
C	2.793412	-2.283930	0.711034
H	1.844182	-2.644190	1.123698
H	3.419192	-3.167368	0.531737
H	3.284806	-1.687232	1.486885

E = -608.026167208
G = -607.858173

Mo-O-2-II

Mo	-1.134666	0.003315	-0.277826
O	0.597580	0.251199	0.539062
C	-0.023400	-2.653978	-0.366789
C	-2.511466	-0.006745	1.022409
C	-0.885440	-2.709623	0.662971
H	-2.130253	0.314181	2.005205
H	-0.562671	-2.533502	1.685507
H	-1.922752	-2.996987	0.519544
H	1.028504	-2.427102	-0.217305
C	-3.966934	-0.344072	0.996889
H	-4.563834	0.538774	1.264963
H	-4.291542	-0.688803	0.012661
H	-4.207302	-1.117357	1.739835
H	-0.342736	-2.879911	-1.379876
O	-1.819498	-0.588786	-1.693981
C	1.923994	0.168297	0.317242
C	2.794077	0.182446	1.416457
C	2.449048	0.069365	-0.979717
C	4.167777	0.092720	1.215281
H	2.373616	0.265513	2.414048
C	3.826644	-0.018293	-1.166623
H	1.774796	0.073016	-1.832832
C	4.692600	-0.009304	-0.073909
H	4.833774	0.103981	2.073978
H	4.223105	-0.091720	-2.175767
H	5.765688	-0.077615	-0.225041
C	-1.229773	2.085540	-0.777350
H	-0.426784	2.219660	-1.521529
H	-2.175343	2.262153	-1.301723
C	-1.055382	3.075120	0.370971
H	-0.130311	2.890766	0.927437
H	-1.018477	4.111515	0.009314
H	-1.886649	3.006055	1.082626

E = -686.626877145
G = -686.407277

Mo-O-2-TSII

Mo	-1.166161	0.115140	-0.324815
O	0.611325	0.102734	0.506470
C	-0.571834	-2.048437	-0.732095
C	-2.350605	-0.377997	1.134785
C	-1.440381	-2.238475	0.368067
H	-1.847270	-0.353931	2.109520
H	-1.011256	-2.465597	1.339639
H	-2.438299	-2.627949	0.192093
H	0.498347	-2.147972	-0.580522
C	-3.826237	-0.616861	1.198929
H	-4.295394	0.250195	1.681790
H	-4.266106	-0.725512	0.205092
H	-4.080577	-1.493410	1.809022
H	-0.942196	-2.271286	-1.728333
O	-2.161468	0.053719	-1.680814
C	-0.805100	2.237895	-0.525972
H	-0.061701	2.321952	-1.336111
H	-1.735401	2.670107	-0.916098
C	-0.330601	3.000781	0.708235
H	0.599908	2.586046	1.106448
H	-0.150831	4.060566	0.482253
H	-1.076108	2.966028	1.511796
C	1.926026	-0.041800	0.299740
C	2.782000	-0.182244	1.404735
C	2.470472	-0.061740	-0.995076
C	4.149561	-0.343285	1.211025
H	2.353548	-0.159238	2.402356
C	3.842288	-0.224121	-1.173565
H	1.811996	0.061385	-1.851271
C	4.689892	-0.367181	-0.076097
H	4.800262	-0.450258	2.075100
H	4.249331	-0.235595	-2.181338
H	5.758764	-0.492228	-0.220719

E = -686.620099628
G = -686.395419

Mo-O-2-TBP

O	-0.654642	-0.130346	-0.337702
C	0.927482	-0.560003	1.848769
H	-0.108271	-0.633682	2.175082
C	1.811395	-1.662316	-0.440960
C	1.445817	-1.843601	1.111387
H	1.055712	-2.155424	-1.058189
H	0.670884	-2.609856	1.169692
H	2.362088	-2.176461	1.602979
Mo	1.235430	0.273476	-0.036267
C	3.221627	-2.063412	-0.817499
H	3.412602	-1.853632	-1.874651
H	3.959992	-1.513894	-0.227078
H	3.381732	-3.139307	-0.662271
H	1.597026	-0.207769	2.629972
O	2.767517	0.835085	0.415671
C	-1.981263	-0.205212	-0.195201
C	-2.640755	0.524809	0.807219
C	-2.729666	-1.027241	-1.053186
C	-4.022350	0.425666	0.945627
H	-2.057145	1.164175	1.463324
C	-4.109828	-1.115728	-0.903057
H	-2.211707	-1.582587	-1.829510
C	-4.765070	-0.393117	0.095069
H	-4.521710	0.996183	1.724444
H	-4.678699	-1.754198	-1.573955
H	-5.842821	-0.465196	0.206400
C	0.862113	2.069765	-1.134759
H	0.050484	1.865908	-1.842084
H	1.781395	2.291985	-1.690308
C	0.503623	3.204359	-0.181081
H	0.301567	4.134448	-0.728985
H	-0.399966	2.980290	0.397986
H	1.317033	3.411287	0.522645

E = -686.635609280
G = -686.409941

Mo-O-2-TSIII

Mo	1.317845	0.261992	-0.081831
O	-0.523044	0.388386	0.567718
C	1.592433	-1.716142	1.431492
C	2.436098	0.344767	1.492142
C	0.865933	-2.014612	0.259487
H	2.021196	0.658435	2.452422
H	3.508734	0.156764	1.502381
H	-0.217827	-2.024439	0.357021
H	1.050469	-1.535723	2.354100
C	1.437424	-2.910928	-0.812010
H	1.009256	-2.694885	-1.794249
H	2.521830	-2.803401	-0.892462
H	1.210416	-3.958480	-0.574534
H	2.599552	-2.109905	1.541698
O	2.360377	-0.191346	-1.318504
C	-1.800597	0.106930	0.276892
C	-2.181954	-0.347360	-0.995957
C	-2.779762	0.265833	1.270922
C	-3.517940	-0.638105	-1.261952
H	-1.426547	-0.456016	-1.770403
C	-4.109654	-0.028960	0.990885
H	-2.475822	0.623455	2.250170
C	-4.488817	-0.483068	-0.273697
H	-3.799469	-0.985924	-2.252453
H	-4.857884	0.098947	1.768807
H	-5.529140	-0.710110	-0.486224
C	0.878722	2.170361	-0.991064
H	0.174233	1.947204	-1.808628
H	1.810166	2.504118	-1.465041
C	0.311264	3.260869	-0.085710
H	0.081080	4.172697	-0.653187
H	-0.610822	2.937845	0.406235
H	1.023522	3.541952	0.698950

E = -686.614664566
g = -686.391180

Mo-O-2-IV

Mo	-1.335841	-0.197704	-0.062914
O	0.426147	-0.616767	0.552354
C	-0.075867	2.747698	0.319383
C	-2.664591	-0.329073	1.269107
C	-0.576236	2.317003	1.488454
H	-2.437270	-0.825339	2.218909
H	-3.671490	0.084046	1.200865
H	-1.552222	2.642108	1.840522
H	0.000641	1.681299	2.153428
C	-0.769435	3.678183	-0.622375
H	-0.926376	3.199631	-1.595275
H	-1.744854	3.987619	-0.237465
H	-0.161067	4.574641	-0.792558
H	0.923315	2.419540	0.028997
O	-1.954897	0.742958	-1.305450
C	1.733270	-0.468234	0.240686
C	2.140685	-0.049031	-1.033123
C	2.691791	-0.748891	1.222290
C	3.497802	0.091320	-1.313563
H	1.392808	0.155094	-1.795791
C	4.044131	-0.602743	0.928667
H	2.357779	-1.079104	2.201050
C	4.454830	-0.181848	-0.336787
H	3.806353	0.414183	-2.304127
H	4.782420	-0.821513	1.695328
H	5.511534	-0.071307	-0.560637
C	-1.620157	-2.118022	-0.955214
H	-0.835755	-2.169319	-1.728498
H	-2.582085	-2.106867	-1.478147
C	-1.525794	-3.317807	-0.017479
H	-2.353601	-3.320540	0.700137
H	-1.565991	-4.263574	-0.574237
H	-0.591410	-3.317912	0.554394

E = -686.627265840
G = -686.409356

Mo-O-2-V

Mo	1.231458	-0.277596	0.203574
O	-0.489234	0.474112	0.445616
C	2.245551	-0.169346	1.784627
H	2.011531	0.611619	2.516059
H	3.025745	-0.866785	2.089768
O	1.632372	-1.731800	-0.520589
C	-1.805625	0.269802	0.167630
C	-2.264686	-0.950943	-0.338173
C	-2.699756	1.317232	0.407085
C	-3.621404	-1.115250	-0.604895
H	-1.561157	-1.761115	-0.514967
C	-4.053067	1.139139	0.133597
H	-2.319417	2.253572	0.802962
C	-4.519958	-0.074127	-0.372000
H	-3.975906	-2.064746	-0.996054
H	-4.746281	1.954796	0.319351
H	-5.576844	-0.208365	-0.581614
C	2.271494	1.163690	-0.960792
H	2.028305	2.134247	-0.504405
H	1.756576	1.129226	-1.935743
C	3.778138	1.018923	-1.145339
H	4.036364	0.044077	-1.570213
H	4.173014	1.790227	-1.819662
H	4.297585	1.109051	-0.186259

E = -568.756179451
G = -568.611488

Mo-O-2-TSA

O	-0.669672	0.775941	-0.242341
C	0.091166	-1.793477	-0.302296
H	-0.769842	-1.718177	-0.960696
C	2.420187	-0.530983	-1.024418
C	1.455908	-1.878453	-1.019830
H	2.219133	0.009933	-1.956087
H	1.265777	-2.047075	-2.080474
H	2.075560	-2.669773	-0.597319
Mo	1.055742	-0.053322	0.393380
C	3.888849	-0.840990	-0.835138
H	4.463324	0.090510	-0.836862
H	4.077658	-1.347082	0.115986
H	4.280128	-1.472756	-1.643498
H	-0.039256	-2.543301	0.476177
O	1.490311	-0.491583	1.948925
C	-1.939035	0.350358	-0.161654
C	-2.458398	-0.240160	1.002786
C	-2.793202	0.542443	-1.261938
C	-3.793454	-0.634167	1.056697
H	-1.806473	-0.374341	1.862756
C	-4.125760	0.147997	-1.193609
H	-2.391315	1.010191	-2.156300
C	-4.636563	-0.445026	-0.037701
H	-4.177357	-1.087790	1.967172
H	-4.771558	0.305354	-2.054051
H	-5.677495	-0.750740	0.010128

C	1.319245	2.087449	0.658293
H	0.598831	2.399114	1.423710
H	2.325776	2.129369	1.104127
C	1.214773	2.970508	-0.575792
H	0.230459	2.868125	-1.039485
H	1.352967	4.028692	-0.316433
H	1.975117	2.721406	-1.325883

E = -686.617643102
G = -686.390778

Mo-O-2-SBP

O	0.875181	0.534459	-0.651210
C	-0.659174	-1.897684	-0.527716
C	-2.231192	-1.073403	0.861945
C	-1.998758	-2.329850	0.031071
H	-1.643066	-1.146592	1.789501
H	-2.020291	-3.284286	0.580857
H	-2.743522	-2.393491	-0.771244
H	0.174242	-2.104455	0.156812
Mo	-0.986853	0.217420	-0.461628
C	-3.678502	-0.733957	1.178020
H	-4.161616	-1.592291	1.667543
H	-3.785441	0.118970	1.854104
H	-4.245805	-0.517756	0.266308
H	-0.382178	-2.203168	-1.543627
O	-2.048844	0.477031	-1.727038
C	2.106066	0.179420	-0.210054
C	3.167047	0.171804	-1.122800
C	2.330187	-0.155561	1.131265
C	4.442279	-0.180647	-0.692232
H	2.970877	0.441203	-2.155869
C	3.612019	-0.503921	1.549413
H	1.503481	-0.128853	1.836165
C	4.670970	-0.519970	0.642077
H	5.263098	-0.188330	-1.403953
H	3.782632	-0.761767	2.590957
H	5.668688	-0.792212	0.973019
C	-1.504319	1.573801	1.096719
H	-2.588694	1.677249	1.171667
H	-1.135416	1.238319	2.073419
C	-0.869300	2.905956	0.669361
H	-1.247324	3.723942	1.297020
H	0.221038	2.897329	0.754713
H	-1.117488	3.176708	-0.365452

E = -686.650798911
G = -686.424708

Mo-O-2-TSB

C	-2.004428	-1.960457	-0.844603
C	-0.272820	-1.837422	0.741035
C	-1.665222	-2.087207	0.559993
H	0.374488	-2.209955	-0.052791
H	-2.325144	-2.499369	1.327675
H	-2.284285	-0.771820	0.912930
O	0.461946	0.812852	-0.084357
H	-1.311801	-2.395287	-1.564354
Mo	-1.277511	0.025168	-0.284698
C	0.346110	-1.703949	2.105992
H	0.589515	-2.686299	2.533751
H	1.275390	-1.129205	2.066063
H	-0.329395	-1.201711	2.808538
H	-3.047996	-1.986633	-1.150914
O	-1.829367	0.551594	-1.803651
C	-2.382187	1.387707	0.965304
H	-3.456058	1.169356	0.951053
H	-2.043563	1.223129	1.998998
C	-2.108285	2.822724	0.516498
H	-2.567830	3.536065	1.214386
H	-1.036521	3.040158	0.478475
H	-2.519451	3.010056	-0.479178
C	1.779240	0.532005	-0.138710
C	2.628189	1.029983	0.859124
C	2.315495	-0.209455	-1.200064
C	3.995675	0.776461	0.794477
H	2.201031	1.616291	1.667095
C	3.684641	-0.459779	-1.248956
H	1.651897	-0.563541	-1.984426
C	4.531514	0.027796	-0.253849
H	4.646780	1.168040	1.571589
H	4.091567	-1.034373	-2.076889
H	5.598660	-0.167950	-0.298080

E = -686.602764212
G = -686.379415

Mo-O-2-TSB$_{transX}$

Mo	0.993515	-0.066525	-0.262083
O	-0.777858	-0.736516	-0.592531
C	1.967968	0.172811	1.778539
C	1.817252	1.948354	0.249423
C	1.330154	1.418223	1.490991
H	2.878296	1.782230	0.053530
H	0.632500	1.929418	2.153322
H	-0.048504	0.929998	0.753958
H	3.036631	0.120151	1.581831
C	1.191231	3.123021	-0.437960
H	1.551516	4.073330	-0.021216
H	1.428156	3.112950	-1.505735
H	0.099743	3.108405	-0.330523
H	1.627395	-0.445769	2.605010
O	1.687552	0.165583	-1.795323
C	1.739386	-2.058835	0.123542
H	1.274522	-2.441798	1.038898
H	1.258894	-2.565446	-0.725079
C	3.239008	-2.318422	0.108593
H	3.444587	-3.396597	0.141237
H	3.704739	-1.924760	-0.800359
H	3.750068	-1.874026	0.969052
C	-2.054559	-0.469024	-0.242177
C	-2.993726	-0.213407	-1.249675
C	-2.459230	-0.486465	1.098736
C	-4.320062	0.036436	-0.910552
H	-2.662877	-0.213076	-2.283715
C	-3.790148	-0.235648	1.424914
H	-1.728104	-0.713967	1.869795
C	-4.725591	0.028719	0.425078
H	-5.042476	0.238742	-1.696840
H	-4.097810	-0.254897	2.467149
H	-5.762556	0.222031	0.683308

E = -686.603357325
G = -686.380711

Mo-O-2-B

C	1.363670	1.966270	-0.818080
C	-0.907585	2.738167	-0.063053
C	0.422348	2.642190	0.104578
H	-1.355485	2.304774	-0.958642

H	0.865287	3.075527	1.003355
H	2.241081	0.956604	0.916498
O	-0.084468	-0.776532	-0.648980
H	0.939084	1.835651	-1.827114
Mo	1.634792	-0.083573	-0.235735
C	-1.842134	3.429875	0.878098
H	-2.349294	4.269990	0.386500
H	-2.630529	2.749865	1.223371
H	-1.316480	3.819971	1.755133
H	2.324592	2.479434	-0.894785
O	2.983990	-0.543496	-1.097602
C	1.950289	-1.063268	1.644164
H	2.942504	-0.854757	2.052171
H	1.226029	-0.657658	2.364172
C	1.747721	-2.564275	1.419898
H	1.921382	-3.115816	2.353947
H	0.734363	-2.805090	1.083190
H	2.450265	-2.962698	0.679393
C	-1.407139	-0.859095	-0.381986
C	-1.925852	-0.499103	0.868297
C	-2.260499	-1.330476	-1.387146
C	-3.293836	-0.614026	1.103835
H	-1.256011	-0.140288	1.643360
C	-3.625942	-1.432407	-1.140259
H	-1.835476	-1.609614	-2.346297
C	-4.148971	-1.076360	0.103709
H	-3.691924	-0.341442	2.077456
H	-4.284542	-1.796562	-1.923889
H	-5.214687	-1.162583	0.293380

E = -686.638064736
G = -686.416787

Mo-O-2-TSC

C	-2.187216	-0.115167	-1.284924
C	-4.184016	-1.515138	-0.668437
C	-3.532578	-0.341922	-0.724675
H	-1.812917	-0.999526	-1.819797
H	-4.053398	0.546554	-0.356267
H	-2.221140	0.718695	-1.991609
H	-1.705406	0.913044	0.877265
O	1.174910	-0.563291	0.511462
C	0.053224	2.236986	1.021159
H	1.102962	2.429454	0.757303
H	0.024046	1.964949	2.084818
C	-0.801246	3.468220	0.747392
H	-0.787849	3.729567	-0.315248
H	-1.846012	3.311056	1.037855
H	-0.428926	4.336194	1.306873
C	-1.885737	-0.392075	1.819629
H	-2.953989	-0.242980	1.686578
H	-1.445607	0.076545	2.698621
C	-1.264711	-1.474311	1.227560
H	-0.320044	-1.844637	1.602103
H	-1.825505	-2.107701	0.548451
H	-3.687963	-2.405663	-1.060863
C	-5.569748	-1.708976	-0.136696
H	-6.241203	-2.106756	-0.908424
H	-5.586810	-2.431137	0.690080
H	-5.996469	-0.768751	0.226878
Mo	-0.342678	0.462634	-0.110277
O	0.083036	1.163064	-1.582561
C	2.489093	-0.623152	0.159343
C	3.000799	-0.063870	-1.017534
C	3.345576	-1.296875	1.041193
C	4.360567	-0.180164	-1.297727
H	2.333985	0.451315	-1.701949
C	4.702378	-1.398231	0.751314
H	2.928528	-1.728920	1.945781
C	5.218079	-0.841898	-0.419417
H	4.750511	0.254080	-2.214471
H	5.358475	-1.919326	1.443394
H	6.276871	-0.925419	-0.646004

E = -765.163017510
G = -764.890854

Mo-O-2-C

C	1.137076	1.758414	-1.080609
C	-0.984881	2.882296	-0.345899
C	0.321123	2.607445	-0.186521
H	-1.506248	2.469489	-1.210923
H	0.834120	3.036957	0.675626
O	-0.554107	-0.700306	-0.741044
H	0.627623	1.572827	-2.042393
Mo	1.271997	-0.295885	-0.435561
C	-1.794427	3.751391	0.563752
H	-2.188010	4.625983	0.030017
H	-2.664171	3.211241	0.958145
H	-1.202236	4.112208	1.410515
H	2.131683	2.164144	-1.279442
O	2.418019	-0.988639	-1.429970
C	1.246553	-1.493937	1.356128
H	2.161237	-1.456421	1.948545
H	0.446928	-1.050232	1.969468
C	0.912288	-2.936126	0.968346
H	0.833508	-3.560925	1.868570
H	-0.037377	-3.022589	0.431791
H	1.693843	-3.375399	0.339016
C	2.602011	0.774724	0.997730
H	2.695297	1.832842	0.740859
H	2.141154	0.737460	1.992813
C	4.015910	0.184422	1.045717
H	4.623064	0.695809	1.804996
H	4.028925	-0.883948	1.284830
H	4.523279	0.300937	0.082929
C	-1.834695	-0.706891	-0.312668
C	-2.215042	-0.085381	0.884617
C	-2.790397	-1.364620	-1.098458
C	-3.546972	-0.132798	1.289007
H	-1.471211	0.433107	1.480307
C	-4.117530	-1.399489	-0.684067
H	-2.471043	-1.839369	-2.021016
C	-4.501466	-0.786211	0.509793
H	-3.838959	0.344691	2.220273
H	-4.855620	-1.910934	-1.295533
H	-5.538286	-0.818593	0.831061

E = -765.225955961
G = -764.950206

Mo-N-3-I

Mo	-0.683526	0.386700	0.117352
O	-1.349388	1.861010	-0.887317
N	1.005887	0.040928	0.055433
C	-0.933235	0.693952	1.944410
H	-1.968615	1.077948	2.039160
Si	-1.814101	3.474184	-0.914097
H	-2.780053	3.674280	-2.034686

H	-2.465416	3.841085	0.382898
H	-0.617817	4.345451	-1.125330
C	-0.148361	0.651885	3.213325
H	-0.609905	-0.043854	3.927319
H	0.878059	0.323266	3.034570
H	-0.121974	1.635337	3.701083
C	2.344420	-0.239120	-0.095188
C	3.236009	0.752154	-0.543479
C	4.586326	0.455424	-0.687600
C	5.063638	-0.822052	-0.389526
C	4.181332	-1.808132	0.055232
C	2.828446	-1.525789	0.204649
H	2.850358	1.741053	-0.771657
H	5.270451	1.224716	-1.034684
H	6.119737	-1.048461	-0.504039
H	4.549655	-2.803680	0.286555
H	2.127894	-2.280945	0.547266
N	-1.714978	-1.320545	-0.159698
C	-2.627538	-1.986065	0.643250
C	-1.665088	-2.003342	-1.370862
C	-3.151979	-3.051059	-0.044867
H	-2.819378	-1.637701	1.648077
C	-2.536838	-3.061894	-1.333964
H	-1.004765	-1.677101	-2.164635
H	-3.890662	-3.749358	0.326388
H	-2.716121	-3.768549	-2.133604

E = -723.628759860
G = -723.433084

Mo-N-3-Ianti

H	-2.279632	1.722136	3.195495
O	-1.464318	1.849055	-0.565255
Si	-1.442386	3.363216	-1.289815
H	-2.663192	3.501495	-2.137663
H	-1.438869	4.424669	-0.237045
H	-0.222630	3.514242	-2.142068
C	-2.347124	0.796741	2.608029
H	-3.074700	0.964581	1.805849
H	-2.762387	0.023082	3.268025
C	-0.987225	0.378726	2.108522
H	-0.230762	0.214570	2.878567
C	2.397734	-0.094606	0.110945
C	3.277147	0.977608	-0.124980
C	2.909910	-1.398859	0.241228
C	4.643285	0.742717	-0.228573
H	2.870356	1.979540	-0.221246
C	4.278105	-1.618360	0.132607
H	2.218578	-2.215647	0.423524
C	5.148433	-0.552267	-0.101376
H	5.318006	1.574680	-0.410015
H	4.668043	-2.627474	0.232090
H	6.216760	-0.729837	-0.183984
N	1.045167	0.123837	0.223981
Mo	-0.666849	0.329087	0.254436
N	-1.528122	-1.415230	-0.264911
C	-2.350026	-2.288095	0.428035
C	-1.416223	-1.904727	-1.562343
C	-2.760663	-3.294026	-0.410566
H	-2.566337	-2.115002	1.472229
C	-2.164159	-3.048341	-1.684827
H	-0.802465	-1.396866	-2.296096
H	-3.411597	-4.117750	-0.148056
H	-2.272851	-3.646915	-2.579724

E = -723.626236962

G = -723.430310

Mo-N-3-TSrot1

Mo	-0.785738	0.096217	0.352286
O	-1.446224	1.858124	0.134301
N	0.782751	0.069402	-0.462536
C	-0.574734	-0.189340	2.198394
H	-0.848780	-1.236981	2.415034
Si	-1.152298	3.159544	-0.897915
H	-2.349792	4.049697	-0.861221
H	0.048752	3.914247	-0.427761
H	-0.923214	2.674756	-2.293030
C	0.008443	0.592390	3.337442
H	0.907650	0.114343	3.748103
H	0.277258	1.609603	3.037727
H	-0.718429	0.671704	4.156932
C	2.161378	0.052335	-0.328682
C	2.950860	0.658480	-1.323400
C	4.337419	0.644331	-1.220404
C	4.956899	0.015375	-0.139389
C	4.179844	-0.600142	0.844377
C	2.793045	-0.582940	0.756605
H	2.453537	1.134468	-2.163120
H	4.938481	1.120969	-1.989872
H	6.040543	0.000029	-0.065786
H	4.659736	-1.096669	1.683504
H	2.173485	-1.058654	1.511402
N	-1.764668	-1.412401	-0.460180
C	-3.069155	-1.735957	-0.080322
C	-1.423772	-2.238412	-1.525701
C	-3.524828	-2.749568	-0.879290
H	-3.553362	-1.217848	0.737371
C	-2.475684	-3.069770	-1.800042
H	-0.450062	-2.147283	-1.984255
H	-4.496386	-3.221248	-0.814301
H	-2.501328	-3.830570	-2.568859

E = -723.599781125
G = -723.403072

Mo-N-3-TSrot2

Mo	-0.701642	0.172415	0.364736
O	-1.338167	1.964553	0.217219
N	0.830386	0.126705	-0.520422
C	-0.398588	-0.125548	2.195250
H	0.211240	0.728726	2.541133
Si	-1.156159	3.186033	-0.927136
H	-2.221463	4.202169	-0.677535
H	0.188549	3.822713	-0.781706
H	-1.297535	2.645413	-2.314890
C	-0.625952	-1.211279	3.205564
H	-1.169554	-0.816874	4.074777
H	-1.211071	-2.037844	2.792622
H	0.320713	-1.622704	3.581619
C	2.208475	0.135687	-0.376862
C	2.988298	0.892428	-1.271468
C	4.373364	0.904627	-1.153394
C	5.003090	0.152243	-0.160235
C	4.236920	-0.613433	0.720652
C	2.850487	-0.623303	0.619559
H	2.484953	1.462759	-2.046223
H	4.966067	1.498761	-1.843555
H	6.086118	0.157679	-0.076837
H	4.724284	-1.207140	1.489453
H	2.239811	-1.214932	1.295405
N	-1.785858	-1.252010	-0.439363
C	-3.109606	-1.483616	-0.047337

C	-1.487543	-2.159369	-1.452839
C	-3.614656	-2.518268	-0.783604
H	-3.569136	-0.885893	0.729266
C	-2.580242	-2.948691	-1.679636
H	-0.510406	-2.145158	-1.912800
H	-4.611050	-2.931412	-0.699683
H	-2.647001	-3.750304	-2.403178

E = -723.599322385
G = -723.402216

Mo-N-3-TSI

Mo	0.654296	-0.275163	0.334680
O	1.846380	-1.324756	-0.731241
N	-1.041762	0.079916	0.203408
C	-0.889391	-3.239733	-0.355118
C	0.893662	-0.565582	2.173132
C	-0.255635	-3.458468	0.799397
H	1.931219	-0.924900	2.304443
Si	2.855949	-1.604009	-2.040076
H	0.793917	-3.736956	0.827972
H	-0.769652	-3.382495	1.753576
H	-0.375734	-3.330104	-1.308248
H	4.207280	-1.024454	-1.780506
H	2.980261	-3.081505	-2.238553
H	2.281056	-0.998147	-3.281322
C	0.082444	-0.504539	3.423780
H	0.493041	0.251702	4.107234
H	-0.956871	-0.243234	3.214748
H	0.106082	-1.460537	3.964557
H	-1.940703	-2.967663	-0.386702
C	-2.347828	0.276440	-0.173695
C	-2.820311	-0.159502	-1.426964
C	-4.146422	0.053438	-1.785977
C	-5.022014	0.694783	-0.908563
C	-4.559496	1.130240	0.334357
C	-3.234764	0.929043	0.703703
H	-2.132416	-0.655945	-2.105051
H	-4.498856	-0.283050	-2.757208
H	-6.057315	0.857731	-1.193341
H	-5.234823	1.635854	1.019093
H	-2.859852	1.275260	1.661560
N	1.473028	1.554356	0.180533
C	2.317489	2.237125	1.036765
C	1.374251	2.304391	-0.981865
C	2.756561	3.387172	0.426713
H	2.530393	1.840817	2.019359
C	2.153286	3.430449	-0.865454
H	0.740094	1.982575	-1.797892
H	3.426955	4.120787	0.855018
H	2.271335	4.203855	-1.613158

E = -802.184417363
G = -801.942732

Mo-N-3-II

Mo	0.626394	0.174900	0.485405
O	2.149088	-1.015539	0.747710
N	-1.112162	0.277548	0.337050
C	0.134773	-0.819600	2.686476
C	1.095811	1.972874	0.891524
C	0.711240	0.368231	3.040062
H	2.191473	2.060561	0.979905
Si	3.609278	-1.465776	0.055401
H	1.779740	0.435271	3.220291
H	0.109287	1.219745	3.340671
H	0.742039	-1.713034	2.585881
H	4.110627	-0.460651	-0.927988
H	4.605461	-1.580387	1.171813
H	3.496228	-2.807156	-0.596026
C	0.364670	3.253025	1.106182
H	0.645647	3.971391	0.323430
H	-0.717645	3.117225	1.076435
H	0.647439	3.718015	2.061037
H	-0.944220	-0.938320	2.700801
C	-2.437062	-0.057492	0.216853
C	-2.842638	-1.403715	0.119282
C	-4.190711	-1.719311	-0.001609
C	-5.153992	-0.709694	-0.026761
C	-4.759054	0.625968	0.066923
C	-3.414815	0.956322	0.187454
H	-2.086668	-2.183421	0.127223
H	-4.491390	-2.760353	-0.080932
H	-6.205895	-0.961995	-0.122963
H	-5.504278	1.416222	0.042036
H	-3.096935	1.992182	0.250873
N	1.056425	0.100325	-1.526267
C	1.095839	1.135816	-2.433968
C	1.184777	-1.072401	-2.244457
C	1.256186	0.633765	-3.707789
H	0.998854	2.159137	-2.098904
C	1.310742	-0.781907	-3.587007
H	1.172209	-2.034356	-1.748117
H	1.334952	1.213859	-4.618209
H	1.437481	-1.500950	-4.386029

E = -802.190693781
G = -801.940742

Mo-N-3-TSII

Mo	0.543490	-0.622728	0.111418
N	-1.145855	-0.185623	0.248408
O	2.092412	-0.875821	-1.036716
Si	3.265871	-0.036861	-1.894258
H	4.410674	-0.974147	-2.130264
H	2.717583	0.367439	-3.230007
H	3.747604	1.166509	-1.160101
C	0.839876	-1.597520	1.715393
H	1.888979	-1.934692	1.744494
C	0.036637	-1.971893	2.911918
H	0.429980	-1.441759	3.790720
H	0.121742	-3.044446	3.135047
H	-1.015901	-1.706947	2.798866
C	0.120773	-3.105185	-0.405038
H	1.121554	-3.523874	-0.361731
H	-0.596748	-3.472111	0.321502
C	-0.273183	-2.343024	-1.468316
H	0.408462	-2.153928	-2.290297
H	-1.319635	-2.090864	-1.610714
C	-2.422660	0.217914	-0.049714
C	-2.770206	0.642071	-1.348657
C	-4.072622	1.037778	-1.630115
C	-5.047680	1.020072	-0.631846
C	-4.709921	0.606429	0.658120
C	-3.411699	0.209414	0.953834
H	-2.004252	0.663420	-2.118818
H	-4.327583	1.365196	-2.634264
H	-6.063560	1.331451	-0.856357
H	-5.463628	0.597487	1.440622
H	-3.136387	-0.103067	1.956090
N	1.272681	1.241494	0.582705
C	2.340399	1.552268	1.396713
C	0.886263	2.408644	-0.043128
C	2.626342	2.897376	1.295240

H	2.819703	0.786595	1.992084
C	1.695844	3.446138	0.370832
H	0.038559	2.422674	-0.715967
H	3.402771	3.427777	1.831329
H	1.615232	4.480518	0.062336

E = -802.189723264
G = -801.939167

Mo-N-3-TBP

O	-2.584540	-0.559000	0.149337
C	-0.558994	-1.951461	1.401141
H	-1.472961	-2.137011	1.961697
C	-0.630033	-1.801386	-1.336550
C	-0.536178	-2.687032	0.003656
H	-1.626191	-1.904143	-1.771109
H	-1.397379	-3.355113	-0.022368
H	0.403151	-3.235792	-0.066597
Si	-4.164067	-1.016500	-0.072690
H	-5.073632	0.170260	-0.015233
H	-4.330503	-1.682178	-1.407242
H	-4.582783	-1.989869	0.987989
N	1.101772	-0.144195	0.086693
C	2.463839	0.010224	0.094461
C	3.158145	0.339282	-1.086235
C	3.180318	-0.153315	1.296358
C	4.539218	0.492404	-1.057975
H	2.597663	0.476666	-2.005290
C	4.561209	0.000845	1.307857
H	2.633831	-0.389443	2.204109
C	5.245372	0.321662	0.133896
H	5.068001	0.749267	-1.971528
H	5.106994	-0.125040	2.238639
H	6.324463	0.443316	0.148995
Mo	-0.633618	-0.339469	0.116185
N	-0.950992	1.670623	0.212985
C	-2.171588	2.320101	0.361132
C	0.021263	2.662881	0.146020
C	-1.970870	3.676576	0.385205
H	-3.083499	1.751080	0.439085
C	-0.567960	3.896780	0.245210
H	1.062274	2.400946	0.031246
H	-2.741167	4.429685	0.490848
H	-0.056171	4.850329	0.222537
C	0.458551	-2.068091	-2.349808
H	0.381325	-1.357404	-3.178935
H	1.456241	-1.973978	-1.913684
H	0.364890	-3.075423	-2.778071
H	0.341441	-2.127262	1.984156

E = -802.210956006
G = -801.956031

Mo-N-3-TSIII

Mo	-0.722224	0.519901	-0.202110
O	-2.468978	0.329875	0.658820
N	1.021360	0.507337	-0.274279
C	-1.090863	2.953993	0.178421
C	-1.101664	1.524463	-1.782104
C	-0.624174	2.322759	1.328415
H	-2.147364	1.657857	-2.075725
H	-0.377678	1.985738	-2.451453
Si	-3.939630	-0.468797	0.690222
H	-5.013510	0.575671	0.780818
H	-4.172825	-1.287799	-0.536102
H	-4.045038	-1.337977	1.903895
H	-1.385821	1.950951	2.011451
H	-2.156720	3.077036	0.022694
C	0.733307	2.599339	1.920623
H	1.146618	1.725639	2.431584
H	1.452427	2.918469	1.162218
H	0.644955	3.401848	2.664484
H	-0.437229	3.612550	-0.387109
C	2.356145	0.251466	-0.082449
C	3.325902	1.091655	-0.660867
C	4.677041	0.820744	-0.478185
C	5.079363	-0.284738	0.272850
C	4.120085	-1.125134	0.841019
C	2.765388	-0.865173	0.671746
H	3.000828	1.943821	-1.250092
H	5.420546	1.473969	-0.926509
H	6.136287	-0.492987	0.411305
H	4.429787	-1.991964	1.418026
H	2.008078	-1.519575	1.092333
N	-0.866750	-1.509683	-0.566608
C	-0.376853	-2.194570	-1.656502
C	-1.253196	-2.454321	0.365765
C	-0.466727	-3.552536	-1.432058
H	-0.002135	-1.657634	-2.517141
C	-1.021574	-3.719018	-0.133894
H	-1.659074	-2.158060	1.323902
H	-0.178911	-4.334008	-2.123578
H	-1.238501	-4.652375	0.369510

E = -802.183381356
G = -801.931356

Mo-N-3-IV

Mo	-0.707338	0.323482	-0.514418
O	-2.132724	0.858847	0.687228
N	1.029016	0.191955	-0.496506
C	-0.189051	2.952347	-0.006321
C	-1.105840	0.227262	-2.357942
C	-0.951980	2.897898	-1.126112
H	-2.163043	0.286090	-2.647250
H	-0.413474	0.136015	-3.193863
Si	-3.504231	0.274185	1.464773
H	-0.524509	3.087531	-2.106821
H	-2.031433	2.810911	-1.062387
H	-4.095715	-0.899067	0.758797
H	-3.193565	-0.077909	2.884532
H	-4.505102	1.390799	1.473750
C	1.257772	3.333209	0.016516
H	1.844293	2.691124	0.678793
H	1.702735	3.301335	-0.981291
H	1.348932	4.358008	0.399121
H	-0.692126	2.852217	0.954679
C	2.334294	0.044390	-0.099314
C	2.686847	-0.002305	1.263987
C	4.016283	-0.167681	1.634757
C	5.011950	-0.282176	0.663383
C	4.668788	-0.235387	-0.689064
C	3.343325	-0.075192	-1.074317
H	1.905101	0.079030	2.013440
H	4.276809	-0.209862	2.688706
H	6.049130	-0.410662	0.958682
H	5.439701	-0.329046	-1.448957
H	3.062282	-0.046682	-2.122392
N	-1.132333	-1.619108	-0.041753
C	-1.119042	-2.103588	1.253322
C	-1.380592	-2.692534	-0.872124
C	-1.362858	-3.459885	1.241363

H	-0.931019	-1.446477	2.092735
C	-1.533062	-3.835881	-0.120782
H	-1.421282	-2.550148	-1.942965
H	-1.419910	-4.105222	2.108429
H	-1.746353	-4.826370	-0.501122

E = -802.186353729
G = -801.936696

Mo-N-3-TSIV

Mo	-0.761374	-0.023157	-0.527209
O	-2.084625	0.984131	0.413952
N	0.965637	-0.051940	-0.373265
C	0.099747	3.299703	-0.737552
C	-1.046765	-0.253098	-2.370320
C	-0.766601	2.998949	-1.713867
H	-0.329922	-0.417092	-3.173250
H	-2.086885	-0.121383	-2.698982
Si	-3.125254	1.199181	1.715668
H	-0.274832	3.373719	0.283865
H	-0.446184	2.927536	-2.750794
H	-1.821875	2.851559	-1.509783
H	-4.250363	0.221154	1.647251
H	-2.383618	1.026217	3.003184
H	-3.668207	2.590988	1.654025
C	1.554520	3.583475	-0.937744
H	1.794426	4.605752	-0.619597
H	2.177655	2.910843	-0.338242
H	1.844237	3.475137	-1.986756
C	2.281012	-0.046919	0.021611
C	2.678013	0.538264	1.239554
C	4.015793	0.520775	1.617763
C	4.975240	-0.069734	0.793731
C	4.586895	-0.650872	-0.414527
C	3.252288	-0.645997	-0.802469
H	1.924694	0.995963	1.874229
H	4.311610	0.970951	2.561363
H	6.019134	-0.079600	1.093115
H	5.328986	-1.116486	-1.057158
H	2.934838	-1.104031	-1.733727
N	-1.238533	-1.866440	0.108522
C	-1.083589	-2.243636	1.434647
C	-1.847523	-2.920438	-0.548819
C	-1.599663	-3.504609	1.612022
H	-0.606723	-1.584404	2.148505
C	-2.087163	-3.937435	0.342498
H	-2.048406	-2.850538	-1.608089
H	-1.620946	-4.059427	2.540930
H	-2.552314	-4.887751	0.115723

E = -802.183464345
G = -801.938913

Mo-N-3-V

Mo	0.827801	0.009249	0.413255
O	2.049935	1.409766	0.047793
N	-0.861217	0.333568	0.334661
C	1.004265	-0.556481	2.188957
H	0.263617	-0.736298	2.966848
H	2.051879	-0.617998	2.518531
Si	2.622166	2.988448	0.119620
H	3.760827	3.118968	-0.835977
H	1.536630	3.943906	-0.259163
H	3.086921	3.291733	1.507218
C	-2.219652	0.524174	0.247250
C	-2.768840	1.812876	0.367421
C	-4.145469	1.987785	0.284502
C	-4.985033	0.891624	0.079586
C	-4.441424	-0.388620	-0.041464
C	-3.067102	-0.579640	0.041698
H	-2.102998	2.655527	0.526053
H	-4.565605	2.985119	0.379602
H	-6.059739	1.034581	0.014645
H	-5.092143	-1.243774	-0.200969
H	-2.626432	-1.567514	-0.049660
N	1.199613	-1.671780	-0.621416
C	0.993312	-1.730803	-1.996666
C	1.774068	-2.875562	-0.243859
C	1.443233	-2.935924	-2.472197
H	0.534144	-0.904718	-2.524908
C	1.941560	-3.667828	-1.351171
H	2.008355	-3.059714	0.794638
H	1.416870	-3.264473	-3.502858
H	2.367954	-4.662314	-1.364788

E = -684.320021651
G = -684.152104

Mo-N-3-TSA

Mo	0.633107	-0.320164	0.297957
C	0.540839	-2.269701	1.218890
N	-1.070374	-0.007644	0.362777
O	1.727303	-1.157589	-1.075354
H	1.399470	-2.924155	1.052030
C	0.664321	-1.470766	2.543749
C	1.287899	-0.068973	2.244010
H	2.383676	-0.160016	2.181266
H	-0.317349	-1.327702	3.003748
H	1.314402	-2.001148	3.254038
Si	1.944585	-2.663591	-1.765196
H	2.525449	-2.475885	-3.130426
H	2.894340	-3.496057	-0.958359
H	0.648289	-3.403502	-1.887926
C	0.878304	1.075258	3.147598
H	-0.210755	1.172940	3.189410
H	1.242162	0.913984	4.172079
H	1.288427	2.025057	2.791950
H	-0.387474	-2.835652	1.137226
C	-2.384601	0.044786	-0.050877
C	-3.354091	0.582910	0.814375
C	-4.684572	0.640532	0.415095
C	-5.063502	0.169626	-0.842572
C	-4.103208	-0.362721	-1.705364
C	-2.770654	-0.429784	-1.318269
H	-3.043289	0.946593	1.788746
H	-5.429117	1.055994	1.088228
H	-6.103922	0.217508	-1.150425
H	-4.395363	-0.728362	-2.685635
H	-2.014806	-0.840636	-1.980734
N	1.337595	1.392690	-0.576818
C	2.558383	1.628186	-1.187799
C	0.700866	2.632873	-0.453962
C	2.706266	2.969993	-1.420119
H	3.211939	0.798502	-1.412901
C	1.512806	3.615878	-0.946810
H	-0.290167	2.693690	-0.026695
H	3.559032	3.449237	-1.883747
H	1.287065	4.673580	-0.989857

E = -802.190307440
G = -801.938377

Mo-N-3-SBP

O	-1.051263	1.838210	-0.977344
C	-0.404773	1.766145	1.740582
C	-1.089545	-0.351556	2.114662
C	-0.335103	0.740677	2.854806
H	-2.169946	-0.138138	2.162039
Si	-1.601047	3.414306	-1.194683
H	-0.475518	4.372724	-0.974185
H	-2.101762	3.538831	-2.594502
H	-2.707363	3.724197	-0.237459
H	-0.758032	1.046609	3.825044
H	0.702164	0.430199	3.026025
H	-1.349790	2.324906	1.748788
N	1.098492	-0.138844	0.083468
C	2.445175	-0.322278	-0.146639
C	3.034056	-1.568616	0.131208
C	3.237337	0.725070	-0.650336
C	4.393290	-1.756724	-0.093229
H	2.411394	-2.368545	0.518928
C	4.594719	0.521887	-0.869948
H	2.772078	1.682626	-0.863139
C	5.177342	-0.716016	-0.592988
H	4.842982	-2.721719	0.122908
H	5.201678	1.334150	-1.259890
H	6.238548	-0.868811	-0.766264
Mo	-0.549488	0.360540	0.097415
N	-1.756350	-1.159907	-0.451501
C	-3.087133	-1.423402	-0.188211
C	-1.371902	-1.989327	-1.501792
C	-3.544388	-2.378867	-1.064056
H	-3.614297	-0.897092	0.595193
C	-2.447965	-2.741907	-1.901937
H	-0.352678	-1.985986	-1.863804
H	-4.551041	-2.773966	-1.104906
H	-2.450395	-3.479046	-2.693982
C	-0.820437	-1.795392	2.493878
H	-1.117064	-1.974911	3.538019
H	-1.372133	-2.497810	1.863355
H	0.246495	-2.029743	2.413347
H	0.428941	2.465980	1.617590

E = -802.214366395
G = -801.962210

Mo-N-3-TSB

C	0.413024	0.793171	2.114304
C	-1.932904	0.601349	1.862014
C	-0.758074	-0.024100	2.383624
H	-1.910755	1.689641	1.924357
H	-0.759605	-0.875797	3.069532
H	-0.381067	-0.995046	1.355119
O	-1.020937	1.856174	-0.737659
Si	-2.207295	3.006181	-1.021943
H	-2.887496	3.392645	0.254850
H	-1.572126	4.220844	-1.617267
H	-3.221850	2.457591	-1.971517
H	0.285604	1.871102	2.224385
C	2.663003	-0.121543	-0.248585
C	3.544005	0.818589	-0.817919
C	3.190731	-1.240387	0.425405
C	4.917494	0.643301	-0.701656
H	3.127681	1.672266	-1.343930
C	4.567261	-1.404173	0.531336
H	2.503125	-1.971281	0.840858
C	5.435177	-0.465159	-0.028069
H	5.590199	1.374602	-1.141307
H	4.965727	-2.271667	1.050426
H	6.509795	-0.598424	0.056231
N	1.305572	0.043706	-0.376605
Mo	-0.362022	0.282040	0.143740
C	-3.299417	-0.028474	1.908793
H	-3.758887	0.078024	2.901920
H	-3.974018	0.445725	1.189448
H	-3.270001	-1.093603	1.663040
H	1.399591	0.420630	2.376277
N	-1.301367	-1.356291	-0.598919
C	-1.782064	-2.546347	-0.088911
C	-1.530448	-1.375641	-1.968539
C	-2.326214	-3.295600	-1.103792
H	-1.686616	-2.774411	0.963552
C	-2.169177	-2.543941	-2.306039
H	-1.215674	-0.551282	-2.594862
H	-2.782534	-4.271446	-1.002006
H	-2.486870	-2.830604	-3.299882

E = -802.169433769
G = -801.919849

Mo-N-3-TSB*TransX*

O	-1.574335	1.507370	-1.141724
C	-2.300808	0.786225	1.771915
C	-0.024298	0.266845	2.219555
C	-1.034212	1.310021	2.158794
H	-0.404517	-0.687318	2.590632
Si	-1.941739	3.121691	-1.400126
H	-0.780756	3.823796	-2.030803
H	-3.124165	3.199578	-2.308100
H	-2.261957	3.802574	-0.103258
H	-0.873100	2.321493	2.541679
H	-0.515518	1.874830	0.887077
H	-2.562836	-0.180318	2.188015
N	0.920519	0.074259	-0.479921
C	2.282642	-0.098081	-0.572004
C	2.878955	-1.311001	-0.177656
C	3.087053	0.928056	-1.101330
C	4.252114	-1.484503	-0.310077
H	2.250527	-2.099460	0.225511
C	4.459649	0.743762	-1.218349
H	2.615361	1.854857	-1.413016
C	5.047523	-0.460128	-0.825774
H	4.704868	-2.423955	-0.005214
H	5.074750	1.542645	-1.623191
H	6.120071	-0.600068	-0.923686
Mo	-0.720069	0.317247	0.096522
N	-1.542431	-1.552037	-0.007300
C	-2.773420	-2.073812	0.368301
C	-0.893572	-2.563103	-0.728153
C	-2.903380	-3.352517	-0.106257
H	-3.489143	-1.474444	0.909076
C	-1.696387	-3.667872	-0.805654
H	0.093973	-2.393533	-1.130382
H	-3.767802	-3.991918	0.017805
H	-1.455665	-4.598832	-1.302141
C	1.385338	0.601889	2.627674
H	1.452007	0.764231	3.712059
H	2.080196	-0.201344	2.371790
H	1.741467	1.512109	2.131885
H	-3.125630	1.457804	1.550505

E = -802.166416892

Mo-N-3-B

C	1.797827	-0.430549	-1.501612

C	4.051342	0.201046	-0.577931
C	3.096094	-0.705484	-0.843018
H	1.793490	0.528487	-2.042364
H	3.263656	-1.739148	-0.535296
H	1.485385	-1.229674	-2.174509
H	0.845718	-1.614453	0.031699
O	0.954140	1.723026	0.405033
Si	1.883604	2.905246	1.155705
H	2.712335	3.596403	0.120589
H	0.969425	3.897091	1.796876
H	2.777949	2.303930	2.188929
H	3.888242	1.235981	-0.884441
C	5.354332	-0.097476	0.092595
H	6.202140	0.155031	-0.556927
H	5.476247	0.495591	1.007835
H	5.435924	-1.155004	0.360963
N	-1.084963	-0.252496	-0.960501
C	-2.272451	-0.286169	-1.655242
C	-2.979940	-1.497081	-1.757961
C	-2.780749	0.873731	-2.266649
C	-4.176680	-1.539000	-2.463880
H	-2.574265	-2.381570	-1.277486
C	-3.980426	0.816352	-2.966360
H	-2.224817	1.802483	-2.180988
C	-4.681017	-0.386627	-3.068738
H	-4.720336	-2.476413	-2.540334
H	-4.370420	1.715106	-3.435791
H	-5.617217	-0.425565	-3.617932
Mo	0.318886	-0.028652	0.007420
N	-0.127146	-0.802458	1.806737
C	0.338532	-1.872336	2.548348
C	-1.043125	-0.117389	2.599378
C	-0.246322	-1.855817	3.789638
H	1.053644	-2.558635	2.118383
C	-1.130738	-0.734354	3.822176
H	-1.561957	0.756337	2.225744
H	-0.069036	-2.564685	4.587690
H	-1.758205	-0.423955	4.647478

E = -802.197389155
G = -801.950371

Mo-N-3-TSC

C	-1.832572	0.521205	0.860471
C	-4.127885	1.199642	0.098713
C	-3.278622	0.317197	0.649030
H	-1.572105	1.591751	0.809112
H	-3.690158	-0.626018	1.016716
H	-1.531781	0.144981	1.839992
H	-1.258759	-1.443185	-0.345731
O	0.101004	1.579923	-1.598024
Si	1.085763	2.917205	-1.373927
H	0.888207	3.859948	-2.516787
H	0.728699	3.619020	-0.098765
H	2.528139	2.519519	-1.312789
C	-2.142868	-1.364145	-1.613357
H	-3.032203	-1.480376	-0.999246
H	-1.724664	-2.277476	-2.027447
C	-1.924549	-0.153602	-2.257682
H	-1.273532	-0.104882	-3.124736
H	-2.581039	0.689707	-2.074751
H	-3.731603	2.155715	-0.250090
C	-5.600424	0.991969	-0.063096
H	-6.172245	1.760002	0.473110
H	-5.900398	1.061265	-1.116640
H	-5.913283	0.013490	0.314249
N	0.799378	0.086397	0.860040
C	1.382937	0.171246	2.094269
C	1.156141	-0.844286	3.045092
C	2.211297	1.261357	2.427735
C	1.742490	-0.760870	4.301873
H	0.526752	-1.684806	2.769707
C	2.794184	1.327180	3.686731
H	2.385523	2.035541	1.687498
C	2.561772	0.321449	4.627480
H	1.563961	-1.546759	5.030367
H	3.434014	2.168546	3.937478
H	3.020567	0.379996	5.610161
Mo	-0.216045	-0.030564	-0.554803
N	0.749916	-1.590837	-1.443427
C	0.694372	-2.962554	-1.311441
C	1.857344	-1.297619	-2.225001
C	1.733333	-3.534358	-2.008784
H	-0.068706	-3.425559	-0.700835
C	2.473650	-2.469410	-2.598445
H	2.105189	-0.275005	-2.474846
H	1.941238	-4.593414	-2.087596
H	3.344700	-2.553903	-3.235059

E = -880.731783466
G = -880.432733

Mo-N-3-C

C	1.015808	-1.943603	0.784050
C	3.447343	-2.394068	0.320182
C	2.459215	-1.936486	1.106650
H	0.803912	-2.544883	-0.112236
H	2.734323	-1.520510	2.077759
H	0.400319	-2.305038	1.610613
H	-0.259619	2.310169	2.528610
O	1.186394	-0.297899	-1.493085
Si	2.456027	-0.353536	-2.596783
H	3.721432	0.147098	-1.984056
H	2.643080	-1.762924	-3.056795
H	2.088519	0.501634	-3.764316
C	-0.252886	1.318673	2.987078
H	-1.285384	0.953989	3.006323
H	0.070322	1.435105	4.030804
C	0.664861	0.340266	2.256084
H	1.697377	0.721413	2.255750
H	0.680645	-0.605669	2.803055
H	3.187529	-2.840071	-0.641710
C	4.902074	-2.374466	0.671892
H	5.321460	-3.388655	0.692392
H	5.486558	-1.812040	-0.067622
H	5.072356	-1.919553	1.652654
N	-1.434341	-0.369277	0.178520
C	-2.725088	-0.757829	-0.113240
C	-3.662614	-0.879005	0.926926
C	-3.112391	-1.029273	-1.437796
C	-4.965916	-1.269115	0.639417
H	-3.349704	-0.664271	1.943525
C	-4.420045	-1.413907	-1.709442
H	-2.379412	-0.930344	-2.232878
C	-5.349711	-1.536419	-0.675290
H	-5.686737	-1.362620	1.446734
H	-4.715308	-1.620268	-2.734336
H	-6.369736	-1.838480	-0.893855
Mo	0.244397	-0.000508	0.118943
N	0.428082	2.015599	0.150580
C	1.548484	2.794061	0.367070
C	-0.582506	2.860261	-0.297667
C	1.268220	4.097921	0.034654
H	2.471047	2.355449	0.722727

C	-0.095875	4.140345	-0.387062
H	-1.572051	2.474397	-0.498009
H	1.959721	4.929130	0.080506
H	-0.650844	5.012600	-0.706363

E = -880.787585835
G = -880.486399

Mo-N-3'-I

O	-0.119437	2.054928	-0.829844
Si	0.235022	3.693216	-0.872246
H	-0.624893	4.343916	-1.905446
H	-0.031738	4.313786	0.463925
H	1.673889	3.897037	-1.225266
C	-0.051127	0.730627	1.976072
C	2.316253	-1.519168	-0.418675
N	1.212152	-0.647659	-0.092587
Mo	-0.114525	0.406678	0.133757
N	-1.827532	-0.649644	-0.048415
C	-2.865827	-0.874061	0.840610
C	-2.199122	-1.223587	-1.258439
C	-3.873334	-1.558482	0.207326
H	-2.789226	-0.525738	1.860760
C	-3.447782	-1.780761	-1.137084
H	-1.541134	-1.181417	-2.117324
H	-4.810408	-1.869370	0.650470
H	-3.997810	-2.290528	-1.917281
C	0.715664	0.326186	3.190052
H	1.225602	1.183859	3.649015
H	0.041238	-0.086554	3.952767
H	1.461704	-0.435844	2.952930
H	-0.801174	1.530823	2.138063
C	3.627178	-0.821574	-0.024311
H	3.641051	-0.603275	1.047342
H	4.481375	-1.466168	-0.256753
H	3.742891	0.119513	-0.569709
C	2.149394	-2.836372	0.354712
H	1.204213	-3.319685	0.092975
H	2.970389	-3.520746	0.115840
H	2.154370	-2.654143	1.433113
C	2.285359	-1.781291	-1.933336
H	2.375870	-0.843700	-2.489767
H	3.116852	-2.434860	-2.216860
H	1.349914	-2.269831	-2.220943

E = -649.869987445
G = -649.642021

Mo-N-3'-Ianti

O	0.060468	2.097665	-0.579452
Si	0.902827	3.357516	-1.296281
H	-0.044651	4.148669	-2.136740
H	1.492230	4.239197	-0.242132
H	2.004702	2.827323	-2.158943
C	-0.254205	0.592735	2.121852
C	2.306176	-1.657725	-0.015987
N	1.244817	-0.695833	0.164685
Mo	-0.072613	0.386979	0.256700
N	-1.757652	-0.623310	-0.216892
C	-2.864048	-0.988179	0.530349
C	-1.994432	-1.039458	-1.521800
C	-3.783777	-1.605551	-0.281171
H	-2.894069	-0.781021	1.590233
C	-3.228812	-1.635890	-1.595951
H	-1.260512	-0.869859	-2.300115
H	-4.745843	-1.995024	0.025349
H	-3.686540	-2.047713	-2.485897
C	-1.184234	1.670958	2.620927
H	-1.934713	1.241550	3.298471
H	-0.633606	2.434306	3.186868
H	-1.729660	2.183728	1.819758
H	0.321559	0.074978	2.889737
C	3.643646	-0.988987	0.336174
H	3.637172	-0.635882	1.371402
H	4.465131	-1.703606	0.219297
H	3.832237	-0.133929	-0.319509
C	2.037417	-2.852240	0.912569
H	1.073072	-3.311025	0.678178
H	2.823433	-3.605702	0.794723
H	2.020913	-2.531317	1.958106
C	2.300278	-2.108022	-1.485513
H	2.472716	-1.256333	-2.150596
H	3.093287	-2.843928	-1.654672
H	1.341378	-2.565909	-1.744601

E = -649.867589574
G = -649.640071

Mo-N-3'-TSI

Mo	0.031076	0.331908	0.337589
O	0.756232	1.952401	-0.408350
N	-1.195508	-0.746933	-0.201125
C	-2.483460	2.459262	-0.358032
C	-0.184651	0.326382	2.206867
C	-2.136915	2.761387	0.895949
H	0.502426	1.089800	2.617868
Si	1.852843	2.843132	-1.305786
H	-2.728802	2.432598	1.745732
H	-1.260218	3.364903	1.110991
H	-3.371584	1.872829	-0.576365
H	2.002302	2.262856	-2.677045
H	1.338575	4.243024	-1.434899
H	3.185639	2.872418	-0.631471
C	-1.039859	-0.350585	3.225839
H	-1.598421	0.377879	3.829875
H	-1.747013	-1.040078	2.760814
H	-0.416536	-0.922336	3.927578
H	-1.896752	2.798682	-1.206347
C	-2.079149	-1.610453	-0.946946
N	1.680080	-0.833405	0.224337
C	2.446898	-1.423367	1.209732
C	2.254619	-1.164963	-0.992194
C	3.495159	-2.102166	0.634434
H	2.171739	-1.310778	2.248632
C	3.373526	-1.935693	-0.776006
H	1.828599	-0.813997	-1.923706
H	4.264290	-2.653236	1.159681
H	4.033814	-2.329637	-1.537771
C	-2.279624	-1.046319	-2.362256
H	-1.322198	-0.980041	-2.888016
H	-2.945218	-1.694522	-2.941980
H	-2.721155	-0.046156	-2.322157
C	-3.424079	-1.686282	-0.207024
H	-4.113568	-2.343711	-0.747010
H	-3.286084	-2.085497	0.801724
H	-3.881258	-0.695833	-0.127135
C	-1.429400	-3.002760	-1.013103
H	-0.450333	-2.949509	-1.496927
H	-1.287130	-3.407848	-0.007589
H	-2.066356	-3.689311	-1.581457

E = -728.424195156
G = -728.148884

Mo-N-3'-II

Mo	0.100094	-0.614595	0.062255
O	1.826049	-1.132173	-0.723951
N	-1.496242	0.010634	-0.152375
C	-0.523055	-2.528770	-1.264266
C	-0.006285	-1.302364	1.841430
C	-0.406845	-3.085034	-0.012509
H	0.975468	-1.684510	2.164557
Si	3.470590	-0.833087	-0.747888
H	-1.282230	-3.298355	0.592040
H	0.525304	-3.544555	0.300989
H	-1.501578	-2.297817	-1.670890
H	3.866500	-0.100746	-1.991914
H	4.168149	-2.162581	-0.762584
H	3.936602	-0.070537	0.449272
C	-1.071087	-1.423400	2.876276
H	-1.145020	-2.450964	3.259211
H	-2.045331	-1.103706	2.502306
H	-0.808309	-0.796623	3.740120
H	0.317640	-2.548653	-1.949289
C	-2.630693	0.748883	-0.651380
N	0.977952	1.248519	0.339329
C	1.594837	1.966932	-0.664108
C	0.815624	2.103094	1.404619
C	1.830737	3.258348	-0.234778
H	1.822614	1.508604	-1.617796
C	1.334991	3.344549	1.093410
H	0.342076	1.759538	2.314299
H	2.318890	4.040214	-0.802370
H	1.372169	4.205088	1.749258
C	-3.832583	-0.200656	-0.780015
H	-4.712317	0.352783	-1.124592
H	-4.071361	-0.658750	0.184556
H	-3.631029	-0.998185	-1.502020
C	-2.935049	1.863961	0.363775
H	-3.769914	2.477708	0.008797
H	-2.058311	2.502094	0.501787
H	-3.207573	1.437021	1.333642
C	-2.274337	1.358024	-2.017292
H	-3.115958	1.942436	-2.404027
H	-2.040784	0.572481	-2.743522
H	-1.405786	2.016144	-1.924163

E = -728.430980373
G = -728.149538

Mo-N-3'-TSII

Mo	0.107368	-0.605483	0.031201
O	1.870140	-1.095945	-0.694661
N	-1.498766	0.005931	-0.154569
C	-0.380167	-3.048649	-0.064196
C	-0.004785	-1.393653	1.773681
C	-0.455858	-2.463416	-1.315312
H	0.977646	-1.776980	2.089741
Si	3.514295	-0.802552	-0.666212
H	4.209440	-2.133541	-0.650008
H	3.944545	-0.033835	0.540658
H	3.953861	-0.078197	-1.900470
H	0.400179	-2.502054	-1.980225
H	0.533424	-3.541929	0.252314
H	-1.278449	-3.287810	0.495562
C	-2.656604	0.732291	-0.613972
H	-1.423579	-2.242632	-1.752453
C	-1.077877	-1.571586	2.791965
H	-1.123076	-2.606597	3.157943
H	-2.058048	-1.274529	2.414312
H	-0.842670	-0.949581	3.667103
C	-3.838816	-0.240728	-0.751275
H	-4.734369	0.300662	-1.073507
H	-4.056666	-0.725390	0.205280
H	-3.627474	-1.017188	-1.493110
C	-2.971106	1.812604	0.435146
H	-3.828550	2.412129	0.111100
H	-2.109357	2.470792	0.573867
H	-3.214247	1.354162	1.398503
C	-2.334746	1.385824	-1.968043
H	-3.193809	1.964503	-2.323712
H	-2.099528	0.625552	-2.720069
H	-1.477045	2.057343	-1.871401
N	0.954855	1.271092	0.329170
C	0.726820	2.130679	1.378399
C	1.631969	1.985123	-0.637806
C	1.263570	3.371101	1.093454
H	0.200995	1.790306	2.260167
C	1.839173	3.279079	-0.201755
H	1.915733	1.523079	-1.574414
H	1.259950	4.234830	1.746182
H	2.358340	4.059288	-0.743463

E = -728.430972156
G = -728.147575

Mo-N-3'-TBP

Mo	0.241170	-0.302892	-0.010731
O	2.198616	-0.566564	-0.105803
C	0.171700	-1.862668	1.315039
H	1.156266	-1.984429	1.771663
C	0.204587	-1.818460	-1.425180
C	0.138387	-2.654141	-0.089437
H	1.133414	-1.970386	-1.970374
H	1.005477	-3.314691	-0.076026
H	-0.796094	-3.215641	-0.089486
Si	3.742548	-1.066575	-0.434754
H	4.653466	0.103290	-0.643293
H	3.780702	-1.913218	-1.675450
H	4.276448	-1.890256	0.698783
C	-0.946282	-2.207068	2.270446
H	-0.919137	-1.541586	3.139047
H	-0.851006	-3.236072	2.643660
H	-1.926286	-2.103453	1.797556
H	-0.675736	-1.949860	-2.047673
N	-1.472199	-0.074573	-0.127221
C	-2.863250	0.127898	-0.439703
N	0.643643	1.690355	0.177312
C	1.832228	2.336621	-0.129018
C	-0.233636	2.665694	0.631886
C	1.706623	3.679731	0.126846
H	2.676746	1.776480	-0.497089
C	0.386340	3.890300	0.622602
H	-1.229727	2.395687	0.947460
H	2.475441	4.427867	-0.017085
H	-0.051343	4.829431	0.936036
C	-3.457518	-1.186003	-0.976485
H	-4.514153	-1.039614	-1.222809
H	-3.389569	-1.984436	-0.231405
H	-2.940558	-1.507679	-1.884643
C	-3.613496	0.555582	0.833616
H	-3.220675	1.496689	1.227067

H	-3.525121	-0.205228	1.614194
H	-4.675598	0.697436	0.608501
C	-2.959486	1.225572	-1.514969
H	-4.010085	1.428750	-1.748134
H	-2.454833	0.908669	-2.432235
H	-2.489082	2.149444	-1.169093

E = -728.448780115
G = -728.160726

Mo-N-3'-TSIII

O	-1.626342	-1.537146	-0.148551
C	0.954107	-2.493677	-0.638415
C	0.212076	-0.981589	2.165676
C	0.953445	-2.807924	0.713664
H	-0.605128	-1.529177	2.645886
H	1.054550	-0.755259	2.816137
Si	-3.178374	-1.390941	-0.763971
H	1.880714	-2.809365	1.280113
H	0.120253	-3.354207	1.140829
H	-3.330988	-0.176785	-1.617277
H	-3.452062	-2.602386	-1.609204
H	-4.183654	-1.381666	0.344736
C	2.215992	-2.284501	-1.432209
H	2.072413	-1.580670	-2.256062
H	3.035301	-1.925147	-0.805531
H	2.524673	-3.240934	-1.874390
H	0.074930	-2.798245	-1.201463
Mo	-0.006001	-0.527306	0.324206
N	-1.237096	1.139492	0.154049
C	-2.358332	1.387853	0.913120
C	-1.205680	2.090885	-0.841529
C	-3.024649	2.490749	0.414561
H	-2.592856	0.770584	1.769991
C	-2.289756	2.937259	-0.714326
H	-0.416213	2.094359	-1.581117
H	-3.926618	2.928961	0.821896
H	-2.520407	3.779873	-1.353415
N	1.442890	0.401312	0.124458
C	2.515907	1.333886	-0.116457
C	3.789532	0.800672	0.562200
H	4.602159	1.525736	0.448936
H	3.619035	0.641364	1.630836
H	4.112262	-0.144378	0.116027
C	2.752327	1.513413	-1.624194
H	1.850368	1.884204	-2.118861
H	3.554842	2.238783	-1.793191
H	3.042885	0.569290	-2.092809
C	2.111705	2.675789	0.523436
H	1.966590	2.556748	1.600629
H	2.899804	3.417858	0.355815
H	1.176561	3.045136	0.096119

E = -728.420330166
G = -728.135157

Mo-N-3'-IV

Mo	0.090903	-0.499215	0.459541
O	-0.886078	-1.853455	-0.553099
N	1.220288	0.765808	0.158285
C	1.998954	-2.271261	-0.358917
C	0.118016	-0.611885	2.349495
C	1.609803	-2.637084	0.887311
H	-0.545271	-1.346564	2.824680
H	0.728402	-0.043453	3.050375
Si	-2.414829	-2.313300	-1.066491
H	-2.669806	-1.852704	-2.467161
H	-3.488641	-1.809657	-0.160963
H	-2.447278	-3.813263	-1.065902
C	1.825689	1.947041	-0.416233
N	-1.583568	0.683756	0.282526
C	-2.258998	1.395834	1.248766
C	-2.119083	1.048884	-0.937687
C	-3.217733	2.191218	0.658277
H	-1.997405	1.278797	2.291326
C	-3.126216	1.972193	-0.743821
H	-1.747309	0.621367	-1.860119
H	-3.912031	2.843460	1.172056
H	-3.736071	2.422805	-1.516389
H	1.354622	-2.543425	-1.193185
H	2.255771	-2.483518	1.747287
H	0.713835	-3.229897	1.039166
C	3.344142	-1.702642	-0.686513
H	3.277747	-0.885213	-1.408407
H	3.960769	-2.485964	-1.146131
H	3.861196	-1.343935	0.206988
C	3.263883	2.074809	0.109024
H	3.271980	2.103616	1.202426
H	3.714388	3.000514	-0.263821
H	3.883144	1.235892	-0.219982
C	1.809650	1.859304	-1.949853
H	0.781557	1.773717	-2.313374
H	2.378303	0.994019	-2.304127
H	2.254849	2.759737	-2.385805
C	0.983810	3.149415	0.048464
H	1.393839	4.072978	-0.374950
H	0.998388	3.228164	1.138777
H	-0.055215	3.041503	-0.273397

E = -728.424752711
G = -728.142529

Mo-N-3'-TSIV

Mo	-0.024410	-0.312829	0.511298
O	-0.252669	-1.993403	-0.404645
N	0.795687	1.131838	0.080652
C	2.966856	-1.739523	-0.055144
C	0.058586	-0.295803	2.394321
C	2.484168	-2.048623	1.157402
H	-0.330988	-1.190216	2.900102
H	0.497635	0.443884	3.062175
Si	-1.142946	-3.055337	-1.347561
H	-1.336574	-2.497648	-2.722754
H	-2.473581	-3.332087	-0.728983
H	-0.376822	-4.336457	-1.459134
N	-1.942587	0.294930	0.304542
C	-2.877433	0.672945	1.248313
C	-2.532654	0.449719	-0.939702
C	-4.042810	1.043569	0.619862
H	-2.620981	0.650027	2.297785
C	-3.823145	0.900308	-0.781260
H	-1.991305	0.212357	-1.846658
H	-4.951933	1.374890	1.104348
H	-4.532756	1.093961	-1.575280
H	2.485874	-2.176279	-0.929742
H	2.935565	-1.656422	2.065614
H	1.666965	-2.752265	1.274163
C	4.165543	-0.881923	-0.307878
H	3.942742	-0.075668	-1.015205
H	4.968888	-1.477472	-0.759732
H	4.549615	-0.438773	0.615270

C	1.267191	2.339587	-0.556009
C	1.596237	2.060913	-2.030284
H	2.369464	1.292405	-2.120126
H	1.958659	2.971582	-2.518695
H	0.704877	1.717661	-2.564079
C	0.144070	3.385441	-0.451039
H	0.453501	4.315589	-0.939987
H	-0.083606	3.599900	0.596504
H	-0.769142	3.021875	-0.929782
C	2.515608	2.824315	0.197102
H	2.876152	3.761600	-0.239612
H	3.318643	2.084461	0.141056
H	2.281926	3.000924	1.250813

E = -728.422794261
G = -728.144592

Mo-N-3'-V

Mo	0.063650	0.425317	0.424725
O	-0.187620	2.165126	-0.295373
N	-1.124496	-0.758441	0.113272
C	0.063549	0.482042	2.299485
H	0.638022	1.336465	2.687129
H	-0.469276	-0.094538	3.052345
Si	-1.082181	3.527651	-0.697117
H	-2.334766	3.129729	-1.410989
H	-0.253706	4.390484	-1.590244
H	-1.440764	4.281783	0.542678
C	-2.084573	-1.783420	-0.221284
N	1.872459	-0.357365	0.001065
C	2.989952	-0.559512	0.795123
C	2.229258	-0.698741	-1.298998
C	4.029999	-1.002001	0.016688
H	2.936137	-0.373997	1.858172
C	3.544664	-1.088954	-1.323402
H	1.512736	-0.629200	-2.107749
H	5.027547	-1.241242	0.361157
H	4.100578	-1.403142	-2.197083
C	-3.493233	-1.259818	0.096698
H	-3.579261	-1.005043	1.156827
H	-4.240492	-2.025094	-0.137830
H	-3.715471	-0.365412	-0.492623
C	-1.950052	-2.094381	-1.720437
H	-0.942410	-2.451715	-1.951217
H	-2.151667	-1.201956	-2.320539
H	-2.666766	-2.871403	-2.005771
C	-1.765395	-3.030843	0.616976
H	-2.468301	-3.835430	0.376793
H	-1.845537	-2.808361	1.684733
H	-0.749181	-3.378940	0.412910

E = -610.561921812
G = -610.361251

Mo-N-3'-TSA

O	1.070957	-1.662345	-0.745826
C	-1.009244	-2.073685	1.098045
H	-0.441533	-3.005226	1.149030
C	0.198151	-0.192102	2.365222
C	-0.939800	-1.270799	2.426927
H	1.160552	-0.658028	2.626503
H	-0.718809	-1.949867	3.261617
H	-1.887791	-0.762496	2.620972
Si	0.848898	-3.164164	-1.434550
H	-0.550314	-3.339324	-1.941931
H	1.797147	-3.308695	-2.582430
H	1.132069	-4.260924	-0.451738
Mo	0.049010	-0.371739	0.313343
N	1.587031	0.863804	-0.272610
C	2.905312	0.547673	-0.550030
C	1.506965	2.257943	-0.235201
C	3.643516	1.697733	-0.662138
H	3.193925	-0.487304	-0.656374
C	2.745127	2.797495	-0.456677
H	0.560562	2.742324	-0.040656
H	4.702976	1.759795	-0.875465
H	2.990765	3.851355	-0.485830
C	-0.032925	1.079842	3.152938
H	0.767676	1.802555	2.969632
H	-0.981197	1.548203	2.872880
H	-0.060534	0.876035	4.232710
H	-2.027750	-2.267536	0.765208
N	-1.325959	0.559476	-0.118014
C	-2.358647	1.101287	-0.980810
C	-3.537738	0.116758	-0.986170
H	-3.936015	-0.020256	0.023570
H	-4.340405	0.502189	-1.623303
H	-3.225465	-0.857817	-1.371464
C	-1.789052	1.271358	-2.397573
H	-2.547607	1.706197	-3.056739
H	-0.916215	1.929973	-2.388518
H	-1.485401	0.304776	-2.810562
C	-2.797517	2.457943	-0.408699
H	-3.595582	2.883904	-1.025385
H	-3.172056	2.345037	0.612731
H	-1.962044	3.163601	-0.395182

E = -728.431974869
G = -728.147689

Mo-N-3'-SBP

O	-0.285299	1.997375	-0.815837
C	0.699931	1.498695	1.765423
C	-0.508337	-0.372738	2.139752
C	0.622361	0.395267	2.803406
H	-1.463160	0.130241	2.364700
Si	-0.369118	3.675476	-0.878054
H	-1.113800	4.214976	0.301782
H	1.011137	4.249710	-0.891554
H	-1.082439	4.057727	-2.132025
H	0.444549	0.714298	3.843203
H	1.538755	-0.206974	2.792794
H	-0.035600	2.292471	1.951452
N	1.316840	-0.582394	-0.220652
C	2.568502	-1.101813	-0.731806
Mo	-0.080688	0.343419	0.097249
N	-1.744159	-0.732979	-0.321991
C	-3.043282	-0.552303	0.116304
C	-1.785259	-1.675241	-1.343714
C	-3.890858	-1.338271	-0.626946
H	-3.269672	0.138110	0.917396
C	-3.085662	-2.058643	-1.559186
H	-0.874446	-2.003826	-1.823601
H	-4.966548	-1.391150	-0.521016
H	-3.425654	-2.778286	-2.292246
C	3.711061	-0.209644	-0.224754
H	4.673130	-0.596813	-0.576204
H	3.595090	0.814163	-0.592095
H	3.726744	-0.186021	0.868463
C	2.738853	-2.539214	-0.217472
H	1.910578	-3.170625	-0.550886

H	3.674425	-2.964480	-0.595486
H	2.767289	-2.557351	0.875524
C	2.513900	-1.081659	-2.267355
H	2.357235	-0.063526	-2.635501
H	3.455013	-1.459111	-2.680519
H	1.700351	-1.712727	-2.636824
C	-0.626219	-1.861479	2.403669
H	-0.803492	-2.046640	3.473748
H	-1.449449	-2.314385	1.844607
H	0.296755	-2.383010	2.128938
H	1.673398	1.953868	1.554894

E = -728.456125526
G = -728.171980

Mo-N-3'-TSB

C	0.515975	-1.078276	-2.171266
C	-1.640224	-1.673842	-1.411983
C	-0.918210	-0.828869	-2.312806
H	-1.173900	-2.642551	-1.236737
H	-1.357547	-0.300175	-3.165994
H	-0.832937	0.413299	-1.666101
O	0.006487	-1.814781	1.021347
Si	0.939902	-2.478020	2.240703
H	1.435239	-3.823060	1.811438
H	2.118498	-1.608069	2.557839
H	0.102309	-2.633549	3.468964
H	0.809117	-2.123158	-2.059771
Mo	-0.100810	-0.338381	-0.216756
C	-3.130076	-1.613071	-1.215413
H	-3.666600	-2.181797	-1.988932
H	-3.409549	-2.041146	-0.247439
H	-3.506494	-0.586267	-1.231454
H	1.208228	-0.478298	-2.754420
N	-1.513031	1.013662	0.349874
C	-1.561863	1.346961	1.695493
C	-2.489612	1.754127	-0.287001
C	-2.569953	2.257362	1.904534
H	-0.873250	0.903399	2.402546
C	-3.160367	2.522292	0.634088
H	-2.627773	1.682792	-1.356853
H	-2.853689	2.684704	2.857335
H	-3.980213	3.197045	0.425605
N	1.377366	0.567280	-0.047423
C	2.656536	1.191227	-0.286643
C	3.035468	1.953659	0.995417
H	3.999063	2.456967	0.862885
H	2.278206	2.706059	1.232847
H	3.115666	1.265656	1.841892
C	2.523340	2.172223	-1.462546
H	3.471905	2.692968	-1.630588
H	2.254832	1.645644	-2.383029
H	1.749123	2.915730	-1.253139
C	3.706028	0.110292	-0.589886
H	4.689275	0.568591	-0.740118
H	3.777543	-0.597146	0.241386
H	3.443870	-0.446203	-1.494108

E = -728.407125685
G = -728.125835

Mo-N-3'-B

C	-0.897107	-1.847201	-1.113832
C	-3.372621	-1.473597	-0.854324
C	-2.230390	-1.376138	-1.555185
H	-0.956998	-2.588273	-0.301922
H	-2.261671	-0.884953	-2.529229
H	-0.296030	-2.246204	-1.930419
H	-0.104997	0.072986	-1.736841
O	-0.949104	-0.386260	1.523520
Si	-2.199846	-0.196979	2.625293
H	-2.832987	-1.529337	2.874336
H	-1.640725	0.325652	3.908808
H	-3.232129	0.751104	2.109185
H	-3.345812	-1.961064	0.122063
C	-4.706546	-0.979918	-1.315982
H	-5.433768	-1.799577	-1.377505
H	-5.123357	-0.245896	-0.614780
H	-4.642170	-0.508380	-2.301083
N	1.675048	-0.749232	-0.143100
C	3.069871	-1.109000	-0.029024
Mo	0.059425	-0.212166	-0.094252
C	3.184735	-2.397605	0.798657
H	2.644713	-3.217220	0.315561
H	4.235528	-2.688455	0.899269
H	2.769000	-2.251419	1.800047
C	3.614759	-1.323961	-1.449427
H	3.512012	-0.409919	-2.040183
H	4.673850	-1.598618	-1.405810
H	3.069317	-2.125653	-1.955264
C	3.809111	0.047459	0.661300
H	3.429269	0.198550	1.676194
H	4.878504	-0.179223	0.724305
H	3.680207	0.977120	0.100717
N	0.117219	1.783647	-0.383425
C	-0.231317	2.627661	-1.420695
C	0.565969	2.582247	0.662964
C	-0.032626	3.931020	-1.038003
H	-0.591226	2.217682	-2.353157
C	0.477341	3.902488	0.295295
H	0.898921	2.145533	1.595814
H	-0.228166	4.809394	-1.638939
H	0.740619	4.753269	0.910361

E = -728.439891502
G = -728.162562

Mo-N-3'-TSC

Mo	-0.228991	0.091817	-0.025395
C	-1.781693	-0.797070	-1.293858
C	-4.136455	-0.321371	-0.567536
C	-3.113067	-0.165466	-1.422757
H	-1.841349	-1.725524	-0.705511
H	-3.275560	0.457380	-2.304883
H	-1.348073	-1.039171	-2.265023
H	-0.520365	1.178376	-1.398463
O	-0.867156	-0.395081	1.737627
Si	-0.593955	-1.461082	2.996122
H	-1.908922	-1.991112	3.472560
H	0.267388	-2.614032	2.577801
H	0.080981	-0.738522	4.118240
C	-1.310032	2.317420	-0.785440
H	-2.120487	2.191137	-1.498698
H	-0.539619	3.030456	-1.067716
C	-1.547928	2.066561	0.562593
H	-0.926426	2.529104	1.321002
H	-2.488813	1.629235	0.879356
H	-3.986500	-0.948155	0.313752
C	-5.491154	0.292089	-0.726708
H	-6.272391	-0.476831	-0.780953
H	-5.743943	0.929912	0.130114

H	-5.554150	0.902116	-1.633116
N	0.908366	-1.102829	-0.513738
C	2.035707	-1.921586	-0.879598
C	2.363886	-1.668720	-2.359727
H	3.207796	-2.294483	-2.667923
H	1.505984	-1.909263	-2.994767
H	2.632472	-0.620540	-2.514068
C	1.660101	-3.395103	-0.652423
H	1.401103	-3.571704	0.395187
H	0.806551	-3.680921	-1.274593
H	2.506983	-4.037894	-0.913810
C	3.224440	-1.517419	0.010276
H	3.449621	-0.453752	-0.104369
H	3.004628	-1.717022	1.062731
H	4.107082	-2.099761	-0.275064
N	1.287091	1.524590	-0.000049
C	2.102716	2.010758	-0.989507
C	1.848761	1.870774	1.210305
C	3.170830	2.679462	-0.420143
H	1.861664	1.843532	-2.030977
C	3.009080	2.588197	0.987230
H	1.373837	1.599371	2.144615
H	3.964939	3.185408	-0.954074
H	3.646475	3.018645	1.748790

E = -806.972581895
G = -806.643064

Mo-N-3'-C

C	0.519898	-1.912921	1.206590
C	2.908408	-1.631587	0.433036
C	1.949323	-1.585894	1.383521
H	0.336577	-2.753743	0.533752
H	2.235320	-1.199995	2.363104
H	-0.016655	-2.047622	2.141487
H	-1.351030	-0.252151	3.253777
O	0.479395	-1.251157	-1.428128
Si	-0.060232	-2.379460	-2.535785
H	0.962737	-2.530420	-3.613902
H	-0.257830	-3.703576	-1.861875
H	-1.361797	-1.960087	-3.145982
C	-0.319175	0.091708	3.388851
H	0.266530	-0.767094	3.735494
H	-0.321146	0.814863	4.215972
C	0.246549	0.717445	2.121658
H	-0.255854	1.676849	1.938157
H	1.305225	0.966522	2.261244
H	2.644644	-1.982179	-0.562803
C	4.338610	-1.256404	0.656219
H	4.998451	-2.118689	0.495455
H	4.662758	-0.484274	-0.052766
H	4.509398	-0.885993	1.671901
Mo	0.006669	-0.128879	0.072779
N	-1.688937	0.005622	0.122081
C	-3.124937	0.174113	0.133979
C	-3.756098	-1.090860	0.733917
H	-4.846439	-0.992428	0.754602
H	-3.497913	-1.970758	0.137759
H	-3.402591	-1.250613	1.756212
C	-3.459295	1.405881	0.989218
H	-3.104693	1.273917	2.014805
H	-2.991048	2.303412	0.575295
H	-4.543250	1.559142	1.013579
C	-3.603129	0.378402	-1.312034
H	-3.152536	1.274260	-1.749005
H	-3.339398	-0.481181	-1.934211
H	-4.691279	0.498782	-1.328929
N	0.917996	1.612836	-0.424191
C	2.205821	2.060034	-0.188888
C	0.301815	2.558170	-1.240697
C	2.410999	3.241636	-0.855999
H	2.878172	1.486650	0.433366
C	1.190754	3.560349	-1.531087
H	-0.724808	2.428281	-1.552988
H	3.327619	3.816882	-0.868310
H	0.998131	4.426220	-2.150840

E = -807.029274255
G = -806.694454

Mo-O-3-I

Mo	0.375391	0.368243	0.274377
O	1.599376	-0.833346	-0.510472
C	0.348509	1.946989	-0.741818
H	0.457976	1.686798	-1.807935
Si	2.957788	-1.831758	-0.450915
H	2.635556	-3.096800	-1.171827
H	4.093741	-1.133173	-1.121908
H	3.314872	-2.127862	0.969013
C	0.308727	3.406058	-0.429806
H	-0.575284	3.866856	-0.891151
H	0.266358	3.588327	0.646326
H	1.186062	3.921068	-0.842615
N	-1.490466	-0.291809	-0.000935
C	-2.470749	0.042537	-0.923025
C	-1.977594	-1.363430	0.745003
C	-3.541334	-0.799954	-0.774069
H	-2.312550	0.864017	-1.607052
C	-3.226473	-1.698679	0.292532
H	-1.394842	-1.788346	1.552617
H	-4.454952	-0.778756	-1.353370
H	-3.853901	-2.489583	0.681557
O	0.556657	0.896771	1.851589

E = -512.547436949
G = -512.435091

Mo-O-3-Ianti

Mo	0.360821	0.341915	0.526531
O	1.603402	-0.570102	-0.557519
C	0.334741	2.157820	0.017800
H	0.281013	2.935990	0.783421
Si	2.913847	-1.618613	-0.748359
H	2.605452	-2.543188	-1.876929
H	4.127570	-0.809141	-1.062761
H	3.133983	-2.396928	0.507190
C	0.498351	2.640175	-1.395267
H	1.406700	3.249898	-1.489309
H	0.557274	1.829129	-2.127247
H	-0.347621	3.282915	-1.673206
N	-1.495758	-0.214086	0.036963
C	-2.483417	0.390579	-0.724285
C	-1.961943	-1.480975	0.382751
C	-3.538896	-0.472238	-0.867889
H	-2.345238	1.396410	-1.092902
C	-3.205583	-1.669038	-0.160566
H	-1.371041	-2.139559	1.007030
H	-4.454789	-0.274449	-1.409047
H	-3.818089	-2.555038	-0.058923
O	0.507502	0.373197	2.192695

E = -512.545431198
G = -512.432486

Mo-O-3-TSrot1

Mo	0.389855	0.410122	0.173462
O	1.876976	-0.386817	-0.647619
C	0.265659	2.164560	-0.491720
H	1.310826	2.522218	-0.535853
Si	3.055728	-1.549645	-0.279732
H	3.735425	-1.899667	-1.559669
H	4.031457	-0.969242	0.687442
H	2.404933	-2.758701	0.306936
C	-0.788552	3.227410	-0.562812
H	-0.712849	3.776906	-1.510812
H	-1.795169	2.803901	-0.504767
H	-0.680660	3.962482	0.247049
N	-1.373697	-0.453583	0.034902
C	-1.942181	-0.852039	-1.178689
C	-2.242063	-0.846074	1.052977
C	-3.140127	-1.459939	-0.925945
H	-1.447185	-0.641895	-2.117661
C	-3.330364	-1.456677	0.495611
H	-1.984757	-0.653506	2.084434
H	-3.818133	-1.859108	-1.668471
H	-4.176992	-1.860948	1.034071
O	0.705606	0.456708	1.846029

E = -512.504592771
G = -512.393473

Mo-O-3-TSrot2

Mo	0.325184	0.292639	0.239962
O	1.443263	-0.900293	-0.659133
C	0.728639	2.016863	-0.289165
H	-0.354601	2.224007	-0.019999
Si	2.671938	-2.054540	-0.505741
H	2.232772	-3.294692	-1.208008
H	3.907374	-1.516068	-1.146043
H	2.909737	-2.324379	0.941935
C	1.640448	3.186888	-0.355563
H	1.707346	3.718317	0.603311
H	2.646669	2.858809	-0.633530
H	1.309788	3.905066	-1.116531
N	-1.616963	-0.079053	0.025025
C	-2.474452	0.492795	-0.912988
C	-2.322953	-1.080680	0.681472
C	-3.685592	-0.144259	-0.852491
H	-2.135667	1.296029	-1.552786
C	-3.590294	-1.143536	0.164845
H	-1.857406	-1.647452	1.475631
H	-4.551610	0.082082	-1.460026
H	-4.372610	-1.818968	0.484374
O	0.686398	0.097158	1.889359

E = -512.505911137
G = -512.396204

Mo-O-3-TSI

Mo	-0.314663	-0.306478	0.179758
O	-0.701323	1.373582	-0.625325
C	-3.349467	0.371690	0.930017
C	-0.576344	-1.748484	-1.005404
C	-3.466902	-0.424285	-0.138054
H	-0.560963	-1.393763	-2.049003
Si	-0.618492	3.051371	-0.676410
H	-3.500882	-0.022829	-1.147216
H	-3.567355	-1.501006	-0.034017
H	-3.281464	1.451007	0.827624
H	0.392119	3.472442	-1.689846
H	-1.964213	3.577208	-1.060935
H	-0.247159	3.592419	0.666872
C	-0.852951	-3.205261	-0.830819
H	-0.057327	-3.796867	-1.303989
H	-0.906125	-3.488303	0.222556
H	-1.790696	-3.491796	-1.326104
H	-3.326783	-0.029189	1.938756
N	1.686001	-0.239342	0.128377
C	2.599822	-0.796237	-0.749970
C	2.399425	0.565478	1.007429
C	3.859460	-0.347350	-0.443785
H	2.265255	-1.471980	-1.524032
C	3.731666	0.523559	0.681451
H	1.899260	1.086989	1.813443
H	4.774391	-0.614932	-0.955761
H	4.529932	1.043813	1.194303
O	-0.630369	-0.901033	1.718253

E = -591.105708162
G = -590.946148

Mo-O-3-II

Mo	-0.611989	-0.143083	0.250772
O	-0.249304	1.665915	-0.313386
C	-2.823371	1.237960	0.884609
C	-1.156806	-1.347494	-1.113294
C	-3.154488	0.642265	-0.281617
H	-0.995133	-0.938388	-2.123514
Si	1.042532	2.600935	-0.860991
H	-2.964573	1.127624	-1.234809
H	-3.726866	-0.280185	-0.304451
H	-2.337790	2.207996	0.898697
H	2.011735	1.792068	-1.655320
H	0.457126	3.667978	-1.733711
H	1.728704	3.254730	0.293869
C	-1.782016	-2.702649	-1.089142
H	-1.120087	-3.422695	-1.589768
H	-1.966057	-3.056471	-0.072957
H	-2.725755	-2.711547	-1.652084
H	-3.091645	0.794275	1.838040
N	1.366840	-0.578289	0.200139
C	2.087915	-1.384631	-0.661865
C	2.275001	-0.004870	1.074690
C	3.422923	-1.322533	-0.344751
H	1.580309	-1.947173	-1.432837
C	3.543188	-0.440140	0.769127
H	1.944731	0.655644	1.866277
H	4.223926	-1.851800	-0.843935
H	4.453139	-0.166359	1.287006
O	-1.051399	-0.859507	1.707565

E = -591.107454219
G = -590.943320

Mo-O-3-TSII

Mo	-0.628688	-0.139691	0.194322
O	-0.119903	1.591504	-0.473833
C	-2.526100	1.291401	1.017645
C	-1.398821	-1.159592	-1.218875
C	-3.094364	0.651106	-0.042772

H	-1.291346	-0.656736	-2.191570
Si	1.118013	2.734717	-0.416948
H	-3.128613	1.115627	-1.023921
H	-3.684321	-0.250076	0.091383
H	-2.092533	2.278304	0.900055
H	2.162075	2.338434	0.569419
H	1.703773	2.892695	-1.781578
H	0.518222	4.044720	-0.003820
C	-2.062317	-2.492594	-1.269458
H	-1.428463	-3.184724	-1.841596
H	-2.218037	-2.917658	-0.275965
H	-3.022958	-2.442132	-1.800036
H	-2.638848	0.905244	2.025812
N	1.345987	-0.684314	0.091109
C	2.192717	-0.555407	-0.990337
C	2.114319	-1.083356	1.169354
C	3.479841	-0.864531	-0.605241
H	1.814692	-0.249543	-1.956868
C	3.428343	-1.203053	0.776230
H	1.649448	-1.274761	2.126614
H	4.354162	-0.859657	-1.243295
H	4.254713	-1.513748	1.402128
O	-0.932958	-1.011336	1.601575

E = -591.106336740
G = -590.939888

Mo-O-3-TBP

O	0.473886	1.506949	0.117528
C	1.731779	-0.136869	-1.678352
H	1.868748	0.876538	-2.047192
C	1.888700	-0.716869	1.008936
C	2.617316	-0.467711	-0.413716
H	2.051590	0.143212	1.659820
H	3.284628	0.378712	-0.254132
H	3.160467	-1.388511	-0.624133
Si	0.887768	3.121676	0.227079
H	-0.336332	3.960056	0.404803
H	1.800185	3.330719	1.395680
H	1.599611	3.549896	-1.019407
Mo	0.278769	-0.404879	-0.230562
N	-1.719352	-0.219887	-0.010394
C	-2.449406	0.929069	0.278208
C	-2.632904	-1.265887	-0.120510
C	-3.780644	0.613120	0.349862
H	-1.946381	1.873622	0.411750
C	-3.898020	-0.788116	0.095445
H	-2.283856	-2.262751	-0.347988
H	-4.585314	1.305071	0.562107
H	-4.809449	-1.371211	0.074299
C	2.215499	-2.032771	1.673010
H	1.616506	-2.150426	2.581397
H	1.999955	-2.877311	1.013279
H	3.271929	-2.075650	1.969713
H	1.798176	-0.896083	-2.453002
O	0.182867	-2.051828	-0.605908

E = -591.116533877
G = -590.946705

Mo-O-3-TSIII

O	-0.208968	1.495978	0.397607
C	-2.595168	0.269991	-0.438478
C	-1.014922	-1.060250	1.927204
C	-2.805372	-0.122806	0.894924
H	-0.954808	-0.423932	2.812743
H	-1.347487	-2.079700	2.116967
Si	0.324086	2.901026	-0.362746
H	-3.353622	-1.038701	1.099631
H	-2.836489	0.634440	1.671552
H	1.119788	2.578428	-1.581682
H	-0.876247	3.706798	-0.760191
H	1.138472	3.698134	0.601294
C	-3.157848	-0.508721	-1.600734
H	-2.542869	-0.402169	-2.498178
H	-3.233912	-1.574881	-1.374423
H	-4.161599	-0.134012	-1.838994
H	-2.438993	1.333724	-0.600711
O	-0.658175	-1.723557	-0.812042
N	1.595436	-0.469507	-0.035857
C	2.531815	0.351385	0.568656
C	2.295663	-1.407590	-0.776075
C	3.797025	-0.055668	0.212831
H	2.221803	1.149014	1.228782
C	3.645247	-1.178300	-0.651410
H	1.760645	-2.164112	-1.332575
H	4.725242	0.397257	0.536719
H	4.434575	-1.746843	-1.125829
Mo	-0.442887	-0.408783	0.211150

E = -591.099182488
G = -590.930898

Mo-O-3-IV

Mo	-0.387249	-0.419162	0.149047
O	-0.334680	1.492056	0.116483
C	-3.142634	0.441437	-0.393384
C	-0.492689	-1.290723	1.821038
C	-2.993174	0.297013	0.939539
H	-0.283609	-0.750364	2.750733
H	-0.823111	-2.320972	1.961279
Si	0.766396	2.770914	0.183764
H	-3.416265	-0.556265	1.463503
H	-2.550617	1.082025	1.544298
H	1.963317	2.412980	0.998082
H	1.171093	3.161850	-1.199381
H	0.051130	3.918995	0.822884
C	-3.870826	-0.510917	-1.283857
H	-3.221122	-0.863617	-2.090944
H	-4.238352	-1.380889	-0.733629
H	-4.726047	-0.004013	-1.747083
H	-2.744767	1.343055	-0.858466
N	1.604237	-0.574781	-0.102576
C	2.243866	-0.113436	-1.244303
C	2.584811	-1.067211	0.743276
C	3.597882	-0.305136	-1.116275
H	1.679294	0.300000	-2.069999
C	3.815442	-0.914762	0.156461
H	2.308637	-1.498005	1.695256
H	4.349840	-0.047190	-1.850524
H	4.765951	-1.211321	0.579890
O	-0.969841	-1.488105	-1.005920

E = -591.106846006
G = -590.943613

Mo-O-3-TSIV

Mo	0.142450	-0.446667	-0.146423
O	0.422121	1.396304	-0.461434
C	3.428604	0.060349	0.351745

C	0.275991	-1.512780	-1.689690
C	3.251483	-0.130880	-0.962650
H	0.570503	-2.561861	-1.718493
H	0.139958	-1.039295	-2.668300
Si	0.182487	3.030086	-0.126315
H	3.189204	1.038196	0.771490
H	3.494054	-1.081474	-1.432208
H	2.900974	0.665341	-1.611701
H	-1.074115	3.496915	-0.779913
H	0.098353	3.236952	1.351070
H	1.350754	3.785104	-0.669447
C	3.939044	-0.962837	1.313259
H	4.821000	-0.589569	1.847115
H	3.174964	-1.193190	2.064631
H	4.208324	-1.893705	0.806501
N	-1.838324	-0.474085	0.094562
C	-2.431938	0.060982	1.233054
C	-2.859995	-0.854374	-0.761472
C	-3.795041	0.029337	1.088428
H	-1.830096	0.400941	2.065975
C	-4.068252	-0.556102	-0.186995
H	-2.625223	-1.314742	-1.710220
H	-4.520584	0.371355	1.814648
H	-5.042734	-0.742955	-0.618411
O	0.707356	-1.361648	1.140114

E = -591.105990140
G = -590.945977

Mo-O-3-V

Mo	0.377517	-0.668525	0.148610
O	1.622423	0.600372	-0.452270
C	0.314146	-2.095552	-1.067148
H	0.432421	-1.854144	-2.129259
H	0.263592	-3.156943	-0.827609
Si	2.984590	1.585497	-0.268774
H	2.676836	2.909901	-0.879677
H	3.301055	1.746111	1.181347
H	4.130269	0.941192	-0.974247
N	-1.458881	0.085211	-0.009299
C	-1.902585	1.052985	0.892388
C	-2.446722	-0.061885	-0.972469
C	-3.130697	1.508803	0.494315
H	-1.309004	1.321067	1.757127
C	-3.477961	0.796551	-0.696769
H	-2.321717	-0.778927	-1.770786
H	-3.725828	2.258218	0.998876
H	-4.388094	0.903659	-1.271917
O	0.549527	-1.376741	1.652339

E = -473.237945740
G = -473.151943

Mo-O-3-TSA

O	-0.754054	1.521699	-0.443148
C	-2.485454	-0.599656	-0.186190
H	-2.903203	-0.057872	-1.032942
C	-0.366869	-1.933463	-0.927773
C	-1.912234	-1.993117	-0.563298
H	-0.253356	-1.623343	-1.974310
H	-2.422825	-2.338708	-1.469552
H	-2.061264	-2.718302	0.239955
Si	-1.764961	2.801167	-0.076584
H	-1.525102	3.302350	1.312709
H	-1.488960	3.898890	-1.052711
H	-3.205383	2.399472	-0.190393
Mo	-0.433192	-0.269299	0.268604
N	1.484535	0.384856	0.071948
C	2.054754	1.300465	-0.793695
C	2.532317	-0.258842	0.740884
C	3.419901	1.228357	-0.698581
H	1.421487	1.922354	-1.407751
C	3.725927	0.228470	0.286029
H	2.322086	-0.989847	1.509147
H	4.130812	1.822678	-1.257852
H	4.709443	-0.066416	0.628156
C	0.436916	-3.177364	-0.610627
H	1.499502	-3.001578	-0.803039
H	0.328237	-3.470609	0.437918
H	0.116873	-4.023828	-1.233074
H	-3.168537	-0.618160	0.661672
O	-0.423395	-0.747443	1.872990

E = -591.103297663
G = -590.934442

Mo-O-3-SBP

O	1.506207	-1.285804	0.317553
C	1.908369	1.314013	-0.561480
C	-0.244088	1.890953	-0.817667
C	1.109797	2.583795	-0.783543
H	-0.398803	1.441483	-1.809043
Si	2.688771	-2.155364	-0.517967
H	4.040205	-1.702390	-0.074229
H	2.496596	-3.597447	-0.193174
H	2.549642	-1.944304	-1.991602
H	1.373409	3.178684	-1.670962
H	1.177919	3.239609	0.091916
H	2.111332	0.779910	-1.497621
Mo	0.364282	0.206912	0.469224
N	-1.431304	-0.494946	-0.055144
C	-2.029242	-0.785885	-1.268494
C	-2.260247	-1.003047	0.949154
C	-3.191177	-1.479866	-1.044515
H	-1.567583	-0.492343	-2.200513
C	-3.340109	-1.615288	0.371493
H	-2.013382	-0.862955	1.993136
H	-3.863579	-1.855133	-1.804711
H	-4.154441	-2.096978	0.895865
C	-1.474163	2.665200	-0.379793
H	-1.632895	3.523818	-1.048378
H	-2.377654	2.049958	-0.404139
H	-1.355944	3.058523	0.635399
H	2.818811	1.352911	0.046337
O	0.368545	0.967904	1.953813

E = -591.134540982
G = -590.965242

Mo-O-3-TSB

C	1.581419	-1.722971	-1.430149
C	2.123885	-1.111516	0.780551
C	1.553517	-2.117023	-0.030672
H	2.918158	-0.527616	0.314344
H	1.259851	-3.102610	0.335568
H	0.053310	-1.801173	0.032055
O	0.865713	1.294234	0.651801
Si	0.855489	2.966714	0.442799
H	2.137877	3.392767	-0.197689
H	-0.290380	3.416906	-0.403901

H	0.750689	3.580380	1.800529
H	2.502415	-1.270866	-1.798009
Mo	0.359876	-0.154896	-0.498066
C	2.051337	-1.076470	2.275697
H	2.979709	-1.444708	2.730400
H	1.899043	-0.047972	2.619691
H	1.225019	-1.686342	2.655572
H	1.053225	-2.327776	-2.164089
O	0.228147	0.562947	-2.030713
N	-1.581831	-0.379878	-0.029990
C	-2.479985	0.649794	-0.297581
C	-2.279848	-1.355109	0.673383
C	-3.701979	0.332536	0.234215
H	-2.170113	1.513210	-0.868222
C	-3.574293	-0.948134	0.856499
H	-1.785381	-2.262582	0.991348
H	-4.597348	0.937119	0.173358
H	-4.350071	-1.502017	1.368212

E = -591.077541865
G = -590.912192

Mo-O-3-TSB$_{transX}$

O	-0.592458	-1.742549	-0.091881
C	-0.191882	1.190018	1.900413
C	-1.495276	1.999534	0.097642
C	-1.506126	1.350542	1.386940
H	-0.716704	2.758246	-0.022791
Si	-1.805157	-2.858068	0.240286
H	-2.624213	-3.113703	-0.982935
H	-1.159996	-4.124668	0.693058
H	-2.698787	-2.327935	1.321921
H	-2.415821	1.122200	1.945143
H	-1.747214	-0.044834	0.765186
H	0.514998	1.998439	1.741141
Mo	-0.304471	0.142767	-0.211592
N	1.707353	0.179681	0.013942
C	2.556037	0.140320	1.110594
C	2.504224	-0.032760	-1.118660
C	3.840106	-0.087971	0.691556
H	2.174687	0.255705	2.112849
C	3.806863	-0.193822	-0.734051
H	2.060437	-0.029246	-2.102801
H	4.710929	-0.167681	1.329041
H	4.649437	-0.351104	-1.394451
C	-2.737319	2.195615	-0.719114
H	-3.271498	3.109063	-0.426964
H	-2.486366	2.272602	-1.780868
H	-3.430474	1.354217	-0.599641
H	-0.027897	0.575494	2.781914
O	-0.417888	0.505461	-1.863929

E = -591.074373795
G = -590.908860

Mo-O-3-B

C	1.685128	-1.627496	0.298001
C	3.330849	0.206809	0.776507
C	2.401731	-0.675183	1.177594
H	3.601035	0.235413	-0.280792
H	2.134146	-0.707811	2.235142
H	-0.142434	-1.159032	1.300510
O	0.466933	0.437697	-1.480628
Si	1.004778	2.032444	-1.670561
H	2.409053	1.988442	-2.173717
H	0.124048	2.692315	-2.676707
H	0.947145	2.764431	-0.372626
H	2.168454	-1.735609	-0.686033
Mo	-0.233107	-0.889368	-0.344045
C	4.060574	1.152367	1.676518
H	5.141951	0.967814	1.651199
H	3.915853	2.193586	1.361979
H	3.725122	1.061602	2.713811
H	1.564078	-2.613459	0.751324
O	-0.844736	-2.292380	-1.006958
N	-1.764589	0.042760	0.528168
C	-2.814571	0.453701	-0.293803
C	-2.045264	0.487849	1.809828
C	-3.718324	1.158783	0.455566
H	-2.835540	0.196116	-1.345036
C	-3.225913	1.182011	1.799160
H	-1.367340	0.266404	2.621245
H	-4.636008	1.602214	0.092308
H	-3.696688	1.651926	2.652394

E = -591.115782361
G = -590.951547

Mo-O-3-TSC

C	1.869475	0.126007	-1.228375
C	4.071201	-0.201485	-0.074924
C	3.021107	-0.669995	-0.768359
H	2.068238	1.206295	-1.157482
H	3.030060	-1.721308	-1.066431
H	1.627436	-0.107417	-2.267700
H	0.482313	-1.415468	-0.119258
O	-0.484453	1.728210	0.844647
Si	-1.115058	3.238572	0.417612
H	-1.190369	4.047440	1.671508
H	-0.217145	3.916630	-0.564396
H	-2.486239	3.104083	-0.163451
C	1.005534	-1.474182	1.343226
H	1.887920	-1.987579	0.969128
H	0.198571	-2.107410	1.703934
C	1.121002	-0.177837	1.812355
H	0.377556	0.236201	2.482962
H	2.057787	0.360230	1.711041
H	4.082024	0.854976	0.201958
C	5.264009	-1.006218	0.333362
H	6.185548	-0.595882	-0.098501
H	5.400398	-0.994714	1.422357
H	5.176711	-2.048912	0.012897
Mo	-0.157936	0.213903	-0.300127
N	-1.705615	-1.029872	-0.020009
C	-1.853181	-2.412666	-0.049363
C	-2.986486	-0.487598	0.068103
C	-3.180621	-2.732215	0.037353
H	-0.990952	-3.055488	-0.153403
C	-3.905522	-1.500626	0.118773
H	-3.134334	0.582745	0.094843
H	-3.596196	-3.731111	0.042409
H	-4.977078	-1.382530	0.211085
O	-0.560285	0.889953	-1.793095

E = -669.641066802
G = -669.425338

Mo-O-3-C

C	1.731921	-1.389716	-0.637048
C	3.444655	-0.220944	0.778793
C	2.454178	-1.114583	0.623634

H	3.776313	0.349319	-0.090676
H	2.152605	-1.700794	1.492747
O	0.702553	1.126111	-1.148574
Si	1.554131	2.537058	-0.781527
H	1.684403	2.718273	0.693644
H	2.908803	2.458236	-1.404774
H	0.796428	3.679403	-1.370176
H	2.224341	-0.922607	-1.500124
Mo	-0.243088	-0.457043	-0.758469
C	4.172857	0.037623	2.059834
H	5.245359	-0.170088	1.955212
H	4.088598	1.089067	2.362862
H	3.786898	-0.581910	2.875097
H	1.606236	-2.457639	-0.828379
O	-0.907258	-1.217155	-2.084949
C	-0.499034	-2.022039	0.777664
H	0.195395	-2.848535	0.608838
H	-0.229904	-1.571291	1.741314
C	-1.926118	-2.573359	0.832435
H	-1.989085	-3.370465	1.585576
H	-2.660534	-1.808477	1.097252
H	-2.225998	-3.009515	-0.126224
N	-1.636742	0.392373	0.397811
C	-2.836122	0.823192	-0.174811
C	-1.624536	0.826982	1.710178
C	-3.546650	1.531057	0.756926
H	-3.082291	0.569392	-1.196756
C	-2.770971	1.538112	1.960101
H	-0.784942	0.614554	2.356993
H	-4.516266	1.986622	0.607040
H	-3.030735	2.017254	2.894871

E = -669.707698952
G = -669.489090

Mo-O-4-I

Mo	-0.668183	0.646444	0.191240
O	0.942974	0.122439	-0.665590
C	-1.504466	1.916229	-0.910908
H	-1.310070	1.664632	-1.966687
C	-2.271752	3.174172	-0.673109
H	-3.280224	3.087962	-1.099920
H	-2.369470	3.395549	0.391998
H	-1.789384	4.026534	-1.169369
N	-1.963033	-0.872164	0.079409
C	-3.011909	-1.138975	-0.786780
C	-1.829773	-1.978371	0.916167
C	-3.520382	-2.382530	-0.515290
H	-3.303806	-0.405953	-1.525033
C	-2.764944	-2.919165	0.573474
H	-1.082253	-1.996433	1.699262
H	-4.345049	-2.859948	-1.027896
H	-2.904460	-3.881080	1.048635
O	-0.730063	1.314717	1.725333
C	2.252416	-0.113321	-0.381787
C	3.005594	-0.835924	-1.312386
C	2.844712	0.355981	0.795622
C	4.349707	-1.090895	-1.056328
H	2.523450	-1.187781	-2.218862
C	4.190997	0.094054	1.037126
H	2.252116	0.922831	1.509801
C	4.948525	-0.628795	0.115930
H	4.932152	-1.654399	-1.779957
H	4.648429	0.460168	1.952043
H	5.997865	-0.829568	0.309715

E = -738.378515425
G = -738.203100

Mo-O-4-Ianti

Mo	-0.663511	-0.679556	-0.454109
O	0.891606	-0.197942	0.518182
C	-1.407512	-2.201477	0.374842
H	-1.844434	-2.990940	-0.242358
C	-1.363523	-2.473124	1.850884
H	-0.799930	-3.393640	2.052813
H	-0.906905	-1.663214	2.427444
H	-2.380075	-2.629852	2.235648
N	-2.080475	0.682756	-0.091144
C	-3.191599	0.685865	0.736242
C	-1.984646	1.953138	-0.655621
C	-3.776136	1.925788	0.707353
H	-3.472454	-0.208803	1.272404
C	-3.004052	2.736338	-0.181593
H	-1.199350	2.190585	-1.362493
H	-4.662077	2.225668	1.251438
H	-3.188393	3.769587	-0.444113
O	-0.660250	-1.044839	-2.087660
C	2.198009	0.137396	0.341296
C	2.868018	0.752034	1.403580
C	2.866079	-0.128910	-0.858472
C	4.206968	1.102772	1.257494
H	2.326890	0.947596	2.323870
C	4.206113	0.226440	-0.989014
H	2.335133	-0.611569	-1.675474
C	4.881593	0.842414	0.064455
H	4.725434	1.582009	2.083259
H	4.723622	0.018119	-1.921244
H	5.926620	1.116718	-0.043453

E = -738.376759919
G = -738.201298

Mo-O-4-TSrot1

Mo	0.669265	-0.684508	0.196363
O	-1.044177	-0.772727	-0.580882
C	1.624231	-2.150183	-0.489877
H	0.859194	-2.950965	-0.499648
C	3.046836	-2.606749	-0.576150
H	3.215921	-3.149158	-1.516064
H	3.742807	-1.763681	-0.550207
H	3.306238	-3.291012	0.243686
N	1.775984	0.934275	-0.006935
C	2.039915	1.544525	-1.236470
C	2.373798	1.713796	0.983157
C	2.794443	2.663885	-1.021221
H	1.681799	1.108697	-2.159770
C	3.006403	2.771732	0.392904
H	2.277121	1.432752	2.021859
H	3.166346	3.334674	-1.784188
H	3.563008	3.545172	0.904902
O	0.482709	-0.850848	1.880803
C	-2.271051	-0.225752	-0.319368
C	-3.155554	-0.075304	-1.390272
C	-2.643707	0.147536	0.974102
C	-4.421954	0.454473	-1.159114
H	-2.839629	-0.379603	-2.383132
C	-3.914396	0.678385	1.186773
H	-1.943539	0.017034	1.794437
C	-4.806817	0.834345	0.126882
H	-5.110708	0.570594	-1.991347

H	-4.205600	0.970305	2.191994
H	-5.795096	1.249047	0.301318

E = -738.336300205
G = -738.162813

Mo-O-4-TSrot2

Mo	-0.681764	0.578909	0.205304
O	0.892573	-0.037765	-0.596689
C	-1.114364	2.229731	-0.506720
H	-2.185216	1.949854	-0.264786
C	-0.820081	3.667165	-0.734311
H	-1.056614	4.283970	0.143191
H	0.241283	3.798125	-0.965819
H	-1.391398	4.059581	-1.585189
N	-2.210515	-0.686831	0.057260
C	-3.256863	-0.647006	-0.862697
C	-2.347037	-1.858155	0.794354
C	-4.023058	-1.772130	-0.711847
H	-3.351679	0.177205	-1.556138
C	-3.445454	-2.541938	0.344859
H	-1.649402	-2.090810	1.586827
H	-4.905790	-2.019196	-1.286386
H	-3.807961	-3.484710	0.732230
O	-0.293813	0.752011	1.852206
C	2.201858	-0.322728	-0.355806
C	2.909407	-1.019412	-1.339450
C	2.824603	0.071301	0.831564
C	4.250888	-1.323306	-1.126127
H	2.397574	-1.312363	-2.250576
C	4.166274	-0.245263	1.029561
H	2.255168	0.608563	1.584136
C	4.884710	-0.939103	0.055780
H	4.802368	-1.864878	-1.889646
H	4.652368	0.057679	1.952818
H	5.931634	-1.178305	0.216646

E = -738.337036111
G = -738.164309

Mo-O-4-TSI

Mo	0.800053	0.514405	-0.164597
O	-0.789231	-0.108653	0.688028
C	-1.780243	2.681427	-1.006810
C	1.744143	1.641613	1.010626
C	-1.022240	3.321124	-0.112630
H	1.457868	1.424203	2.052399
H	-1.296240	3.367894	0.938299
H	-0.117502	3.845439	-0.407317
H	-2.697376	2.174917	-0.720619
C	2.718894	2.757546	0.829868
H	3.672095	2.506288	1.314789
H	2.917682	2.959773	-0.224828
H	2.357392	3.678058	1.307800
H	-1.506012	2.647300	-2.057538
N	1.973397	-1.104167	-0.058667
C	2.940403	-1.475746	0.860191
C	1.821368	-2.163606	-0.945515
C	3.380344	-2.742611	0.572087
H	3.228670	-0.795871	1.649063
C	2.665518	-3.182362	-0.584114
H	1.135310	-2.095568	-1.779862
H	4.134191	-3.295543	1.116867
H	2.772619	-4.131539	-1.092372
O	1.074123	1.117956	-1.705219
C	-2.056916	-0.515664	0.449301
C	-2.946860	-0.584738	1.527585
C	-2.485741	-0.873011	-0.835304
C	-4.256330	-1.005390	1.315505
H	-2.593598	-0.310119	2.516558
C	-3.798421	-1.294180	-1.032943
H	-1.789097	-0.824923	-1.668630
C	-4.689547	-1.360948	0.037669
H	-4.942051	-1.057652	2.156746
H	-4.123563	-1.573116	-2.031441
H	-5.711750	-1.690531	-0.121747

E = -816.938304152
G = -816.715946

Mo-O-4-II

Mo	-0.954952	-0.495742	-0.205974
O	0.804538	-0.360878	0.594826
C	0.035341	-2.454191	-1.117175
C	-2.067007	-1.276973	1.149462
C	-0.752589	-2.993743	-0.116584
H	-1.561509	-1.336876	2.123362
H	-0.316418	-3.276421	0.836748
H	-1.727553	-3.413098	-0.343328
H	1.101817	-2.323180	-0.962709
C	-3.490168	-1.716295	1.148883
H	-4.071544	-1.012842	1.761278
H	-3.920566	-1.725802	0.145344
H	-3.610486	-2.704687	1.612264
H	-0.322908	-2.444125	-2.141754
N	-1.070506	1.548413	-0.025108
C	-0.412358	2.349209	0.892069
C	-1.965160	2.359911	-0.705162
C	-0.872113	3.640931	0.786892
H	0.340153	1.929851	1.543752
C	-1.864476	3.648027	-0.236852
H	-2.597359	1.939963	-1.474796
H	-0.530047	4.487133	1.368845
H	-2.428165	4.501105	-0.592110
O	-1.943586	-0.520445	-1.565300
C	2.109848	-0.169637	0.320174
C	3.070243	-0.606410	1.242987
C	2.516864	0.458757	-0.865460
C	4.422766	-0.419111	0.973912
H	2.738466	-1.082552	2.160854
C	3.873680	0.638288	-1.120925
H	1.764871	0.823694	-1.559851
C	4.832341	0.200380	-0.207360
H	5.161642	-0.759636	1.694362
H	4.181270	1.130748	-2.039363
H	5.888985	0.344748	-0.411623

E = -816.941461923
G = -816.713386

Mo-O-4-TSII

Mo	-0.960566	-0.483071	-0.212270
O	0.802159	-0.351691	0.586316
C	0.000691	-2.403490	-1.127407
C	-2.035065	-1.332342	1.140780
C	-0.789108	-2.954463	-0.120750
H	-1.514288	-1.410294	2.104661
H	-0.336361	-3.274066	0.813137
H	-1.753566	-3.391708	-0.358747
H	1.071729	-2.304907	-0.980774

C	-3.455218	-1.783402	1.153417
H	-4.029900	-1.091372	1.784454
H	-3.899933	-1.778156	0.156072
H	-3.564097	-2.779342	1.602662
H	-0.358924	-2.409449	-2.151567
N	-1.065048	1.559971	-0.017286
C	-0.385790	2.355872	0.889737
C	-1.969961	2.378050	-0.676941
C	-0.844153	3.648715	0.799564
H	0.376639	1.931157	1.526007
C	-1.856356	3.663322	-0.204962
H	-2.617260	1.963773	-1.437012
H	-0.489850	4.490962	1.379934
H	-2.424780	4.519565	-0.544745
O	-1.981023	-0.489541	-1.548618
C	2.109476	-0.175091	0.314255
C	3.064195	-0.621032	1.238761
C	2.525012	0.447338	-0.871693
C	4.418976	-0.448814	0.971042
H	2.726355	-1.092391	2.156900
C	3.883946	0.611768	-1.125788
H	1.777639	0.818520	-1.567711
C	4.836730	0.164680	-0.210506
H	5.153279	-0.796536	1.692741
H	4.197980	1.099414	-2.044631
H	5.895131	0.297213	-0.413714

E = -816.941443782
G = -816.711414

Mo-O-4-TBP

O	0.829391	-0.077731	0.346090
C	-0.049974	-1.745628	-1.555526
H	1.014046	-1.589800	-1.719334
C	-1.077003	-2.120940	0.969004
C	-0.359312	-2.718510	-0.359328
H	-0.344272	-2.054451	1.776135
H	0.590766	-3.124705	-0.013472
H	-1.034108	-3.493958	-0.721077
Mo	-0.994358	-0.462645	-0.220732
N	-1.438498	1.488931	0.063413
C	-0.631891	2.480691	0.613586
C	-2.661037	2.080845	-0.242516
C	-1.330526	3.658933	0.656970
H	0.371750	2.252020	0.936893
C	-2.625363	3.404321	0.109185
H	-3.446856	1.490182	-0.690692
H	-0.960070	4.601031	1.039846
H	-3.432198	4.115616	-0.010498
C	-2.347105	-2.828985	1.379162
H	-2.801042	-2.317305	2.233479
H	-3.076306	-2.840177	0.564717
H	-2.144089	-3.863685	1.685785
H	-0.599999	-1.992592	-2.459708
O	-2.462399	-0.778662	-0.997495
C	2.150709	0.094921	0.198029
C	2.670787	0.664065	-0.974991
C	3.021161	-0.291399	1.228661
C	4.046231	0.830427	-1.111570
H	1.985798	0.981382	-1.755718
C	4.393295	-0.118333	1.077135
H	2.604267	-0.714355	2.137846
C	4.913630	0.439721	-0.091442
H	4.441128	1.274235	-2.021493
H	5.060822	-0.418739	1.880320
H	5.985330	0.574233	-0.203102

E = -816.952963961
G = -816.720709

Mo-O-4-TSIII

Mo	-1.053417	-0.563597	-0.179588
O	0.725328	-0.052927	-0.745280
C	-0.441770	-2.892492	-0.810332
C	-1.867831	-1.316381	-1.747267
C	0.104561	-2.532156	0.428170
H	-1.405087	-1.188005	-2.728480
H	-2.827353	-1.831338	-1.754717
H	1.133299	-2.176196	0.419709
H	0.167011	-2.828060	-1.706102
C	-0.376371	-3.138399	1.722159
H	-0.271089	-2.446852	2.561925
H	-1.426607	-3.433452	1.663775
H	0.221670	-4.030337	1.948824
H	-1.273841	-3.590756	-0.846179
N	-1.416513	1.440331	0.043878
C	-2.456853	1.986062	0.781613
C	-0.790483	2.487914	-0.612459
C	-2.480863	3.347318	0.602559
H	-3.091671	1.343956	1.375493
C	-1.416594	3.668157	-0.291617
H	0.055909	2.302867	-1.257174
H	-3.175396	4.038162	1.062923
H	-1.141148	4.651611	-0.650174
O	-2.133103	-0.966055	1.041362
C	1.974662	0.224719	-0.324174
C	2.227185	0.598822	1.003399
C	3.034165	0.137871	-1.237898
C	3.531231	0.873438	1.406877
H	1.396042	0.696964	1.696398
C	4.331823	0.416318	-0.819705
H	2.820489	-0.142266	-2.265048
C	4.588684	0.782134	0.502145
H	3.718559	1.167647	2.435969
H	5.148072	0.347574	-1.533752
H	5.603162	0.999152	0.822683

E = -816.934204080
G = -816.704759

Mo-O-4-IV

Mo	0.860182	0.731128	-0.150935
O	-0.550256	-0.399830	-0.760889
C	-1.787336	2.524278	0.307645
C	1.667149	1.671434	-1.566724
C	-1.369058	2.666784	-0.960721
H	1.515348	1.318705	-2.592378
H	2.242066	2.592419	-1.469606
H	-0.797634	3.538490	-1.270632
H	-1.648485	1.958632	-1.734656
C	-1.514574	3.488843	1.414949
H	-0.928671	3.010302	2.207639
H	-0.956750	4.360673	1.062761
H	-2.454419	3.832513	1.863094
H	-2.390910	1.651608	0.561159
N	2.249012	-0.687418	0.110978
C	2.223888	-1.538185	1.208555
C	3.275997	-1.112970	-0.714634
C	3.206054	-2.485746	1.070076
H	1.519243	-1.384718	2.015337
C	3.878431	-2.213878	-0.160981

H	3.488138	-0.583259	-1.632040
H	3.432304	-3.276059	1.773643
H	4.714201	-2.760436	-0.577527
O	1.055271	1.657031	1.233486
C	-1.704107	-1.002935	-0.399497
C	-2.546755	-1.486706	-1.407811
C	-2.062859	-1.157623	0.946125
C	-3.741264	-2.113087	-1.066197
H	-2.246481	-1.367159	-2.444078
C	-3.260449	-1.789292	1.273120
H	-1.397601	-0.793846	1.725289
C	-4.105518	-2.266777	0.272055
H	-4.390658	-2.486679	-1.853119
H	-3.530470	-1.910283	2.318555
H	-5.037683	-2.758800	0.532446

E = -816.938235781
G = -816.715940

Mo-O-4-V

Mo	-0.719309	-0.912745	-0.008967
O	0.832935	-0.064559	-0.669032
C	-1.366390	-2.062841	-1.342621
H	-1.235600	-1.757741	-2.386578
H	-1.794017	-3.053204	-1.190057
N	-2.172554	0.446419	0.093937
C	-2.177377	1.401849	1.110043
C	-3.219769	0.751965	-0.762768
C	-3.194664	2.290601	0.885704
H	-1.459416	1.357574	1.919117
C	-3.860500	1.875246	-0.310167
H	-3.413471	0.127363	-1.622657
H	-3.447326	3.138519	1.508295
H	-4.716842	2.349401	-0.771088
O	-0.719805	-1.815878	1.398297
C	2.122556	0.221473	-0.338718
C	2.779699	-0.455262	0.693589
C	2.782922	1.210649	-1.073137
C	4.102023	-0.133352	0.988054
H	2.256159	-1.225998	1.253869
C	4.103836	1.522834	-0.764841
H	2.249589	1.719363	-1.869767
C	4.768762	0.854433	0.263436
H	4.612309	-0.660883	1.788988
H	4.615889	2.293212	-1.334526
H	5.799930	1.100673	0.497880

E = -699.068992343
G = -698.919694

Mo-O-4-TSA

O	-0.839786	0.679786	-0.203335
C	-0.759464	-2.038612	-0.272178
H	-1.448262	-1.810862	-1.084145
C	1.701723	-1.669778	-1.050270
C	0.556014	-2.722651	-0.730041
H	1.561499	-1.283865	-2.067451
H	0.350343	-3.240949	-1.673584
H	0.917826	-3.439753	0.010306
Mo	0.627682	-0.543940	0.291034
N	1.621940	1.214307	0.119444
C	1.392348	2.344943	-0.642728
C	2.886910	1.357961	0.703038
C	2.481393	3.173070	-0.566359
H	0.457222	2.455254	-1.169584
C	3.439068	2.540522	0.296213
H	3.264268	0.609428	1.385938
H	2.589166	4.130988	-1.058341
H	4.402725	2.932189	0.594769
C	3.120988	-2.140557	-0.809397
H	3.822966	-1.315004	-0.960730
H	3.254000	-2.512789	0.210979
H	3.395929	-2.947169	-1.502448
H	-1.262119	-2.536442	0.554982
O	0.999728	-1.036018	1.850672
C	-2.179104	0.576492	-0.107044
C	-2.807507	0.244626	1.102388
C	-2.964464	0.851620	-1.236976
C	-4.196681	0.181789	1.171885
H	-2.196629	0.049367	1.979856
C	-4.352666	0.789521	-1.153267
H	-2.468679	1.119615	-2.165590
C	-4.977464	0.452427	0.047812
H	-4.671799	-0.074695	2.115232
H	-4.950087	1.006445	-2.035073
H	-6.060709	0.405198	0.108172

E = -816.939569626
G = -816.708130

Mo-O-4-SBP

O	1.113591	0.051822	-0.920617
C	0.363544	-2.065481	0.666510
C	-1.712010	-1.408338	1.199712
C	-0.879910	-2.680066	1.278649
H	-1.444194	-0.748837	2.037937
H	-0.767547	-3.125598	2.278579
H	-1.295357	-3.447152	0.615060
H	0.979122	-1.522498	1.394711
Mo	-0.634425	-0.566118	-0.517214
N	-1.664669	1.087683	-0.048764
C	-1.772175	1.854992	1.097754
C	-2.285478	1.796111	-1.079954
C	-2.423501	3.025756	0.800299
H	-1.367279	1.509849	2.038658
C	-2.753217	2.986732	-0.590114
H	-2.353233	1.377740	-2.075533
H	-2.643963	3.824867	1.495798
H	-3.282454	3.743219	-1.153828
C	-3.219805	-1.515455	1.061934
H	-3.645579	-1.999806	1.952739
H	-3.692301	-0.534753	0.955717
H	-3.496845	-2.122687	0.193834
H	1.010924	-2.682612	0.034613
O	-1.308985	-1.473608	-1.743874
C	2.334569	0.268881	-0.375095
C	3.461205	-0.272990	-1.003968
C	2.476965	1.054980	0.774869
C	4.724620	-0.034759	-0.471610
H	3.326472	-0.870185	-1.900378
C	3.747852	1.289507	1.293119
H	1.594922	1.494844	1.232149
C	4.874115	0.744258	0.676652
H	5.598165	-0.458194	-0.959444
H	3.857306	1.905279	2.181514
H	5.862902	0.929209	1.085580

E = -816.968492820
G = -816.736593

Mo-O-4-TSB

C	-2.787172	-1.302051	-1.150489
C	-2.025936	-1.850500	1.010477
C	-3.000069	-1.136052	0.281151
H	-1.642764	-2.750927	0.530280
H	-3.873011	-0.660486	0.732834
H	-2.431616	0.272857	0.205878
O	0.491644	-1.106071	0.553700
H	-2.557493	-2.308318	-1.500981
Mo	-0.938936	-0.333700	-0.504087
C	-1.796253	-1.723626	2.483357
H	-2.258899	-2.553604	3.032409
H	-0.722252	-1.745377	2.695517
H	-2.204309	-0.787650	2.878909
H	-3.375863	-0.707986	-1.846525
O	-0.399823	-0.393673	-2.111943
C	1.819321	-0.834639	0.344265
C	2.523742	-0.147637	1.338681
C	2.484239	-1.293622	-0.796824
C	3.889372	0.077300	1.186074
H	1.989905	0.200394	2.217447
C	3.850698	-1.061721	-0.936525
H	1.923533	-1.815312	-1.566137
C	4.559628	-0.376981	0.050286
H	4.430813	0.613205	1.961071
H	4.362674	-1.420433	-1.825451
H	5.624519	-0.197879	-0.065361
N	-0.766707	1.630437	-0.120044
C	0.341754	2.331978	-0.592530
C	-1.517798	2.521384	0.639175
C	0.290348	3.619479	-0.129447
H	1.066285	1.848273	-1.231512
C	-0.896942	3.741171	0.658527
H	-2.435615	2.201113	1.112519
H	1.011406	4.398272	-0.339886
H	-1.249215	4.627227	1.169843

E = -816.908984580
G = -816.681241

Mo-O-4-TSB$_{transX}$

O	-0.812515	-0.772819	-0.502582
C	0.902714	0.713527	2.137391
C	0.807608	2.530528	0.612001
C	0.123125	1.795169	1.655533
H	1.892241	2.594852	0.742888
H	-0.820205	2.119832	2.099823
H	-0.784969	1.104204	0.651819
H	1.973656	0.863309	2.227591
Mo	0.597555	0.490402	-0.221098
N	2.178478	-0.758402	-0.002330
C	2.633026	-1.569366	1.027068
C	2.901214	-1.121388	-1.148275
C	3.603011	-2.413645	0.555246
H	2.208560	-1.497361	2.016231
C	3.777615	-2.122936	-0.834438
H	2.728900	-0.609922	-2.083398
H	4.134932	-3.156658	1.135002
H	4.480049	-2.588714	-1.512989
C	0.166082	3.679840	-0.108252
H	0.296650	4.619872	0.443308
H	0.606397	3.803001	-1.101700
H	-0.910340	3.517374	-0.237323
H	0.458026	-0.023483	2.800877
O	0.930144	1.179190	-1.736734
C	-2.150918	-0.829560	-0.291944
C	-3.008316	0.128097	-0.845924
C	-2.671408	-1.891180	0.456869
C	-4.381701	0.027704	-0.632640
H	-2.590559	0.927575	-1.451541
C	-4.045962	-1.979781	0.658498
H	-1.989505	-2.632736	0.861495
C	-4.906593	-1.022061	0.120200
H	-5.044206	0.772050	-1.066184
H	-4.446475	-2.804726	1.241517
H	-5.977787	-1.097209	0.281533

E = -816.909682413
G = -816.681588

Mo-O-4-B

C	0.385293	2.064286	-1.429583
C	-0.435014	3.429688	0.508749
C	0.538227	3.043373	-0.330613
H	-1.430234	2.998979	0.388348
H	1.537274	3.463084	-0.201728
H	2.112515	1.050665	-0.665471
O	-0.746040	-0.048801	0.267415
H	-0.664984	1.936815	-1.738015
Mo	0.801482	0.034906	-0.827568
C	-0.268522	4.424801	1.611951
H	-0.939522	5.282712	1.477584
H	-0.520206	3.983010	2.584526
H	0.757296	4.801255	1.665508
H	0.991816	2.308166	-2.304048
O	0.894131	-0.651639	-2.346458
C	-2.010026	-0.543997	0.281316
C	-2.753066	-0.409042	1.459040
C	-2.569717	-1.167282	-0.840541
C	-4.053932	-0.901193	1.509228
H	-2.293814	0.073631	2.315660
C	-3.872948	-1.652508	-0.775665
H	-1.983811	-1.268618	-1.751159
C	-4.619671	-1.522542	0.395620
H	-4.628102	-0.798277	2.425753
H	-4.305371	-2.135578	-1.647367
H	-5.635275	-1.904039	0.439896
N	2.174743	-0.893504	0.282140
C	2.021071	-2.268111	0.461911
C	3.267008	-0.497696	1.033923
C	2.984835	-2.715556	1.326375
H	1.242300	-2.817338	-0.052014
C	3.780271	-1.584349	1.692505
H	3.577771	0.536931	1.036843
H	3.117575	-3.737608	1.655680
H	4.631751	-1.581056	2.359939

E = -816.946982320
G = -816.721350

Mo-O-4-TSC

C	2.048722	-1.016896	1.277317
C	3.744387	-2.393046	0.046517
C	3.383137	-1.286978	0.717840
H	1.427054	-1.925205	1.310558
H	4.149560	-0.533458	0.915542
H	2.124657	-0.614056	2.289251
H	1.998127	1.002302	0.032472
O	-0.916018	-0.715462	-0.599642
C	2.318001	0.589454	-1.405598
H	3.337973	0.376956	-1.093849

H	2.140869	1.577648	-1.823417
C	1.484224	-0.461456	-1.752984
H	0.615168	-0.290013	-2.376781
H	1.810807	-1.486780	-1.616246
H	2.991078	-3.164076	-0.128933
C	5.119926	-2.681658	-0.464598
H	5.523762	-3.599709	-0.019337
H	5.117574	-2.839743	-1.550768
H	5.813655	-1.865262	-0.241635
Mo	0.437844	0.260777	0.391695
N	0.094703	2.178602	-0.093874
C	0.894434	3.312944	-0.160268
C	-1.227384	2.605019	-0.190984
C	0.103281	4.419941	-0.311468
H	1.968434	3.235140	-0.067880
C	-1.253716	3.966708	-0.337370
H	-2.042497	1.894533	-0.166003
H	0.447526	5.442261	-0.395024
H	-2.139641	4.575032	-0.463091
O	-0.151750	0.207370	1.971177
C	-2.183903	-1.132871	-0.329371
C	-2.817007	-0.979435	0.910366
C	-2.866220	-1.751482	-1.387702
C	-4.119699	-1.445566	1.077583
H	-2.287339	-0.509325	1.732273
C	-4.167029	-2.208091	-1.206528
H	-2.355849	-1.862016	-2.339487
C	-4.801690	-2.057967	0.027078
H	-4.604014	-1.324736	2.042882
H	-4.686209	-2.684582	-2.033740
H	-5.817719	-2.414743	0.167874

E = -895.472312417
G = -895.195177

Mo-O-4-C

C	0.202168	-2.241620	-0.449893
C	1.922281	-2.015762	1.369736
C	0.685422	-2.328471	0.946503
H	2.658750	-1.676708	0.641395
H	-0.031810	-2.686899	1.685666
O	0.679652	0.373590	-1.204400
H	1.029899	-2.130353	-1.160240
Mo	-0.991134	-0.439595	-0.798806
C	2.389920	-2.121649	2.786344
H	3.228400	-2.824324	2.874670
H	2.756722	-1.155205	3.154414
H	1.591863	-2.461732	3.453572
H	-0.408093	-3.100020	-0.739418
O	-1.832616	-0.725866	-2.208206
C	-2.268189	-1.628570	0.536876
H	-2.137278	-2.697258	0.344283
H	-1.945654	-1.446313	1.568441
C	-3.746384	-1.262219	0.376720
H	-4.359974	-1.883705	1.043105
H	-3.945484	-0.216358	0.625434
H	-4.095639	-1.436420	-0.646066
N	-1.720232	1.044023	0.335575
C	-2.356851	2.135532	-0.254280
C	-1.593946	1.319039	1.685917
C	-2.608459	3.080755	0.704538
H	-2.579158	2.138621	-1.312818
C	-2.117901	2.561019	1.944231
H	-1.132062	0.606724	2.355291
H	-3.093652	4.034629	0.546835
H	-2.151675	3.049195	2.909366
C	1.929133	0.685022	-0.803080
C	2.146382	1.337094	0.418285
C	3.005972	0.382813	-1.646336
C	3.442968	1.682744	0.786546
H	1.295526	1.580626	1.047280
C	4.298674	0.721104	-1.255724
H	2.810754	-0.108865	-2.594324
C	4.522850	1.371032	-0.041434
H	3.610629	2.199005	1.727793
H	5.134098	0.482143	-1.907908
H	5.532545	1.639056	0.255230

E = -895.542745367
G = -895.261460

Mo-N-5-I

Mo	-0.874260	-0.000021	-0.154289
O	-1.634161	1.582328	-0.914135
N	0.847485	0.000000	-0.069197
C	-1.305313	0.000048	1.667542
H	-2.411004	0.000055	1.729049
Si	-2.290306	3.031002	-0.374152
H	-3.125874	3.609966	-1.469231
H	-3.141618	2.794907	0.835013
H	-1.201989	3.995187	-0.022952
C	-0.594683	0.000051	2.983082
H	-0.866869	-0.881366	3.579395
H	0.489919	-0.000017	2.848741
H	-0.866759	0.881552	3.579322
C	2.223069	0.000101	-0.111452
C	2.930690	1.215616	-0.130560
C	4.320162	1.208361	-0.170488
C	5.019090	0.000286	-0.190955
C	4.320299	-1.207882	-0.171363
C	2.930827	-1.215321	-0.131435
H	2.373363	2.147062	-0.115705
H	4.861137	2.150364	-0.186362
H	6.104780	0.000360	-0.222577
H	4.861379	-2.149813	-0.187915
H	2.373603	-2.146839	-0.117232
O	-1.633975	-1.582510	-0.914002
Si	-2.289471	-3.031378	-0.373740
H	-3.141018	-2.795405	0.835282
H	-3.124651	-3.611008	-1.468764
H	-1.200729	-3.994956	-0.022198

E = -595.074934987
G = -594.920379

Mo-N-5-Ianti

Mo	0.807822	0.000007	-0.086680
O	1.550555	-1.579668	-0.865177
N	-0.908484	-0.000036	0.058825
C	1.289179	0.000056	1.731925
H	0.587858	0.000053	2.567945
Si	1.946535	-3.176986	-0.538400
H	2.927809	-3.639942	-1.565596
H	2.550884	-3.304967	0.824146
H	0.722168	-4.033985	-0.606897
C	2.752965	0.000072	2.100732
H	3.002590	-0.884708	2.700886
H	3.422037	0.000099	1.231294
H	3.002563	0.884832	2.700925
C	-2.283660	-0.000056	0.058852
C	-2.991619	-1.215718	0.062281

C	-4.381540	-1.208262	0.067021
C	-5.080622	-0.000090	0.068986
C	-4.381569	1.208099	0.067038
C	-2.991649	1.215588	0.062298
H	-2.434094	-2.147078	0.059559
H	-4.922825	-2.150200	0.068531
H	-6.166763	-0.000104	0.071909
H	-4.922877	2.150023	0.068560
H	-2.434146	2.146961	0.059588
O	1.550446	1.579718	-0.865214
Si	1.946245	3.177076	-0.538411
H	2.550431	3.305126	0.824200
H	2.927587	3.640113	-1.565507
H	0.721808	4.033965	-0.607052

E = -595.071981154
G = -594.918336

Mo-N-5-TSrot

Mo	-1.070237	-0.015627	0.341666
O	-1.648833	1.762201	0.618560
N	0.516123	0.159037	-0.440671
C	-0.880320	-0.781787	2.050410
Si	-1.197392	3.258219	-0.024782
H	-2.170813	4.270409	0.480990
H	0.182646	3.610713	0.422705
H	-1.248316	3.215882	-1.518096
C	1.888530	0.024513	-0.299241
C	2.472315	-0.697799	0.758476
C	3.854376	-0.813976	0.850666
C	4.679485	-0.213428	-0.102345
C	4.109778	0.504542	-1.154848
C	2.728050	0.621579	-1.258591
H	1.819914	-1.158358	1.494934
H	4.292880	-1.376682	1.670750
H	5.759049	-0.306691	-0.025880
H	4.746093	0.973104	-1.900826
H	2.270537	1.171957	-2.075356
O	-2.052266	-1.185730	-0.736617
Si	-1.877968	-1.860987	-2.285864
H	-3.017953	-2.803178	-2.479826
H	-1.934104	-0.774380	-3.307423
H	-0.581368	-2.591725	-2.378070
C	-0.960577	-2.178243	2.595505
H	-1.337974	-2.886825	1.852693
H	0.016934	-2.541207	2.942646
H	-1.638057	-2.210181	3.459231
H	-0.508386	-0.015188	2.749575

E = -595.048885114
G = -594.893475

Mo-N-5-TSI

Mo	0.777372	0.090850	0.003721
O	1.957779	-1.259304	-0.686840
O	1.392707	1.568881	-1.048480
N	-0.952836	0.236012	0.009671
C	-0.424804	-2.929970	0.662809
C	1.225442	0.578047	1.762640
C	0.164966	-2.545835	1.798983
H	2.326767	0.531558	1.845851
H	1.227878	-2.692718	1.967426
H	-0.400445	-2.096108	2.610293
H	0.141666	-3.389326	-0.141837
C	0.518036	0.989495	3.012550
H	0.800621	2.009880	3.305200
H	-0.566626	0.959867	2.885763
H	0.789407	0.336736	3.853951
H	-1.491442	-2.798637	0.503507
C	-2.300843	0.092731	-0.220170
C	-2.778931	-0.739016	-1.250835
C	-4.146710	-0.864440	-1.467917
C	-5.057357	-0.176984	-0.664678
C	-4.588319	0.648949	0.357865
C	-3.223505	0.791612	0.580494
H	-2.064382	-1.267515	-1.874931
H	-4.503573	-1.504320	-2.270368
H	-6.124556	-0.280610	-0.837099
H	-5.291103	1.191979	0.983890
H	-2.848769	1.442028	1.364434
Si	3.513589	-1.798448	-0.981051
H	4.015881	-1.249831	-2.277134
H	4.434330	-1.372359	0.122046
H	3.506702	-3.292714	-1.049473
Si	1.618547	3.186196	-0.667449
H	2.497002	3.320372	0.539477
H	2.276517	3.850079	-1.834552
H	0.312710	3.861250	-0.389329

E = -673.627022615
G = -673.425536

Mo-N-5-TBP

Mo	-0.833161	-0.185937	0.053740
C	-0.697048	-1.487821	1.653576
N	0.914847	-0.030810	-0.002206
O	-2.774721	-0.426906	0.304008
H	-1.582531	-1.531100	2.282949
C	-0.761659	-2.498944	0.446010
C	-0.878141	-1.912892	-1.050856
H	-1.893422	-2.075206	-1.417662
H	0.156519	-3.086410	0.456965
H	-1.649866	-3.113285	0.589632
Si	-4.140604	0.527393	0.367912
H	-5.322766	-0.345375	0.669259
H	-4.044332	1.559300	1.449351
H	-4.399587	1.215452	-0.936706
C	0.174383	-2.411573	-2.013072
H	1.184791	-2.248856	-1.628668
H	0.051157	-3.484026	-2.216480
H	0.086373	-1.888653	-2.970961
H	0.234401	-1.556548	2.210149
C	2.278195	0.050021	0.120878
C	3.103198	0.017729	-1.020532
C	4.484184	0.089691	-0.882159
C	5.064016	0.196316	0.383167
C	4.251184	0.236088	1.517263
C	2.868566	0.166261	1.395170
H	2.641260	-0.055723	-1.999939
H	5.112771	0.065780	-1.767991
H	6.143784	0.253559	0.484583
H	4.697710	0.327383	2.503530
H	2.225848	0.210692	2.268941
O	-1.267958	1.658793	-0.276019
Si	-0.289352	2.978411	-0.621616
H	0.482298	2.762002	-1.886437
H	-1.172376	4.171960	-0.792151
H	0.676355	3.238477	0.491287

E = -673.657712164
G = -673.445049

Mo-N-5-TSIII

Mo	-0.845248	-0.262059	0.331609
C	-0.527069	-2.499302	-0.454529
N	0.894707	-0.089644	0.368335
O	-1.264523	1.602621	-0.085151
O	-2.527484	-0.587534	-0.616797
C	-1.193909	-0.675399	2.163630
C	-1.049503	-2.697408	0.817924
H	-2.235627	-0.765510	2.486867
H	-0.457946	-0.803455	2.955202
H	-2.120135	-2.803588	0.952625
H	-0.417366	-3.074698	1.617211
C	0.880792	-2.884857	-0.823562
H	1.302141	-2.234639	-1.594558
H	0.880883	-3.907428	-1.222840
H	1.550403	-2.859279	0.040247
H	-1.248895	-2.439825	-1.266249
C	2.211312	0.101520	0.025254
C	3.216911	-0.080802	0.993269
C	4.550839	0.121956	0.659062
C	4.904349	0.509835	-0.634265
C	3.911214	0.695353	-1.597454
C	2.573748	0.492184	-1.278338
H	2.929962	-0.373848	1.998496
H	5.319654	-0.020321	1.413533
H	5.947835	0.669357	-0.889567
H	4.180579	1.001909	-2.604414
H	1.793327	0.642055	-2.018510
Si	-0.732620	3.030066	0.600754
H	-1.284562	4.172952	-0.191986
H	0.762494	3.118412	0.599396
H	-1.206998	3.156770	2.018123
Si	-3.625108	0.484517	-1.302006
H	-4.212581	1.430939	-0.304300
H	-4.745602	-0.349743	-1.849985
H	-3.027960	1.250570	-2.438071

E = -673.631452709
G = -673.420374

Mo-N-5-IV

Mo	0.845814	-0.222565	-0.388402
O	2.336628	-0.757492	0.748104
N	-0.885742	-0.009784	-0.411141
C	0.300409	-2.691872	0.210207
C	1.246588	-0.278962	-2.239151
C	1.001970	-2.736355	-0.958981
H	2.301369	-0.342755	-2.530958
H	0.543770	-0.239046	-3.069559
Si	3.390551	0.168329	1.677501
H	0.510900	-2.970190	-1.899232
H	2.086587	-2.730839	-0.954277
H	2.673211	0.923054	2.749345
H	4.326881	-0.798759	2.338957
H	4.209738	1.107408	0.852308
C	-1.154441	-3.030727	0.333354
H	-1.675919	-2.377547	1.037450
H	-1.669147	-2.980446	-0.629616
H	-1.245614	-4.055955	0.715033
H	0.871509	-2.611129	1.133447
C	-2.183657	0.191828	-0.006243
C	-2.493298	0.464745	1.340406
C	-3.812425	0.683854	1.720911
C	-4.839063	0.629521	0.776868
C	-4.537771	0.358204	-0.558840
C	-3.222916	0.141980	-0.954353
H	-1.686703	0.513720	2.066073
H	-4.040561	0.899647	2.761061
H	-5.867872	0.800460	1.079908
H	-5.332846	0.318499	-1.298334
H	-2.975542	-0.061606	-1.991621
O	1.349534	1.582049	0.164317
Si	1.120205	3.018959	-0.658296
H	1.743250	4.124632	0.135102
H	1.765545	2.962901	-2.011596
H	-0.334812	3.322379	-0.845938

E = -673.632258746
G = -673.423586

Mo-N-5-TSIV

Mo	-0.921295	-0.138705	-0.344094
O	-2.129233	1.108485	0.472477
N	0.792329	-0.361602	-0.228324
C	0.355629	3.028965	-0.596388
C	-1.238722	-0.403825	-2.177793
C	-0.414056	2.731807	-1.652774
H	-0.541911	-0.644417	-2.977683
H	-2.283735	-0.275793	-2.488621
Si	-3.116248	1.462447	1.781349
H	-0.130847	3.225865	0.359152
H	0.018114	2.543766	-2.632807
H	-1.495845	2.712093	-1.576943
H	-2.352957	1.335000	3.062332
H	-3.598815	2.870914	1.643904
H	-4.290488	0.538896	1.812187
C	1.845384	3.158267	-0.624659
H	2.144957	4.182725	-0.369854
H	2.318496	2.498328	0.110550
H	2.252260	2.918842	-1.611125
C	2.111913	-0.457513	0.146413
C	2.520158	-0.155197	1.459096
C	3.858449	-0.277591	1.816767
C	4.806822	-0.691464	0.880380
C	4.405641	-0.990546	-0.422492
C	3.070198	-0.880582	-0.792663
H	1.775964	0.162796	2.183193
H	4.162556	-0.047708	2.834276
H	5.850855	-0.783059	1.164975
H	5.138007	-1.317211	-1.155679
H	2.745467	-1.119018	-1.800491
O	-1.631024	-1.711488	0.478247
Si	-1.912272	-3.240472	-0.160594
H	-2.621563	-4.045767	0.881154
H	-2.765075	-3.143031	-1.387179
H	-0.624515	-3.913919	-0.512808

E = -673.627156335
G = -673.424689

Mo-N-5-V

Mo	0.913637	0.000026	0.039971
O	1.677499	1.575245	-0.710272
N	-0.806550	-0.000148	0.091638
C	1.307160	0.000180	1.872242
H	0.650990	0.000169	2.740878
H	2.383446	0.000286	2.097748
Si	2.283135	3.052346	-0.177835
H	3.105392	3.642185	-1.276677
H	1.158251	3.980279	0.152280

H	3.131351	2.852447	1.038191
C	-2.179787	-0.000228	0.021599
C	-2.886232	1.215804	-0.010403
C	-4.274590	1.208060	-0.075296
C	-4.972472	-0.000401	-0.108219
C	-4.274440	-1.208776	-0.075302
C	-2.886081	-1.216347	-0.010408
H	-2.329263	2.147124	0.015691
H	-4.815558	2.149796	-0.100397
H	-6.057413	-0.000467	-0.159178
H	-4.815291	-2.150579	-0.100404
H	-2.328995	-2.147598	0.015694
O	1.677815	-1.575071	-0.710210
Si	2.284469	-3.051773	-0.177827
H	1.160220	-3.980262	0.152873
H	3.106585	-3.641313	-1.276928
H	3.133086	-2.851282	1.037819

E = -555.767649795
G = -555.639046

Mo-N-5-TSA

Mo	-0.683366	-0.354569	0.043173
C	-0.843359	-0.419908	2.185829
N	1.044298	-0.399718	0.019258
O	-1.845097	1.242579	0.203382
H	-1.795243	-0.081863	2.601358
C	-0.808378	-1.953552	1.980081
C	-1.246007	-2.287405	0.512736
H	-2.345447	-2.302742	0.456109
H	0.198397	-2.346123	2.145396
H	-1.502001	-2.448358	2.673659
Si	-2.211599	2.394251	1.354003
H	-2.725017	3.611406	0.652242
H	-3.274216	1.916087	2.297761
H	-1.010404	2.780957	2.162953
C	-0.639001	-3.529570	-0.108070
H	0.453261	-3.502836	-0.053911
H	-0.981321	-4.434123	0.414135
H	-0.921587	-3.625647	-1.160741
H	-0.011881	-0.034096	2.775027
C	2.345371	0.045866	-0.065935
C	3.291443	-0.714133	-0.776763
C	4.608326	-0.276602	-0.860229
C	4.999021	0.910003	-0.238043
C	4.062390	1.664405	0.470837
C	2.741437	1.241735	0.560709
H	2.971842	-1.633437	-1.257137
H	5.334124	-0.865353	-1.414090
H	6.029713	1.245772	-0.304887
H	4.362956	2.588869	0.955866
H	2.002880	1.818887	1.108663
O	-1.192245	-0.139788	-1.783554
Si	-2.364615	0.811811	-2.556493
H	-3.722722	0.642564	-1.959951
H	-1.963025	2.247577	-2.561735
H	-2.410739	0.320158	-3.969456

E = -673.639684477
G = -673.427937

Mo-N-5-SBP

O	-1.412374	1.730355	-0.846953
C	-1.112362	1.145500	1.802557
C	-1.102638	-1.111613	1.696270
C	-0.768798	-0.024780	2.705489
H	-2.193381	-1.264888	1.671968
Si	-2.050468	3.274767	-0.672624
H	-1.040458	4.188760	-0.056014
H	-2.404709	3.771083	-2.035485
H	-3.280525	3.260347	0.178962
H	-1.309142	-0.077545	3.663894
H	0.305143	-0.035103	2.926031
H	-2.186095	1.376732	1.818755
Mo	-0.740852	0.122510	-0.078120
C	-0.379893	-2.442654	1.799531
H	-0.653122	-2.959233	2.731607
H	-0.619784	-3.119802	0.972603
H	0.706023	-2.300671	1.807666
H	-0.544940	2.074730	1.919543
O	-1.593273	-1.261957	-1.057987
Si	-2.606480	-2.579614	-1.294668
H	-3.510738	-2.775602	-0.119354
H	-3.428572	-2.319957	-2.513791
H	-1.789419	-3.814424	-1.497981
N	0.977322	0.071753	-0.010660
C	2.344909	0.029950	-0.168596
C	2.967717	-1.126405	-0.671134
C	3.126960	1.144366	0.182462
C	4.349407	-1.158905	-0.820672
H	2.353061	-1.980137	-0.939062
C	4.508257	1.095813	0.032272
H	2.633328	2.030940	0.567780
C	5.123818	-0.051999	-0.469342
H	4.825126	-2.053662	-1.212326
H	5.107765	1.959547	0.305856
H	6.203141	-0.083781	-0.586383

E = -673.664159279
G = -673.453591

Mo-N-5-TSB

C	-0.408726	0.702822	2.014920
C	-2.453243	-0.378525	1.510811
C	-1.164046	-0.540536	2.107323
H	-2.880476	0.618911	1.614080
H	-0.885136	-1.387081	2.742756
H	-0.399653	-1.202813	1.065159
O	-1.636293	1.760380	-0.539288
Si	-1.411346	3.404252	-0.773296
H	-1.478903	4.119467	0.539711
H	-0.080156	3.669599	-1.403393
H	-2.496509	3.911229	-1.665727
H	-0.964996	1.611216	2.241259
Mo	-0.807694	0.098877	-0.063292
C	-3.419116	-1.516782	1.342833
H	-4.018398	-1.672388	2.251033
H	-4.114142	-1.327670	0.519261
H	-2.898952	-2.453552	1.120444
H	0.629092	0.707927	2.339981
O	-1.482634	-1.407745	-1.053792
Si	-0.879391	-2.809355	-1.745964
H	-1.929828	-3.369711	-2.648519
H	0.362347	-2.527614	-2.530897
H	-0.559289	-3.815199	-0.681986
N	0.913426	0.187401	-0.440458
C	2.252409	0.052146	-0.140127
C	3.162613	1.025155	-0.593486
C	2.731641	-1.047745	0.595651
C	4.516452	0.900722	-0.304377
H	2.784352	1.865797	-1.166865

C	4.088451	-1.160964	0.877554
H	2.025731	-1.805017	0.925464
C	4.985350	-0.189258	0.431169
H	5.211298	1.658197	-0.656402
H	4.449113	-2.014465	1.445215
H	6.044691	-0.283318	0.651551

E = -673.615169582
G = -673.408854

Mo-N-5-B

C	-1.207818	-0.712512	-1.792403
C	-3.600861	-0.478515	-1.028095
C	-2.540912	-0.066377	-1.752914
H	-3.510761	-1.393483	-0.443963
H	-2.639542	0.865272	-2.312012
H	-0.571305	1.276538	-1.102747
O	-1.214819	-1.518455	0.849326
Si	-1.009336	-3.134528	1.229807
H	-1.126330	-3.972858	-0.005985
H	0.334607	-3.373178	1.844244
H	-2.074160	-3.538962	2.196291
H	-1.244284	-1.800789	-1.686031
Mo	-0.447750	0.072666	0.079510
C	-4.919590	0.223513	-0.973543
H	-5.725337	-0.422120	-1.346069
H	-5.186600	0.487523	0.057594
H	-4.915795	1.140483	-1.570400
H	-0.620050	-0.428826	-2.664341
O	-0.921873	1.540095	1.190658
Si	-1.452107	3.125524	0.973738
H	-2.562536	3.186996	-0.024411
H	-1.942130	3.620261	2.295948
H	-0.320624	3.985718	0.510991
N	1.252820	-0.022034	-0.117866
C	2.626451	0.031872	-0.203867
C	3.374061	-1.155474	-0.283175
C	3.283726	1.274346	-0.214827
C	4.760421	-1.093922	-0.367283
H	2.853552	-2.107835	-0.275237
C	4.669881	1.320010	-0.305763
H	2.691709	2.181942	-0.155855
C	5.412046	0.140079	-0.379972
H	5.335014	-2.013959	-0.425775
H	5.174467	2.281973	-0.316816
H	6.495179	0.182372	-0.448224

E = -673.642952312
G = -673.438714

Mo-N-5-TSC

Mo	0.446307	-0.603510	0.114232
C	0.968774	1.336008	-0.907883
C	3.318175	2.227667	-0.813003
C	2.299809	1.646994	-1.468528
H	0.774593	1.958303	-0.023652
H	2.456814	1.405366	-2.522995
H	0.178998	1.533887	-1.636620
H	0.478414	-0.888082	-1.614492
O	1.405127	-0.100258	1.713713
Si	1.227226	0.680411	3.179420
H	1.866747	2.032007	3.111362
H	-0.218339	0.854126	3.537339
H	1.897968	-0.125540	4.244306
C	1.948953	-1.494680	-1.749632
H	2.129649	-0.813063	-2.576541
H	1.550017	-2.468508	-2.019991
C	2.646013	-1.336644	-0.561511
H	2.725134	-2.167275	0.133439
H	3.294036	-0.480813	-0.413804
H	3.178126	2.491438	0.236845
C	4.647436	2.563818	-1.413095
H	4.851107	3.641119	-1.356666
H	5.467769	2.066314	-0.879240
H	4.701270	2.266689	-2.465340
N	-1.170960	0.038912	0.165323
C	-2.363064	0.675769	-0.080015
C	-2.924992	0.659381	-1.370041
C	-3.027261	1.350728	0.960773
C	-4.128624	1.311970	-1.608496
H	-2.402530	0.129171	-2.160606
C	-4.232342	1.995075	0.707493
H	-2.583903	1.353597	1.951551
C	-4.786273	1.979588	-0.573838
H	-4.557996	1.297898	-2.606346
H	-4.742387	2.513691	1.514375
H	-5.728065	2.485541	-0.765212
O	0.107530	-2.504900	0.108510
Si	-1.188373	-3.486025	-0.299312
H	-0.917216	-4.853532	0.238849
H	-2.466670	-2.964123	0.275632
H	-1.326561	-3.567372	-1.789827

E = -752.179331671
G = -751.925507

Mo-N-5-C

C	-1.212072	-1.083373	-1.672098
C	-3.594794	-1.109613	-0.831761
C	-2.631153	-0.648503	-1.651682
H	-3.342217	-1.891295	-0.116401
H	-2.901189	0.148713	-2.345576
O	-0.995060	-1.522798	0.949695
Si	-0.504895	-3.053641	1.419213
H	-0.467591	-3.970672	0.235039
H	0.855122	-3.016500	2.041523
H	-1.490750	-3.581257	2.410564
H	-1.091366	-2.140046	-1.420943
Mo	-0.382645	0.047064	0.008383
C	-5.014057	-0.636765	-0.837108
H	-5.702021	-1.456457	-1.082138
H	-5.316818	-0.265175	0.150062
H	-5.171057	0.164630	-1.565776
H	-0.721175	-0.869308	-2.620449
C	-0.568371	1.575508	-1.576981
H	-0.341232	1.170146	-2.565954
H	-1.617618	1.896982	-1.591057
C	0.340892	2.777077	-1.301582
H	0.174659	3.565072	-2.049671
H	0.164707	3.223805	-0.317792
H	1.399423	2.501581	-1.349739
Si	-2.220000	2.497832	1.586192
H	-1.601511	3.818127	1.912220
H	-3.187148	2.664354	0.458761
H	-2.936659	1.973801	2.787065
O	-1.006217	1.407860	1.173386
N	1.319551	-0.091194	-0.163943
C	2.696451	-0.064680	-0.125791
C	3.430208	-0.881897	-1.002888
C	3.372896	0.772745	0.778717
C	4.819906	-0.855670	-0.972246

H	2.893281	-1.523353	-1.694522
C	4.762817	0.784364	0.800741
H	2.794984	1.398815	1.451461
C	5.490411	-0.026057	-0.072383
H	5.382702	-1.488172	-1.652969
H	5.281494	1.431067	1.502854
H	6.576171	-0.011183	-0.050995

E = -752.237271534
G = -751.978223

Mo-O-5-I

Mo	-0.000018	0.147821	-0.492817
O	-1.544276	-0.940246	-0.318289
C	-0.000085	1.338961	0.956818
H	0.000033	0.761867	1.897381
Si	-2.945211	-1.053534	0.612155
H	-3.393271	-2.477010	0.609111
H	-2.655158	-0.614396	2.013584
H	-4.010839	-0.184680	0.029742
C	-0.000314	2.826203	1.106570
H	0.881352	3.161773	1.668526
H	-0.000451	3.324975	0.134231
H	-0.882027	3.161488	1.668622
O	-0.000204	1.184771	-1.800357
O	1.544514	-0.939835	-0.318289
Si	2.945446	-1.053286	0.612126
H	2.655630	-0.613372	2.013350
H	3.392908	-2.476950	0.609755
H	4.011409	-0.185193	0.029233

E = -383.994526863
G = -383.923837

Mo-O-5-Ianti

42	-0.000293	-0.515376	0.314300
O	1.541364	-0.362669	-0.776173
C	0.004564	0.954926	1.494281
H	0.001908	0.792392	2.574029
Si	3.066535	0.333124	-0.939864
H	3.408793	0.358038	-2.392243
H	3.055536	1.726928	-0.399181
H	4.072172	-0.481166	-0.195074
C	0.009251	2.391054	1.045818
H	0.892809	2.911605	1.436815
H	0.012208	2.509224	-0.043048
H	-0.873763	2.915503	1.432868
O	-0.011625	-1.813811	1.360605
O	-1.533359	-0.336187	-0.783636
Si	-3.070401	0.334775	-0.938015
H	-3.359080	0.501112	-2.392890
H	-4.079354	-0.577290	-0.322312
H	-3.118712	1.664297	-0.256198

E = -383.991410754
G = -383.923307

Mo-O-5-TSrot

Mo	0.015379	0.311858	0.060329
O	1.761222	0.080034	-0.571400
C	-0.451596	2.103691	-0.267993
H	0.465962	2.702005	-0.138104
Si	3.175781	-0.755175	-0.151038
H	4.156821	-0.530567	-1.250724
H	3.700823	-0.221786	1.138509
H	2.874305	-2.212418	-0.022446
C	-1.741633	2.866852	-0.239216
H	-1.756016	3.622035	-1.036237
H	-2.606136	2.213711	-0.390858
H	-1.879884	3.396621	0.713994
O	0.100626	0.059008	1.748395
O	-1.371713	-0.763071	-0.556790
Si	-2.352841	-2.072603	-0.099661
H	-3.462920	-2.150025	-1.090946
H	-1.537443	-3.321766	-0.138422
H	-2.884315	-1.837996	1.272826

E = -383.957295036
G = -383.889006

Mo-O-5-TSI

Mo	-0.087418	0.178381	0.254915
O	1.171837	-1.039073	-0.512697
C	2.782725	1.403754	0.739811
C	-0.710095	1.370480	-1.062853
C	2.400418	1.959261	-0.416043
H	-0.656178	0.895756	-2.055522
Si	2.091541	-2.438360	-0.444518
H	2.597364	1.481476	-1.371453
H	1.911546	2.928860	-0.443365
H	3.303665	0.451020	0.768939
H	1.211995	-3.618981	-0.193700
H	2.800420	-2.603735	-1.749232
H	3.106889	-2.337523	0.651315
C	-1.217456	2.776279	-1.047931
H	-2.249398	2.816683	-1.421775
H	-1.202485	3.202717	-0.042094
H	-0.619745	3.416355	-1.711502
H	2.595657	1.889341	1.692602
O	-0.096765	1.091682	1.661549
O	-1.514915	-1.065036	0.478192
Si	-3.116855	-1.104163	-0.026555
H	-3.215640	-0.718372	-1.470896
H	-3.626193	-2.496945	0.154701
H	-3.946741	-0.162575	0.786304

E = -462.549040031
G = -462.430817

Mo-O-5-II

Mo	0.359035	0.003103	-0.273966
O	-0.359499	1.719140	0.297555
C	2.205112	1.628128	-0.755233
C	1.064259	-1.010701	1.180241
C	2.615641	1.052950	0.411986
H	0.741671	-0.623481	2.158477
H	2.377608	1.506873	1.369460
H	3.348694	0.252646	0.418503
H	1.622641	2.542199	-0.744975
C	1.951740	-2.208743	1.248766
H	1.407173	-3.042707	1.711748
H	2.292883	-2.527567	0.261637
H	2.824142	-2.019057	1.889744
H	2.581531	1.275091	-1.709657
O	1.005733	-0.751541	-1.632761
Si	-1.939681	2.246045	0.538546
H	-1.850342	3.664125	1.013146
H	-2.722629	2.214792	-0.732326
H	-2.643488	1.448195	1.589615

O	-1.490233	-0.564618	-0.396137
Si	-2.205697	-2.053053	-0.128572
H	-3.686825	-1.903015	-0.261478
H	-1.722779	-3.071050	-1.113788
H	-1.882974	-2.542928	1.253001

E = -462.552561275
G = -462.429496

Mo-O-5-TSII

Mo	0.427327	-0.113843	-0.355886
O	-0.958934	1.007606	0.466951
C	1.340780	2.003052	-0.704683
C	1.490888	-0.586224	1.175401
C	2.030454	1.593304	0.435794
H	0.988765	-0.343715	2.120978
H	1.732228	1.967118	1.410461
H	3.046967	1.222780	0.352627
H	0.521949	2.706868	-0.606577
C	2.782649	-1.317318	1.313273
H	2.576781	-2.309893	1.736625
H	3.280357	-1.455671	0.351071
H	3.462613	-0.815533	2.014386
H	1.823571	1.932492	-1.673711
O	1.467724	-0.569485	-1.601102
Si	-2.246759	2.065742	0.400600
H	-2.920592	2.106275	1.734410
H	-1.761549	3.449034	0.073459
H	-3.233937	1.659792	-0.646188
O	-0.951527	-1.414801	-0.701301
Si	-2.187497	-2.112944	0.178415
H	-3.335403	-1.169429	0.360321
H	-2.672829	-3.319966	-0.557701
H	-1.703801	-2.531343	1.535735

E = -462.549632282
G = -462.425482

Mo-O-5-TBP

O	-1.130589	1.203984	-0.094610
C	-0.969963	-0.724387	1.808706
H	-1.587167	0.067547	2.224452
C	-1.140911	-1.427048	-0.844479
C	-1.693227	-1.539531	0.665523
H	-1.829760	-0.830778	-1.443355
H	-2.725088	-1.192316	0.626482
H	-1.617187	-2.595832	0.922118
Si	-2.248480	2.416085	-0.321279
H	-1.568081	3.702663	-0.663836
H	-3.181609	2.048509	-1.436415
H	-3.059961	2.611193	0.924223
Mo	0.184531	-0.218165	0.168592
C	-0.777450	-2.740304	-1.494534
H	-0.336694	-2.560277	-2.480301
H	-0.051765	-3.295168	-0.894320
H	-1.666985	-3.366544	-1.645397
H	-0.510907	-1.364226	2.557356
O	1.153331	-1.578145	0.481794
O	1.564882	0.995316	-0.298185
Si	3.245062	0.925961	-0.170146
H	3.786576	-0.181424	-1.013787
H	3.781270	2.232762	-0.653434
H	3.653218	0.716553	1.252007

E = -462.564796558
G = -462.440135

Mo-O-5-TSIII

Mo	-0.230883	-0.267274	0.161628
O	-0.007532	1.664190	0.062432
C	-2.528967	0.215616	0.910664
C	-0.774795	-0.701516	1.955656
C	-2.369719	0.422752	-0.473441
H	-0.655519	0.011887	2.773519
H	-1.153888	-1.677461	2.254977
Si	1.341214	2.635429	-0.211490
H	0.858656	4.053309	-0.167134
H	2.386595	2.465978	0.842081
H	1.926567	2.377377	-1.561163
H	-2.153207	1.443277	-0.777048
H	-2.478120	1.070509	1.577079
C	-3.043939	-0.458248	-1.494193
H	-2.476205	-0.504921	-2.427099
H	-3.169303	-1.480672	-1.129627
H	-4.035733	-0.050115	-1.728017
H	-3.126258	-0.624707	1.255210
O	-0.575973	-1.682104	-0.685209
O	1.687384	-0.280960	-0.103173
Si	2.790520	-1.536547	-0.246989
H	4.136078	-0.943075	-0.514122
H	2.854035	-2.334827	1.019561
H	2.412611	-2.446029	-1.372395

E = -462.545690866
G = -462.420556

Mo-O-5-IV

Mo	-0.108610	-0.341010	0.040116
O	-0.156731	1.581523	0.158725
C	-2.840741	0.363512	-0.113074
C	0.017529	-1.294428	1.667245
C	-2.535668	0.144383	1.187114
H	0.364911	-0.794182	2.576938
H	-0.271849	-2.336986	1.799451
Si	1.010317	2.771991	-0.096757
H	-2.864817	-0.757207	1.696683
H	-2.083730	0.921822	1.794277
H	2.183772	2.593350	0.811348
H	1.461982	2.772944	-1.519524
H	0.361263	4.083932	0.213049
C	-3.637870	-0.562434	-0.973066
H	-3.117649	-0.779112	-1.910442
H	-3.844935	-1.509006	-0.467623
H	-4.593427	-0.087310	-1.227884
H	-2.555755	1.320422	-0.548654
O	-0.760287	-1.427899	-1.059158
O	1.724982	-0.215732	-0.520008
Si	3.040948	-1.203494	-0.181924
H	2.878022	-2.543251	-0.826077
H	4.269076	-0.542860	-0.719676
H	3.173814	-1.388439	1.299011

E = -462.551482206
G = -462.430030

Mo-O-5-TSIV

O	-0.302907	1.472444	0.324084
C	-3.046783	-0.188702	-0.054898

C	0.363860	-1.332976	1.601373
C	-2.660495	-0.363644	1.219701
H	0.181281	-2.399728	1.724391
H	0.660525	-0.797638	2.509207
Si	-0.125427	3.085481	-0.111829
H	-2.966923	0.808523	-0.488518
H	-2.750862	-1.331366	1.707128
H	-2.310965	0.465214	1.826179
H	1.321176	3.454068	-0.140720
H	-0.729928	3.322421	-1.459028
H	-0.839909	3.918040	0.901849
C	-3.610441	-1.252917	-0.938499
H	-4.602270	-0.961885	-1.304583
H	-2.969189	-1.404626	-1.813822
H	-3.699948	-2.207783	-0.413494
O	-0.466153	-1.449693	-1.100810
O	1.917568	-0.023964	-0.582819
Si	3.397340	-0.695899	-0.140677
H	3.499641	-2.101895	-0.636550
H	4.476574	0.131650	-0.759315
H	3.540390	-0.684646	1.348920
Mo	0.140922	-0.352984	0.010565

E = -462.550404527
G = -462.432356

Mo-O-5-V

Mo	-0.000092	0.544858	-0.092751
O	1.533580	-0.430852	-0.600075
C	-0.000533	0.655509	1.780048
H	0.000142	-0.288904	2.336192
H	-0.001297	1.559523	2.386350
Si	2.947665	-1.092209	0.046615
H	3.365386	-2.224392	-0.830411
H	4.014775	-0.049628	0.080133
H	2.679520	-1.586980	1.432107
O	-0.001113	2.141195	-0.571384
O	-1.532469	-0.432759	-0.600462
Si	-2.947147	-1.092549	0.046553
H	-3.368307	-2.221886	-0.832491
H	-2.678281	-1.591006	1.430584
H	-4.012085	-0.047870	0.083823

E = -344.686274236
G = -344.641947

Mo-O-5-TSA

O	-1.406183	-0.510186	-0.319637
C	0.896376	-1.970876	-0.071808
H	0.371987	-2.492677	-0.870896
C	1.993825	0.249110	-0.928615
C	2.203186	-1.288763	-0.552323
H	1.644126	0.316116	-1.966826
H	2.530500	-1.782126	-1.473094
H	2.987930	-1.355648	0.203920
Si	-2.313989	-1.912645	-0.231702
H	-2.087005	-2.644153	1.054543
H	-3.756913	-1.536498	-0.332987
H	-1.991943	-2.842929	-1.363522
Mo	0.392004	0.057284	0.325038
C	3.183853	1.149697	-0.663589
H	2.934648	2.189540	-0.894540
H	3.496509	1.105329	0.383584
H	4.041399	0.863197	-1.287242
H	1.020233	-2.597085	0.809598
O	0.951112	0.065630	1.902418
O	-0.533291	1.700239	0.226993
Si	-2.099825	2.100479	-0.318618
H	-2.137193	3.593917	-0.223990
H	-2.327569	1.720666	-1.741873
H	-3.154039	1.546257	0.576038

E = -462.553830214
G = -462.425050

Mo-O-5-SBP

O	-1.811156	0.626257	0.353832
C	-0.884279	-1.603867	-0.903100
C	1.324798	-1.219476	-0.777445
C	0.402463	-2.390010	-1.078298
H	1.411310	-0.582109	-1.669845
Si	-3.262567	0.781008	-0.492849
H	-4.116072	-0.422889	-0.267612
H	-3.946630	1.997504	0.032959
H	-3.006434	0.944602	-1.957053
H	0.548923	-2.881954	-2.051419
H	0.494832	-3.153685	-0.297483
H	-1.163608	-1.060892	-1.814591
Mo	-0.094799	-0.153368	0.506763
C	2.686325	-1.488872	-0.161920
H	3.315449	-2.053210	-0.865528
H	3.223049	-0.569233	0.091974
H	2.594799	-2.084792	0.751994
H	-1.763565	-2.118015	-0.500569
O	0.071115	-1.105531	1.865587
O	1.076107	1.317761	0.380052
Si	2.078789	2.356959	-0.492147
H	2.075000	1.993050	-1.942409
H	1.555413	3.743255	-0.320942
H	3.467627	2.263746	0.045240

E = -462.584334012
G = -462.457567

Mo-O-5-TSB

C	0.420814	1.892464	-1.582202
C	-0.264213	2.159171	0.652113
C	0.837087	2.241955	-0.229317
H	-1.233677	2.397697	0.216688
H	1.811811	2.653005	0.041979
H	1.509911	0.888297	-0.084123
O	-1.598770	-0.183187	0.597231
Si	-2.694115	-1.464272	0.445196
H	-3.596420	-1.221580	-0.720702
H	-1.990616	-2.771008	0.276117
H	-3.500570	-1.490896	1.703676
H	-0.523219	2.317074	-1.927041
Mo	-0.014080	0.064806	-0.464868
C	-0.170993	2.199597	2.146852
H	-0.400165	3.199705	2.537002
H	-0.893530	1.503473	2.586376
H	0.828113	1.923133	2.500060
H	1.173515	1.791512	-2.361096
O	-0.461570	-0.641246	-1.940314
O	1.108346	-1.269169	0.325738
Si	2.727358	-1.607145	0.615120
H	2.805253	-2.535851	1.780956
H	3.349720	-2.247274	-0.583019
H	3.465624	-0.339597	0.927255

E = -462.516790823
G = -462.394552

Mo-O-5-B

C	-0.925161	-0.272177	1.729205
C	-2.949204	-0.975684	0.412868
C	-1.768184	-1.242668	0.992199
H	-3.353956	0.034982	0.492079
H	-1.376836	-2.259946	0.925890
H	0.864214	-1.212713	0.932748
O	-0.389930	1.524385	-0.426903
Si	-1.534552	1.753521	-1.650500
H	-2.826443	2.170542	-1.031264
H	-1.023111	2.839928	-2.535358
H	-1.724254	0.500688	-2.438170
H	-1.455150	0.668308	1.937427
Mo	0.768878	0.425574	0.566425
C	-3.791330	-1.973572	-0.317581
H	-4.774450	-2.086162	0.156771
H	-3.979668	-1.656883	-1.351331
H	-3.315026	-2.958150	-0.346710
H	-0.541868	-0.687025	2.664995
O	1.646217	1.127280	1.793706
O	1.958055	-0.205521	-0.766901
Si	2.533679	-1.722046	-1.254710
H	1.392105	-2.661403	-1.474507
H	3.273128	-1.517033	-2.534806
H	3.449208	-2.274462	-0.214051

E = -462.560169241
G = -462.438415

Mo-O-5-TSC

C	1.500825	0.076761	-1.301800
C	3.723127	0.007968	-0.135041
C	2.739395	-0.576274	-0.838152
H	1.601420	1.172759	-1.295653
H	2.875345	-1.619621	-1.133960
H	1.251129	-0.233787	-2.318924
H	0.190267	-1.569684	-0.200851
O	-0.411881	1.688178	0.781879
C	0.756550	-1.731448	1.176548
H	1.656988	-2.171264	0.754446
H	-0.009038	-2.437216	1.492209
C	0.837458	-0.487230	1.785935
H	0.084123	-0.169736	2.499095
H	1.748895	0.095896	1.724177
H	3.610531	1.057982	0.143298
C	4.994322	-0.658985	0.286239
H	5.869956	-0.149339	-0.135631
H	5.117772	-0.634679	1.376688
H	5.026453	-1.704823	-0.034790
Mo	-0.471548	0.075740	-0.258964
O	-1.035982	0.648181	-1.741667
O	-1.947450	-0.949395	0.359804
Si	-2.840593	-2.333613	0.009079
H	-3.511159	-2.183697	-1.315906
H	-1.939253	-3.529379	-0.023768
H	-3.856341	-2.498738	1.089161
Si	-1.157176	3.168402	0.431693
H	-0.509104	3.791590	-0.761589
H	-2.618850	2.989237	0.180240
H	-0.962901	4.045938	1.624927

E = -541.085940971
G = -540.914046

Mo-O-5-C

C	1.349746	-1.108125	-1.024613
C	3.289768	-0.824533	0.551603
C	2.143609	-1.420272	0.187074
H	3.711979	-0.055445	-0.097071
H	1.758494	-2.212855	0.830003
O	0.581807	1.460169	-0.657231
Si	1.886358	2.459595	-0.279816
H	3.046350	2.134892	-1.163175
H	1.441656	3.860132	-0.542374
H	2.278681	2.313200	1.151999
H	1.882696	-0.416450	-1.687047
Mo	-0.541093	-0.057570	-0.592706
C	4.072835	-1.156768	1.783008
H	5.087662	-1.490828	1.532057
H	4.185795	-0.279805	2.433287
H	3.590777	-1.948235	2.365101
H	1.089009	-2.007199	-1.588753
O	-1.387758	-0.200565	-2.020629
C	-0.883755	-2.083394	0.170908
H	-0.331927	-2.848045	-0.379131
H	-0.513448	-2.079342	1.202887
C	-2.378408	-2.412768	0.140936
H	-2.550671	-3.409027	0.570717
H	-2.977527	-1.707246	0.723913
H	-2.771451	-2.424306	-0.880593
Si	-2.862360	1.200753	1.565253
H	-3.820897	1.491589	0.457228
H	-3.510723	0.314857	2.576370
H	-2.426534	2.473309	2.212249
O	-1.486893	0.427779	0.968655

E = -541.154362698
G = -540.979852

ethene

C	0.000000	0.665027	0.000000
H	-0.924084	1.237465	0.000000
H	0.924090	1.237460	0.000000
C	0.000000	-0.665027	0.000000
H	0.924084	-1.237465	0.000000
H	-0.924090	-1.237460	0.000000

E = -78.5600140642
G = -78.530357

propene

C	1.281164	0.220204	0.000005
H	2.241566	-0.287347	0.000116
H	1.302542	1.308092	-0.000048
C	0.132029	-0.454776	-0.000060
H	0.163749	-1.545241	0.000031
C	-1.231907	0.162949	-0.000001
H	-1.808777	-0.151012	-0.878952
H	-1.808259	-0.150395	0.879562
H	-1.178537	1.255641	-0.000378

E = -117.868519219
G = -117.813596