

**Table S1.** Calculated (6-31G\*) and experimental data for 1-chlorosilatrane.<sup>a</sup>

Method	Gas		Xtal												
	SCF	B3LYP	SCF	SCF	SCF	SCF	ONIOM	ONIOM	ONIOM	ONIOM	B3LYP	Exp <sup>b</sup>	Exp <sup>b</sup>	Exp <sup>b</sup>	Exp <sup>c</sup>
Model	0	0	1	2	3	4	1	2	3	4	1				(C <sub>3</sub> )
Si-N	2.571	2.410	2.260	2.130	2.073	2.379	2.392	2.373	2.370	2.368	2.226	2.023			2.023
Cl-Si	2.058	2.086	2.075	2.098	2.129	2.041	2.069	2.062	2.062	2.062	2.096	2.153			2.153
Si-O	1.633	1.668	1.648	1.653	1.654	1.641	1.639	1.639	1.639	1.640	1.680	1.644	1.652	1.651	1.649
O-C	1.401	1.415	1.400	1.401	1.405	1.392	1.393	1.392	1.392	1.392	1.420	1.421	1.419	1.408	1.416
C-C	1.527	1.534	1.524	1.521	1.521	1.523	1.527	1.526	1.526	1.526	1.531	1.443	1.433	1.428	1.435
C-N	1.449	1.467	1.457	1.467	1.471	1.452	1.453	1.454	1.454	1.455	1.473	1.452	1.442	1.454	1.449
Cl-Si-O	104.4	100.2	98.6	95.9	94.5	100.7	100.9	100.5	100.5	100.4	96.9	93.0	93.5	93.4	93.3
Si-O-C	124.6	122.3	125.6	123.3	121.9	127.0	127.5	127.1	127.2	127.2	122.6	119.8	120.4	120.4	120.2
O-C-C	109.8	109.7	108.9	108.4	108.3	109.7	110.0	109.9	109.9	109.9	109.1	111.4	110.3	111.6	111.1
C-C-N	108.8	107.6	107.7	107.2	106.9	108.1	108.1	108.1	108.1	108.1	107.4	110.9	112.5	111.2	111.6
O-Si-N	76.0	79.8	81.4	84.1	84.5	79.3	79.1	79.5	79.5	79.6	83.1	87.1	86.6	86.4	86.7
Si-N-C	98.5	101.2	103.0	104.3	104.9	101.2	101.3	101.5	101.5	101.5	103.3	106.0	105.7	106.0	105.9
O-Si-O	114.4	117.0	117.8	119.0	119.4	116.6	116.5	116.7	116.8	116.8	118.6	119.7	119.4	120.0	119.7
C-N-C	117.9	116.3	115.1	114.1	113.6	116.3	116.2	116.2	116.1	116.1	114.8	113.7	112.3	112.4	112.8
O-Si-N-C	-0.3	-4.4	-14.3	-15.8	-16.3	-11.8	-11.7	-11.8	-12.0	-12.1	-13.9	-9.7	-8.7	-9.1	-9.2
C-O-Si-N	-30.2	-24.1	-9.9	-7.1	-6.2	-13.9	-13.5	-13.3	-12.9	-12.8	-10.6	-3.7	-4.4	-3.9	-4.0
Si-O-C-C	56.1	48.4	31.2	27.8	26.7	36.3	35.5	35.1	34.7	34.6	32.5	16.8	16.7	16.5	16.7

C–C–N–Si	24.1	26.6	31.0	31.7	31.8	29.8	29.2	29.2	29.2	29.3	31.6	20.2	19.4	19.4	19.6	
O–C–C–N	-47.2	-46.1	-39.8	-38.2	-37.5	-41.9	-41.0	-40.9	-40.6	-40.6	-41.2	-23.9	-23.3	-23.2	-23.5	
$q_M(\text{Cl})$	-0.372	-0.304	-0.420	-0.495	-0.546	-0.389						-0.329				
$q_M(\text{Si})$	1.565	1.111	1.720	1.754	1.771	1.717						1.265				
$q_M(\text{N})$	-0.715	-0.481	-0.754	-0.776	-0.784	-0.741						-0.502				
$q_M(\text{O})$	-0.733	-0.533	-0.775	-0.776	-0.781	-0.764						-0.581				
$q_M(\text{C–O})$	0.012	-0.028	-0.003	-0.009	-0.015	0.004						-0.050				
$q_M(\text{C–N})$	-0.134	-0.157	-0.170	-0.180	-0.186	-0.163						-0.188				
$\rho_b(\text{Si–N})$	0.185		0.297	0.379	0.426	0.245										AIM
$\nabla^2\rho_b(\text{Si–N})$	1.231		2.330	3.984	5.013	1.514										
$\rho_b(\text{Cl–Si})$	0.661		0.651	0.609	0.564	0.694										
$\nabla^2\rho_b(\text{Cl–Si})$	6.474		5.935	5.555	4.920	7.019										
$\rho_b(\text{Si–O})$	0.902		0.869	0.863	0.864	0.879										
$\nabla^2\rho_b(\text{Si–O})$	26.062		24.575	24.139	24.076	25.219										
$\rho_b(\text{O–C})$	1.697		1.711	1.717	1.698	1.745										
$\nabla^2\rho_b(\text{O–C})$	0.038		-0.149	-0.504	-0.431	0.039										
$\rho_b(\text{C–C})$	1.798		1.800	1.808	1.810	1.806										
$\nabla^2\rho_b(\text{C–C})$	-17.878		-17.940	-18.086	-18.116	-18.034										
$\rho_b(\text{C–N})$	1.847		1.819	1.777	1.756	1.839										
$\nabla^2\rho_b(\text{C–N})$	-19.631		-18.120	-16.963	-16.242	-18.760										
$q_{NBO}(\text{Cl})$	-0.474		-0.467		-0.536											NBO

$q_{NBO}$ (Si)	2.455	2.436	2.465
$q_{NBO}$ (N)	-0.639	-0.654	-0.684
$q_{NBO}$ (O)	-1.028	-1.036	-1.040
$q_{NBO}$ (C-O)	-0.022	-0.026	-0.033
$q_{NBO}$ (C-N)	-0.222	-0.225	-0.229
BndIdx (Si-Cl) <sup>d</sup>	0.795	0.776	0.675
BndIdx (Si-N)	0.064	0.145	0.220
BndIdx (Si-O)	0.525	0.504	0.500
BndIdx (O-C)	0.884	0.884	0.880
BndIdx (C-C)	0.999	0.999	1.003
BndIdx (C-N)	0.952	0.936	0.919
$\Delta E^{(2)} n \rightarrow Ry^*$ (Si)	7	20	46
$\Delta E^{(2)} n \rightarrow \sigma^*$ (Si-Cl)	24	55	97
$\Delta E^{(2)} n \rightarrow \sigma^*$ (Si-O)	18	48	73

<sup>a</sup> Distances in Å, angles in degrees, Mulliken charges,  $q_M$ , and NBO charges,  $q_{NBO}$ , in e, electron density at the BCP,  $\rho_b$ , in e A<sup>-3</sup>, Laplacian of the electron density at the BCP,  $\nabla^2\rho_b$ , in e A<sup>-5</sup>, donor-acceptor stabilization energy,  $\Delta E^{(2)}$ , in kJ mol<sup>-1</sup>. <sup>b</sup> Experimental, non-symmetrized, crystal structure. <sup>c</sup> Experimental, C<sub>3</sub>-symmetrized, crystal structure. <sup>d</sup> Wiberg bond index in the NAO basis.

Gas, model 0, HF

%chk=Cl\_silatrane.chk  
%mem=256MB

# HF/6-31G(d) Opt IOp(1/8=3) Freq

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	17	0	0.000000	0.000000	2.963278
2	14	0	0.000000	0.000000	0.905538
3	7	0	0.000000	0.000000	-1.665813
4	8	0	0.000000	1.585117	0.511361
5	6	0	0.580527	2.117725	-0.647377
6	6	0	-0.006309	1.433350	-1.880110
7	8	0	1.372752	-0.792559	0.511361
8	6	0	1.543740	-1.561614	-0.647377
9	6	0	1.244472	-0.711211	-1.880110
10	8	0	-1.372752	-0.792559	0.511361
11	6	0	-2.124267	-0.556112	-0.647377
12	6	0	-1.238163	-0.722139	-1.880110
13	1	0	0.377779	3.180843	-0.664063
14	1	0	1.656986	1.985662	-0.610306
15	1	0	-1.032005	1.757532	-2.005031
16	1	0	0.538080	1.723101	-2.777423
17	1	0	2.565801	-1.917588	-0.664063
18	1	0	0.891141	-2.427823	-0.610306
19	1	0	2.038070	0.014976	-2.005031
20	1	0	1.223209	-1.327541	-2.777423
21	1	0	-2.943581	-1.263255	-0.664063
22	1	0	-2.548126	0.442161	-0.610306
23	1	0	-1.006065	-1.772509	-2.005031
24	1	0	-1.761289	-0.395560	-2.777423

Gas, model 0, b3lyp

%chk=Cl-SilatraneB3LYP.chk  
%mem=256MB

# B3LYP/6-31G(d) Opt IOp(1/8=3) Freq

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	17	0	0.000000	0.000000	2.926527

2	14	0	0.000000	0.000000	0.840478
3	7	0	0.000000	0.000000	-1.569576
4	8	0	0.000000	1.641522	0.546348
5	6	0	0.488242	2.192666	-0.662028
6	6	0	-0.110366	1.434525	-1.854136
7	8	0	1.421600	-0.820761	0.546348
8	6	0	1.654783	-1.519163	-0.662028
9	6	0	1.297518	-0.621683	-1.854136
10	8	0	-1.421600	-0.820761	0.546348
11	6	0	-2.143025	-0.673502	-0.662028
12	6	0	-1.187152	-0.812843	-1.854136
13	1	0	0.205273	3.250062	-0.695823
14	1	0	1.586346	2.140630	-0.682576
15	1	0	-1.172398	1.684264	-1.939051
16	1	0	0.376709	1.714257	-2.799893
17	1	0	2.712000	-1.802802	-0.695823
18	1	0	1.060667	-2.444131	-0.682576
19	1	0	2.044814	0.173195	-1.939051
20	1	0	1.296236	-1.183368	-2.799893
21	1	0	-2.917273	-1.447259	-0.695823
22	1	0	-2.647013	0.303501	-0.682576
23	1	0	-0.872416	-1.857458	-1.939051
24	1	0	-1.672945	-0.530890	-2.799893

Xtal, model 1, HF

%chk=Cl\_silatrane.chk  
%mem=128MB

# HF/6-31G(d) Opt(Z-Matrix) IOp(1/8=5) MaxDisk=2GB

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	17	0	0.000000	0.000000	2.920667
2	14	0	0.000000	0.000000	0.845852
3	7	0	0.000000	0.000000	-1.414072
4	8	0	0.000000	-1.629073	0.599661
5	6	0	-0.194721	-2.267693	-0.631088
6	6	0	0.349732	-1.376453	-1.740825
7	8	0	-1.410818	0.814536	0.599661
8	6	0	-1.866519	1.302480	-0.631088
9	6	0	-1.366909	0.385350	-1.740825
10	8	0	1.410818	0.814536	0.599661
11	6	0	2.061240	0.965213	-0.631088
12	6	0	1.017177	0.991103	-1.740825
13	1	0	0.336826	-3.210315	-0.618311
14	1	0	-1.246460	-2.474389	-0.767901

15	1	0	1.422928	-1.459685	-1.765802	67	1	0	3.429744	-4.167894	1.932157
16	1	0	-0.038782	-1.674084	-2.712256	68	1	0	2.472583	-2.871056	1.362185
17	1	0	-2.948627	1.313457	-0.618311	69	1	0	3.541569	0.762178	3.281776
18	1	0	-1.519654	2.316660	-0.767901	70	1	0	5.177471	0.280447	3.160439
19	1	0	-1.975589	-0.502449	-1.765802	71	1	0	2.851252	-0.886299	1.932157
20	1	0	-1.430409	0.870629	-2.712256	72	1	0	4.452927	-0.705792	1.362185
21	1	0	2.611801	1.896858	-0.618311	73	14	0	-4.087813	-2.360100	4.641790
22	1	0	2.766113	0.157729	-0.767901	74	17	0	-4.087813	-2.360100	6.795090
23	1	0	0.552660	1.962135	-1.765802	75	7	0	-4.087813	-2.360100	2.619290
24	1	0	1.469191	0.803456	-2.712256	76	8	0	-5.513607	-3.183283	4.546855
25	14	0	0.000000	4.720200	4.641790	77	6	0	-6.111186	-3.429862	3.287369
26	17	0	0.000000	4.720200	6.795090	78	6	0	-5.168465	-3.240371	2.222870
27	7	0	0.000000	4.720200	2.619290	79	8	0	-4.087813	-0.713735	4.546855
28	8	0	0.000000	6.366565	4.546855	80	6	0	-4.002568	-0.072926	3.287369
29	6	0	0.085246	7.007374	3.287369	81	6	0	-4.309824	-0.984093	2.222870
30	6	0	-0.222011	6.096207	2.222870	82	8	0	-2.662019	-3.183283	4.546855
31	8	0	1.425794	3.897017	4.546855	83	6	0	-2.149685	-3.577512	3.287369
32	6	0	1.938128	3.502788	3.287369	84	6	0	-2.785150	-2.855836	2.222870
33	6	0	1.302663	4.224464	2.222870	85	1	0	-6.518663	-4.394300	3.281776
34	8	0	-1.425794	3.897017	4.546855	86	1	0	-6.919423	-2.736702	3.160439
35	6	0	-2.023373	3.650438	3.287369	87	1	0	-4.745882	-4.167894	1.932157
36	6	0	-1.080652	3.839929	2.222870	88	1	0	-5.703043	-2.871056	1.362185
37	1	0	-0.546244	7.842478	3.281776	89	1	0	-4.634057	0.762178	3.281776
38	1	0	1.089657	7.360747	3.160439	90	1	0	-2.998156	0.280447	3.160439
39	1	0	-1.236561	6.194001	1.932157	91	1	0	-5.324374	-0.886299	1.932157
40	1	0	0.365114	6.374508	1.362185	92	1	0	-3.722699	-0.705792	1.362185
41	1	0	2.977094	3.632123	3.281776	93	1	0	-1.110719	-3.448177	3.281776
42	1	0	1.741952	2.456255	3.160439	94	1	0	-2.345861	-4.624045	3.160439
43	1	0	1.894630	5.054192	1.932157	95	1	0	-2.193183	-2.026108	1.932157
44	1	0	1.250116	3.576848	1.362185	96	1	0	-2.837698	-3.503452	1.362185
45	1	0	-2.430850	2.686000	3.281776	97	14	0	0.000000	4.720200	-3.309210
46	1	0	-2.831609	4.343598	3.160439	98	17	0	0.000000	4.720200	-1.155910
47	1	0	-0.658069	2.912406	1.932157	99	7	0	0.000000	4.720200	-5.331710
48	1	0	-1.615230	4.209244	1.362185	100	8	0	0.000000	6.366565	-3.404145
49	14	0	4.087813	-2.360100	4.641790	101	6	0	0.085246	7.007374	-4.663631
50	17	0	4.087813	-2.360100	6.795090	102	6	0	-0.222011	6.096207	-5.728130
51	7	0	4.087813	-2.360100	2.619290	103	8	0	1.425794	3.897017	-3.404145
52	8	0	5.513607	-3.183283	4.546855	104	6	0	1.938128	3.502788	-4.663631
53	6	0	6.025941	-3.577512	3.287369	105	6	0	1.302663	4.224464	-5.728130
54	6	0	5.390476	-2.855836	2.222870	106	8	0	-1.425794	3.897017	-3.404145
55	8	0	2.662019	-3.183283	4.546855	107	6	0	-2.023373	3.650438	-4.663631
56	6	0	2.064440	-3.429862	3.287369	108	6	0	-1.080652	3.839929	-5.728130
57	6	0	3.007162	-3.240371	2.222870	109	1	0	-0.546244	7.842478	-4.669224
58	8	0	4.087813	-0.713735	4.546855	110	1	0	1.089657	7.360747	-4.790561
59	6	0	4.173059	-0.072926	3.287369	111	1	0	-1.236561	6.194001	-6.018843
60	6	0	3.865802	-0.984093	2.222870	112	1	0	0.365114	6.374508	-6.588815
61	1	0	7.064907	-3.448177	3.281776	113	1	0	2.977094	3.632123	-4.669224
62	1	0	5.829765	-4.624045	3.160439	114	1	0	1.741952	2.456255	-4.790561
63	1	0	5.982443	-2.026108	1.932157	115	1	0	1.894630	5.054192	-6.018843
64	1	0	5.337929	-3.503452	1.362185	116	1	0	1.250116	3.576848	-6.588815
65	1	0	1.656964	-4.394300	3.281776	117	1	0	-2.430850	2.686000	-4.669224
66	1	0	1.256204	-2.736702	3.160439	118	1	0	-2.831609	4.343598	-4.790561

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119      1      0      -0.658069      2.912406      -6.018843
120      1      0      -1.615230      4.209244      -6.588815
121     14      0      -4.087813      -2.360100      -3.309210
122     17      0      -4.087813      -2.360100      -1.155910
123      7      0      -4.087813      -2.360100      -5.331710
124      8      0      -5.513607      -3.183283      -3.404145
125      6      0      -6.111186      -3.429862      -4.663631
126      6      0      -5.168465      -3.240371      -5.728130
127      8      0      -4.087813      -0.713735      -3.404145
128      6      0      -4.002568      -0.072926      -4.663631
129      6      0      -4.309824      -0.984093      -5.728130
130      8      0      -2.662019      -3.183283      -3.404145
131      6      0      -2.149685      -3.577512      -4.663631
132      6      0      -2.785150      -2.855836      -5.728130
133      1      0      -6.518663      -4.394300      -4.669224
134      1      0      -6.919423      -2.736702      -4.790561
135      1      0      -4.745882      -4.167894      -6.018843
136      1      0      -5.703043      -2.871056      -6.588815
137      1      0      -4.634057      0.762178      -4.669224
138      1      0      -2.998156      0.280447      -4.790561
139      1      0      -5.324374      -0.886299      -6.018843
140      1      0      -3.722699      -0.705792      -6.588815
141      1      0      -1.110719      -3.448177      -4.669224
142      1      0      -2.345861      -4.624045      -4.790561
143      1      0      -2.193183      -2.026108      -6.018843
144      1      0      -2.837698      -3.503452      -6.588815
145     14      0      4.087813      -2.360100      -3.309210
146     17      0      4.087813      -2.360100      -1.155910
147      7      0      4.087813      -2.360100      -5.331710
148      8      0      5.513607      -3.183283      -3.404145
149      6      0      6.025941      -3.577512      -4.663631
150      6      0      5.390476      -2.855836      -5.728130
151      8      0      2.662019      -3.183283      -3.404145
152      6      0      2.064440      -3.429862      -4.663631
153      6      0      3.007162      -3.240371      -5.728130
154      8      0      4.087813      -0.713735      -3.404145
155      6      0      4.173059      -0.072926      -4.663631
156      6      0      3.865802      -0.984093      -5.728130
157      1      0      7.064907      -3.448177      -4.669224
158      1      0      5.829765      -4.624045      -4.790561
159      1      0      5.982443      -2.026108      -6.018843
160      1      0      5.337929      -3.503452      -6.588815
161      1      0      1.656964      -4.394300      -4.669224
162      1      0      1.256204      -2.736702      -4.790561
163      1      0      3.429744      -4.167894      -6.018843
164      1      0      2.472583      -2.871056      -6.588815
165      1      0      3.541569      0.762178      -4.669224
166      1      0      5.177471      0.280447      -4.790561
167      1      0      2.851252      -0.886299      -6.018843
168      1      0      4.452927      -0.705792      -6.588815

```

Xtal, model 2, HF

```

%chk=C1_silatrane.chk
%mem=256MB
%RWF=s1,1900MB,s2,1900MB,s3,1900MB,s4,1900MB,s5,1900MB,s6,1900MB,s7,1900
MB

```

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# HF/6-31G(d) Opt(Z-Matrix) IOp(1/8=5)

```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	17	0	0.000000	0.000000	2.871755
2	14	0	0.000000	0.000000	0.773424
3	7	0	0.000000	0.000000	-1.356178
4	8	0	0.000000	-1.644377	0.603503
5	6	0	-0.144918	-2.288913	-0.631860
6	6	0	0.387440	-1.367287	-1.719119
7	8	0	-1.424072	0.822188	0.603503
8	6	0	-1.909798	1.269959	-0.631860
9	6	0	-1.377825	0.348110	-1.719119
10	8	0	1.424072	0.822188	0.603503
11	6	0	2.054715	1.018954	-0.631860
12	6	0	0.990385	1.019176	-1.719119
13	1	0	0.423967	-3.209460	-0.614726
14	1	0	-1.185396	-2.536127	-0.790834
15	1	0	1.462340	-1.419931	-1.735607
16	1	0	0.014252	-1.639273	-2.697711
17	1	0	-2.991457	1.237564	-0.614726
18	1	0	-1.603652	2.294646	-0.790834
19	1	0	-1.960867	-0.556458	-1.735607
20	1	0	-1.426778	0.807294	-2.697711
21	1	0	2.567491	1.971896	-0.614726
22	1	0	2.789048	0.241481	-0.790834
23	1	0	0.498526	1.976389	-1.735607
24	1	0	1.412526	0.831980	-2.697711
25	14	0	0.000000	4.720200	4.644966
26	17	0	0.000000	4.720200	6.798266
27	7	0	0.000000	4.720200	2.622466
28	8	0	0.000000	6.366565	4.550031
29	6	0	0.085246	7.007374	3.290545
30	6	0	-0.222011	6.096207	2.226046
31	8	0	1.425794	3.897017	4.550031
32	6	0	1.938128	3.502788	3.290545
33	6	0	1.302663	4.224464	2.226046
34	8	0	-1.425794	3.897017	4.550031
35	6	0	-2.023373	3.650438	3.290545
36	6	0	-1.080652	3.839929	2.226046
37	1	0	-0.546244	7.842478	3.284952
38	1	0	1.089657	7.360747	3.163615

39	1	0	-1.236561	6.194001	1.935333	91	1	0	-5.324374	-0.886299	1.935333
40	1	0	0.365114	6.374508	1.365361	92	1	0	-3.722699	-0.705792	1.365361
41	1	0	2.977094	3.632123	3.284952	93	1	0	-1.110719	-3.448177	3.284952
42	1	0	1.741952	2.456255	3.163615	94	1	0	-2.345861	-4.624045	3.163615
43	1	0	1.894630	5.054192	1.935333	95	1	0	-2.193183	-2.026108	1.935333
44	1	0	1.250116	3.576848	1.365361	96	1	0	-2.837698	-3.503452	1.365361
45	1	0	-2.430850	2.686000	3.284952	97	14	0	0.000000	4.720200	-3.306034
46	1	0	-2.831609	4.343598	3.163615	98	17	0	0.000000	4.720200	-1.152734
47	1	0	-0.658069	2.912406	1.935333	99	7	0	0.000000	4.720200	-5.328534
48	1	0	-1.615230	4.209244	1.365361	100	8	0	0.000000	6.366565	-3.400969
49	14	0	4.087813	-2.360100	4.644966	101	6	0	0.085246	7.007374	-4.660455
50	17	0	4.087813	-2.360100	6.798266	102	6	0	-0.222011	6.096207	-5.724954
51	7	0	4.087813	-2.360100	2.622466	103	8	0	1.425794	3.897017	-3.400969
52	8	0	5.513607	-3.183283	4.550031	104	6	0	1.938128	3.502788	-4.660455
53	6	0	6.025941	-3.577512	3.290545	105	6	0	1.302663	4.224464	-5.724954
54	6	0	5.390476	-2.855836	2.226046	106	8	0	-1.425794	3.897017	-3.400969
55	8	0	2.662019	-3.183283	4.550031	107	6	0	-2.023373	3.650438	-4.660455
56	6	0	2.064440	-3.429862	3.290545	108	6	0	-1.080652	3.839929	-5.724954
57	6	0	3.007162	-3.240371	2.226046	109	1	0	-0.546244	7.842478	-4.660455
58	8	0	4.087813	-0.713735	4.550031	110	1	0	1.089657	7.360747	-4.787385
59	6	0	4.173059	-0.072926	3.290545	111	1	0	-1.236561	6.194001	-6.015667
60	6	0	3.865802	-0.984093	2.226046	112	1	0	0.365114	6.374508	-6.585639
61	1	0	7.064907	-3.448177	3.284952	113	1	0	2.977094	3.632123	-4.660455
62	1	0	5.829765	-4.624045	3.163615	114	1	0	1.741952	2.456255	-4.787385
63	1	0	5.982443	-2.026108	1.935333	115	1	0	1.894630	5.054192	-6.015667
64	1	0	5.337929	-3.503452	1.365361	116	1	0	1.250116	3.576848	-6.585639
65	1	0	1.656964	-4.394300	3.284952	117	1	0	-2.430850	2.686000	-4.660455
66	1	0	1.256204	-2.736702	3.163615	118	1	0	-2.831609	4.343598	-4.787385
67	1	0	3.429744	-4.167894	1.935333	119	1	0	-0.658069	2.912406	-6.015667
68	1	0	2.472583	-2.871056	1.365361	120	1	0	-1.615230	4.209244	-6.585639
69	1	0	3.541569	0.762178	3.284952	121	14	0	-4.087813	-2.360100	-3.306034
70	1	0	5.177471	0.280447	3.163615	122	17	0	-4.087813	-2.360100	-1.152734
71	1	0	2.851252	-0.886299	1.935333	123	7	0	-4.087813	-2.360100	-5.328534
72	1	0	4.452927	-0.705792	1.365361	124	8	0	-5.513607	-3.183283	-3.400969
73	14	0	-4.087813	-2.360100	4.644966	125	6	0	-6.111186	-3.429862	-4.660455
74	17	0	-4.087813	-2.360100	6.798266	126	6	0	-5.168465	-3.240371	-5.724954
75	7	0	-4.087813	-2.360100	2.622466	127	8	0	-4.087813	-0.713735	-3.400969
76	8	0	-5.513607	-3.183283	4.550031	128	6	0	-4.002568	-0.072926	-4.660455
77	6	0	-6.111186	-3.429862	3.290545	129	6	0	-4.309824	-0.984093	-5.724954
78	6	0	-5.168465	-3.240371	2.226046	130	8	0	-2.662019	-3.183283	-3.400969
79	8	0	-4.087813	-0.713735	4.550031	131	6	0	-2.149685	-3.577512	-4.660455
80	6	0	-4.002568	-0.072926	3.290545	132	6	0	-2.785150	-2.855836	-5.724954
81	6	0	-4.309824	-0.984093	2.226046	133	1	0	-6.518663	-4.394300	-4.660455
82	8	0	-2.662019	-3.183283	4.550031	134	1	0	-6.919423	-2.736702	-4.787385
83	6	0	-2.149685	-3.577512	3.290545	135	1	0	-4.745882	-4.167894	-6.015667
84	6	0	-2.785150	-2.855836	2.226046	136	1	0	-5.703043	-2.871056	-6.585639
85	1	0	-6.518663	-4.394300	3.284952	137	1	0	-4.634057	0.762178	-4.660455
86	1	0	-6.919423	-2.736702	3.163615	138	1	0	-2.998156	0.280447	-4.787385
87	1	0	-4.745882	-4.167894	1.935333	139	1	0	-5.324374	-0.886299	-6.015667
88	1	0	-5.703043	-2.871056	1.365361	140	1	0	-3.722699	-0.705792	-6.585639
89	1	0	-4.634057	0.762178	3.284952	141	1	0	-1.110719	-3.448177	-4.660455
90	1	0	-2.998156	0.280447	3.163615	142	1	0	-2.345861	-4.624045	-4.787385

143	1	0	-2.193183	-2.026108	-6.015667	195	7	0	0.000000	0.000000	-9.304034
144	1	0	-2.837698	-3.503452	-6.585639	196	8	0	1.425794	0.823183	-7.376469
145	14	0	4.087813	-2.360100	-3.306034	197	6	0	2.023373	1.069762	-8.635955
146	17	0	4.087813	-2.360100	-1.152734	198	6	0	1.080652	0.880271	-9.700454
147	7	0	4.087813	-2.360100	-5.328534	199	8	0	0.000000	-1.646365	-7.376469
148	8	0	5.513607	-3.183283	-3.400969	200	6	0	-0.085246	-2.287174	-8.635955
149	6	0	6.025941	-3.577512	-4.660455	201	6	0	0.222011	-1.376007	-9.700454
150	6	0	5.390476	-2.855836	-5.724954	202	8	0	-1.425794	0.823183	-7.376469
151	8	0	2.662019	-3.183283	-3.400969	203	6	0	-1.938128	1.217412	-8.635955
152	6	0	2.064440	-3.429862	-4.660455	204	6	0	-1.302663	0.495736	-9.700454
153	6	0	3.007162	-3.240371	-5.724954	205	1	0	2.430850	2.034200	-8.641548
154	8	0	4.087813	-0.713735	-3.400969	206	1	0	2.831609	0.376602	-8.762885
155	6	0	4.173059	-0.072926	-4.660455	207	1	0	0.658069	1.807794	-9.991167
156	6	0	3.865802	-0.984093	-5.724954	208	1	0	1.615230	0.510956	-10.561139
157	1	0	7.064907	-3.448177	-4.666048	209	1	0	0.546244	-3.122278	-8.641548
158	1	0	5.829765	-4.624045	-4.787385	210	1	0	-1.089657	-2.640547	-8.762885
159	1	0	5.982443	-2.026108	-6.015667	211	1	0	1.236561	-1.473801	-9.991167
160	1	0	5.337929	-3.503452	-6.585639	212	1	0	-0.365114	-1.654308	-10.561139
161	1	0	1.656964	-4.394300	-4.666048	213	1	0	-2.977094	1.088077	-8.641548
162	1	0	1.256204	-2.736702	-4.787385	214	1	0	-1.741952	2.263945	-8.762885
163	1	0	3.429744	-4.167894	-6.015667	215	1	0	-1.894630	-0.333992	-9.991167
164	1	0	2.472583	-2.871056	-6.585639	216	1	0	-1.250116	1.143352	-10.561139
165	1	0	3.541569	0.762178	-4.666048	-----					
166	1	0	5.177471	0.280447	-4.787385	<b>Xtal, model 3, HF</b>					
167	1	0	2.851252	-0.886299	-6.015667	%chk=C1_silatrane.chk					
168	1	0	4.452927	-0.705792	-6.585639	%mem=512MB					
169	14	0	0.000000	0.000000	8.620466	%RWF=s1,1900MB,s2,1900MB,s3,1900MB,s4,1900MB,s5,1900MB,s6,1900MB,s7,1900					
170	17	0	0.000000	0.000000	10.773766	MB					
171	7	0	0.000000	0.000000	6.597966	-----					
172	8	0	0.000000	-1.646365	8.525531	# HF/6-31G(d) Opt(Z-Matrix) IOp(1/8=5) SCF=IntRep					
173	6	0	-0.085246	-2.287174	7.266045	-----					
174	6	0	0.222011	-1.376007	6.201546	Standard orientation:					
175	8	0	-1.425794	0.823183	8.525531	-----					
176	6	0	-1.938128	1.217412	7.266045	Center Atomic Atomic Coordinates (Angstroms)					
177	6	0	-1.302663	0.495736	6.201546	Number Number Type X Y Z					
178	8	0	1.425794	0.823183	8.525531	-----					
179	6	0	2.023373	1.069762	7.266045	1	17	0	0.000000	0.000000	2.868264
180	6	0	1.080652	0.880271	6.201546	2	14	0	0.000000	0.000000	0.739523
181	1	0	0.546244	-3.122278	7.260452	3	7	0	0.000000	0.000000	-1.333429
182	1	0	-1.089657	-2.640547	7.139115	4	8	0	0.000000	-1.649291	0.609206
183	1	0	1.236561	-1.473801	5.910833	5	6	0	-0.129491	-2.296178	-0.631719
184	1	0	-0.365114	-1.654308	5.340861	6	6	0	0.398241	-1.364631	-1.712048
185	1	0	-2.977094	1.088077	7.260452	7	8	0	-1.428328	0.824646	0.609206
186	1	0	-1.741952	2.263945	7.139115	8	6	0	-1.923803	1.260232	-0.631719
187	1	0	-1.894630	-0.333992	5.910833	9	6	0	-1.380926	0.337428	-1.712048
188	1	0	-1.250116	1.143352	5.340861	10	8	0	1.428328	0.824646	0.609206
189	1	0	2.430850	2.034200	7.260452	11	6	0	2.053294	1.035946	-0.631719
190	1	0	2.831609	0.376602	7.139115	12	6	0	0.982684	1.027203	-1.712048
191	1	0	0.658069	1.807794	5.910833	13	1	0	0.451838	-3.208509	-0.612669
192	1	0	1.615230	0.510956	5.340861						
193	14	0	0.000000	0.000000	-7.281534						
194	17	0	0.000000	0.000000	-5.128234						



14	1	0	-1.166033	-2.555410	-0.796379	66	1	0	1.256204	-2.736702	3.166011
15	1	0	1.473296	-1.409006	-1.730514	67	1	0	3.429744	-4.167894	1.937730
16	1	0	0.025436	-1.624193	-2.692515	68	1	0	2.472583	-2.871056	1.367758
17	1	0	-3.004570	1.212952	-0.612669	69	1	0	3.541569	0.762178	3.287348
18	1	0	-1.630033	2.287519	-0.796379	70	1	0	5.177471	0.280447	3.166011
19	1	0	-1.956883	-0.571409	-1.730514	71	1	0	2.851252	-0.886299	1.937730
20	1	0	-1.419310	0.790069	-2.692515	72	1	0	4.452927	-0.705792	1.367758
21	1	0	2.552732	1.995558	-0.612669	73	14	0	-4.087813	-2.360100	4.647362
22	1	0	2.796066	0.267891	-0.796379	74	17	0	-4.087813	-2.360100	6.800662
23	1	0	0.483587	1.980415	-1.730514	75	7	0	-4.087813	-2.360100	2.624862
24	1	0	1.393874	0.834124	-2.692515	76	8	0	-5.513607	-3.183283	4.552428
25	14	0	0.000000	4.720200	4.647362	77	6	0	-6.111186	-3.429862	3.292942
26	17	0	0.000000	4.720200	6.800662	78	6	0	-5.168465	-3.240371	2.228443
27	7	0	0.000000	4.720200	2.624862	79	8	0	-4.087813	-0.713735	4.552428
28	8	0	0.000000	6.366565	4.552428	80	6	0	-4.002568	-0.072926	3.292942
29	6	0	0.085246	7.007374	3.292942	81	6	0	-4.309824	-0.984093	2.228443
30	6	0	-0.222011	6.096207	2.228443	82	8	0	-2.662019	-3.183283	4.552428
31	8	0	1.425794	3.897017	4.552428	83	6	0	-2.149685	-3.577512	3.292942
32	6	0	1.938128	3.502788	3.292942	84	6	0	-2.785150	-2.855836	2.228443
33	6	0	1.302663	4.224464	2.228443	85	1	0	-6.518663	-4.394300	3.287348
34	8	0	-1.425794	3.897017	4.552428	86	1	0	-6.919423	-2.736702	3.166011
35	6	0	-2.023373	3.650438	3.292942	87	1	0	-4.745882	-4.167894	1.937730
36	6	0	-1.080652	3.839929	2.228443	88	1	0	-5.703043	-2.871056	1.367758
37	1	0	-0.546244	7.842478	3.287348	89	1	0	-4.634057	0.762178	3.287348
38	1	0	1.089657	7.360747	3.166011	90	1	0	-2.998156	0.280447	3.166011
39	1	0	-1.236561	6.194001	1.937730	91	1	0	-5.324374	-0.886299	1.937730
40	1	0	0.365114	6.374508	1.367758	92	1	0	-3.722699	-0.705792	1.367758
41	1	0	2.977094	3.632123	3.287348	93	1	0	-1.110719	-3.448177	3.287348
42	1	0	1.741952	2.456255	3.166011	94	1	0	-2.345861	-4.624045	3.166011
43	1	0	1.894630	5.054192	1.937730	95	1	0	-2.193183	-2.026108	1.937730
44	1	0	1.250116	3.576848	1.367758	96	1	0	-2.837698	-3.503452	1.367758
45	1	0	-2.430850	2.686000	3.287348	97	14	0	0.000000	4.720200	-3.303638
46	1	0	-2.831609	4.343598	3.166011	98	17	0	0.000000	4.720200	-1.150338
47	1	0	-0.658069	2.912406	1.937730	99	7	0	0.000000	4.720200	-5.326138
48	1	0	-1.615230	4.209244	1.367758	100	8	0	0.000000	6.366565	-3.398572
49	14	0	4.087813	-2.360100	4.647362	101	6	0	0.085246	7.007374	-4.658058
50	17	0	4.087813	-2.360100	6.800662	102	6	0	-0.222011	6.096207	-5.722557
51	7	0	4.087813	-2.360100	2.624862	103	8	0	1.425794	3.897017	-3.398572
52	8	0	5.513607	-3.183283	4.552428	104	6	0	1.938128	3.502788	-4.658058
53	6	0	6.025941	-3.577512	3.292942	105	6	0	1.302663	4.224464	-5.722557
54	6	0	5.390476	-2.855836	2.228443	106	8	0	-1.425794	3.897017	-3.398572
55	8	0	2.662019	-3.183283	4.552428	107	6	0	-2.023373	3.650438	-4.658058
56	6	0	2.064440	-3.429862	3.292942	108	6	0	-1.080652	3.839929	-5.722557
57	6	0	3.007162	-3.240371	2.228443	109	1	0	-0.546244	7.842478	-4.663652
58	8	0	4.087813	-0.713735	4.552428	110	1	0	1.089657	7.360747	-4.784989
59	6	0	4.173059	-0.072926	3.292942	111	1	0	-1.236561	6.194001	-6.013270
60	6	0	3.865802	-0.984093	2.228443	112	1	0	0.365114	6.374508	-6.583242
61	1	0	7.064907	-3.448177	3.287348	113	1	0	2.977094	3.632123	-4.663652
62	1	0	5.829765	-4.624045	3.166011	114	1	0	1.741952	2.456255	-4.784989
63	1	0	5.982443	-2.026108	1.937730	115	1	0	1.894630	5.054192	-6.013270
64	1	0	5.337929	-3.503452	1.367758	116	1	0	1.250116	3.576848	-6.583242
65	1	0	1.656964	-4.394300	3.287348	117	1	0	-2.430850	2.686000	-4.663652

118	1	0	-2.831609	4.343598	-4.784989	170	17	0	0.000000	0.000000	10.776162
119	1	0	-0.658069	2.912406	-6.013270	171	7	0	0.000000	0.000000	6.600362
120	1	0	-1.615230	4.209244	-6.583242	172	8	0	0.000000	-1.646365	8.527928
121	14	0	-4.087813	-2.360100	-3.303638	173	6	0	-0.085246	-2.287174	7.268442
122	17	0	-4.087813	-2.360100	-1.150338	174	6	0	0.222011	-1.376007	6.203943
123	7	0	-4.087813	-2.360100	-5.326138	175	8	0	-1.425794	0.823183	8.527928
124	8	0	-5.513607	-3.183283	-3.398572	176	6	0	-1.938128	1.217412	7.268442
125	6	0	-6.111186	-3.429862	-4.658058	177	6	0	-1.302663	0.495736	6.203943
126	6	0	-5.168465	-3.240371	-5.722557	178	8	0	1.425794	0.823183	8.527928
127	8	0	-4.087813	-0.713735	-3.398572	179	6	0	2.023373	1.069762	7.268442
128	6	0	-4.002568	-0.072926	-4.658058	180	6	0	1.080652	0.880271	6.203943
129	6	0	-4.309824	-0.984093	-5.722557	181	1	0	0.546244	-3.122278	7.262848
130	8	0	-2.662019	-3.183283	-3.398572	182	1	0	-1.089657	-2.640547	7.141511
131	6	0	-2.149685	-3.577512	-4.658058	183	1	0	1.236561	-1.473801	5.913230
132	6	0	-2.785150	-2.855836	-5.722557	184	1	0	-0.365114	-1.654308	5.343258
133	1	0	-6.518663	-4.394300	-4.663652	185	1	0	-2.977094	1.088077	7.262848
134	1	0	-6.919423	-2.736702	-4.784989	186	1	0	-1.741952	2.263945	7.141511
135	1	0	-4.745882	-4.167894	-6.013270	187	1	0	-1.894630	-0.333992	5.913230
136	1	0	-5.703043	-2.871056	-6.583242	188	1	0	-1.250116	1.143352	5.343258
137	1	0	-4.634057	0.762178	-4.663652	189	1	0	2.430850	2.034200	7.262848
138	1	0	-2.998156	0.280447	-4.784989	190	1	0	2.831609	0.376602	7.141511
139	1	0	-5.324374	-0.886299	-6.013270	191	1	0	0.658069	1.807794	5.913230
140	1	0	-3.722699	-0.705792	-6.583242	192	1	0	1.615230	0.510956	5.343258
141	1	0	-1.110719	-3.448177	-4.663652	193	14	0	0.000000	0.000000	-7.279138
142	1	0	-2.345861	-4.624045	-4.784989	194	17	0	0.000000	0.000000	-5.125838
143	1	0	-2.193183	-2.026108	-6.013270	195	7	0	0.000000	0.000000	-9.301638
144	1	0	-2.837698	-3.503452	-6.583242	196	8	0	1.425794	0.823183	-7.374072
145	14	0	4.087813	-2.360100	-3.303638	197	6	0	2.023373	1.069762	-8.633558
146	17	0	4.087813	-2.360100	-1.150338	198	6	0	1.080652	0.880271	-9.698057
147	7	0	4.087813	-2.360100	-5.326138	199	8	0	0.000000	-1.646365	-7.374072
148	8	0	5.513607	-3.183283	-3.398572	200	6	0	-0.085246	-2.287174	-8.633558
149	6	0	6.025941	-3.577512	-4.658058	201	6	0	0.222011	-1.376007	-9.698057
150	6	0	5.390476	-2.855836	-5.722557	202	8	0	-1.425794	0.823183	-7.374072
151	8	0	2.662019	-3.183283	-3.398572	203	6	0	-1.938128	1.217412	-8.633558
152	6	0	2.064440	-3.429862	-4.658058	204	6	0	-1.302663	0.495736	-9.698057
153	6	0	3.007162	-3.240371	-5.722557	205	1	0	2.430850	2.034200	-8.639152
154	8	0	4.087813	-0.713735	-3.398572	206	1	0	2.831609	0.376602	-8.760489
155	6	0	4.173059	-0.072926	-4.658058	207	1	0	0.658069	1.807794	-9.988770
156	6	0	3.865802	-0.984093	-5.722557	208	1	0	1.615230	0.510956	-10.558742
157	1	0	7.064907	-3.448177	-4.663652	209	1	0	0.546244	-3.122278	-8.639152
158	1	0	5.829765	-4.624045	-4.784989	210	1	0	-1.089657	-2.640547	-8.760489
159	1	0	5.982443	-2.026108	-6.013270	211	1	0	1.236561	-1.473801	-9.988770
160	1	0	5.337929	-3.503452	-6.583242	212	1	0	-0.365114	-1.654308	-10.558742
161	1	0	1.656964	-4.394300	-4.663652	213	1	0	-2.977094	1.088077	-8.639152
162	1	0	1.256204	-2.736702	-4.784989	214	1	0	-1.741952	2.263945	-8.760489
163	1	0	3.429744	-4.167894	-6.013270	215	1	0	-1.894630	-0.333992	-9.988770
164	1	0	2.472583	-2.871056	-6.583242	216	1	0	-1.250116	1.143352	-10.558742
165	1	0	3.541569	0.762178	-4.663652	217	14	0	0.000000	4.720200	12.598362
166	1	0	5.177471	0.280447	-4.784989	218	17	0	0.000000	4.720200	14.751662
167	1	0	2.851252	-0.886299	-6.013270	219	7	0	0.000000	4.720200	10.575862
168	1	0	4.452927	-0.705792	-6.583242	220	8	0	0.000000	6.366565	12.503428
169	14	0	0.000000	0.000000	8.622862	221	6	0	0.085246	7.007374	11.243942

222	6	0	-0.222011	6.096207	10.179443	274	8	0	-2.662019	-3.183283	12.503428
223	8	0	1.425794	3.897017	12.503428	275	6	0	-2.149685	-3.577512	11.243942
224	6	0	1.938128	3.502788	11.243942	276	6	0	-2.785150	-2.855836	10.179443
225	6	0	1.302663	4.224464	10.179443	277	1	0	-6.518663	-4.394300	11.238348
226	8	0	-1.425794	3.897017	12.503428	278	1	0	-6.919423	-2.736702	11.117011
227	6	0	-2.023373	3.650438	11.243942	279	1	0	-4.745882	-4.167894	9.888730
228	6	0	-1.080652	3.839929	10.179443	280	1	0	-5.703043	-2.871056	9.318758
229	1	0	-0.546244	7.842478	11.238348	281	1	0	-4.634057	0.762178	11.238348
230	1	0	1.089657	7.360747	11.117011	282	1	0	-2.998156	0.280447	11.117011
231	1	0	-1.236561	6.194001	9.888730	283	1	0	-5.324374	-0.886299	9.888730
232	1	0	0.365114	6.374508	9.318758	284	1	0	-3.722699	-0.705792	9.318758
233	1	0	2.977094	3.632123	11.238348	285	1	0	-1.110719	-3.448177	11.238348
234	1	0	1.741952	2.456255	11.117011	286	1	0	-2.345861	-4.624045	11.117011
235	1	0	1.894630	5.054192	9.888730	287	1	0	-2.193183	-2.026108	9.888730
236	1	0	1.250116	3.576848	9.318758	288	1	0	-2.837698	-3.503452	9.318758
237	1	0	-2.430850	2.686000	11.238348	289	14	0	-4.087813	-2.360100	-11.254638
238	1	0	-2.831609	4.343598	11.117011	290	17	0	-4.087813	-2.360100	-9.101338
239	1	0	-0.658069	2.912406	9.888730	291	7	0	-4.087813	-2.360100	-13.277138
240	1	0	-1.615230	4.209244	9.318758	292	8	0	-5.513607	-3.183283	-11.349572
241	14	0	4.087813	-2.360100	12.598362	293	6	0	-6.111186	-3.429862	-12.609058
242	17	0	4.087813	-2.360100	14.751662	294	6	0	-5.168465	-3.240371	-13.673557
243	7	0	4.087813	-2.360100	10.575862	295	8	0	-4.087813	-0.713735	-11.349572
244	8	0	5.513607	-3.183283	12.503428	296	6	0	-4.002568	-0.072926	-12.609058
245	6	0	6.025941	-3.577512	11.243942	297	6	0	-4.309824	-0.984093	-13.673557
246	6	0	5.390476	-2.855836	10.179443	298	8	0	-2.662019	-3.183283	-11.349572
247	8	0	2.662019	-3.183283	12.503428	299	6	0	-2.149685	-3.577512	-12.609058
248	6	0	2.064440	-3.429862	11.243942	300	6	0	-2.785150	-2.855836	-13.673557
249	6	0	3.007162	-3.240371	10.179443	301	1	0	-6.518663	-4.394300	-12.614652
250	8	0	4.087813	-0.713735	12.503428	302	1	0	-6.919423	-2.736702	-12.735989
251	6	0	4.173059	-0.072926	11.243942	303	1	0	-4.745882	-4.167894	-13.964270
252	6	0	3.865802	-0.984093	10.179443	304	1	0	-5.703043	-2.871056	-14.534242
253	1	0	7.064907	-3.448177	11.238348	305	1	0	-4.634057	0.762178	-12.614652
254	1	0	5.829765	-4.624045	11.117011	306	1	0	-2.998156	0.280447	-12.735989
255	1	0	5.982443	-2.026108	9.888730	307	1	0	-5.324374	-0.886299	-13.964270
256	1	0	5.337929	-3.503452	9.318758	308	1	0	-3.722699	-0.705792	-14.534242
257	1	0	1.656964	-4.394300	11.238348	309	1	0	-1.110719	-3.448177	-12.614652
258	1	0	1.256204	-2.736702	11.117011	310	1	0	-2.345861	-4.624045	-12.735989
259	1	0	3.429744	-4.167894	9.888730	311	1	0	-2.193183	-2.026108	-13.964270
260	1	0	2.472583	-2.871056	9.318758	312	1	0	-2.837698	-3.503452	-14.534242
261	1	0	3.541569	0.762178	11.238348	313	14	0	4.087813	-2.360100	-11.254638
262	1	0	5.177471	0.280447	11.117011	314	17	0	4.087813	-2.360100	-9.101338
263	1	0	2.851252	-0.886299	9.888730	315	7	0	4.087813	-2.360100	-13.277138
264	1	0	4.452927	-0.705792	9.318758	316	8	0	5.513607	-3.183283	-11.349572
265	14	0	-4.087813	-2.360100	12.598362	317	6	0	6.025941	-3.577512	-12.609058
266	17	0	-4.087813	-2.360100	14.751662	318	6	0	5.390476	-2.855836	-13.673557
267	7	0	-4.087813	-2.360100	10.575862	319	8	0	2.662019	-3.183283	-11.349572
268	8	0	-5.513607	-3.183283	12.503428	320	6	0	2.064440	-3.429862	-12.609058
269	6	0	-6.111186	-3.429862	11.243942	321	6	0	3.007162	-3.240371	-13.673557
270	6	0	-5.168465	-3.240371	10.179443	322	8	0	4.087813	-0.713735	-11.349572
271	8	0	-4.087813	-0.713735	12.503428	323	6	0	4.173059	-0.072926	-12.609058
272	6	0	-4.002568	-0.072926	11.243942	324	6	0	3.865802	-0.984093	-13.673557
273	6	0	-4.309824	-0.984093	10.179443	325	1	0	7.064907	-3.448177	-12.614652

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326      1      0      5.829765  -4.624045  -12.735989      2      14      0      0.000000      0.000000      0.901975
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328      1      0      5.337929  -3.503452  -14.534242      4      8      0      0.000000     -1.612046      0.597381
329      1      0      1.656964  -4.394300  -12.614652      5      6      0     -0.267066     -2.234809     -0.618246
330      1      0      1.256204  -2.736702  -12.735989      6      6      0      0.291205     -1.394066     -1.758890
331      1      0      3.429744  -4.167894  -13.964270      7      8      0     -1.396072      0.806023      0.597381
332      1      0      2.472583  -2.871056  -14.534242      8      6      0     -1.801868      1.348691     -0.618246
333      1      0      3.541569      0.762178  -12.614652      9      6      0     -1.352900      0.444842     -1.758890
334      1      0      5.177471      0.280447  -12.735989     10     8      0      1.396072      0.806023      0.597381
335      1      0      2.851252  -0.886299  -13.964270     11     6      0      2.068934      0.886118     -0.618246
336      1      0      4.452927  -0.705792  -14.534242     12     6      0      1.061694      0.949224     -1.758890
337     14      0      0.000000      4.720200  -11.254638     13     1      0      0.204120     -3.209785     -0.610282
338     17      0      0.000000      4.720200   -9.101338     14     1      0     -1.332672     -2.378119     -0.724142
339      7      0      0.000000      4.720200  -13.277138     15     1      0      1.360936     -1.516225     -1.793901
340      8      0      0.000000      6.366565  -11.349572     16     1      0     -0.116427     -1.716692     -2.712880
341      6      0      0.085246      7.007374  -12.609058     17     1      0     -2.881816      1.428120     -0.610282
342      6      0     -0.222011      6.096207  -13.673557     18     1      0     -1.393176      2.343187     -0.724142
343      8      0      1.425794      3.897017  -11.349572     19     1      0     -1.993557     -0.420493     -1.793901
344      6      0      1.938128      3.502788  -12.609058     20     1      0     -1.428486      0.959175     -2.712880
345      6      0      1.302663      4.224464  -13.673557     21     1      0      2.677696      1.781666     -0.610282
346      8      0     -1.425794      3.897017  -11.349572     22     1      0      2.725847      0.034932     -0.724142
347      6      0     -2.023373      3.650438  -12.609058     23     1      0      0.632621      1.936718     -1.793901
348      6      0     -1.080652      3.839929  -13.673557     24     1      0      1.544912      0.757518     -2.712880
349      1      0     -0.546244      7.842478  -12.614652     25     14     0      0.000000      4.720200      4.646307
350      1      0      1.089657      7.360747  -12.735989     26     17     0      0.000000      4.720200      6.799607
351      1      0     -1.236561      6.194001  -13.964270     27     7      0      0.000000      4.720200      2.623807
352      1      0      0.365114      6.374508  -14.534242     28     8      0      0.000000      6.366565      4.551372
353      1      0      2.977094      3.632123  -12.614652     29     6      0      0.085246      7.007374      3.291886
354      1      0      1.741952      2.456255  -12.735989     30     6      0     -0.222011      6.096207      2.227387
355      1      0      1.894630      5.054192  -13.964270     31     8      0      1.425794      3.897017      4.551372
356      1      0      1.250116      3.576848  -14.534242     32     6      0      1.938128      3.502788      3.291886
357      1      0     -2.430850      2.686000  -12.614652     33     6      0      1.302663      4.224464      2.227387
358      1      0     -2.831609      4.343598  -12.735989     34     8      0     -1.425794      3.897017      4.551372
359      1      0     -0.658069      2.912406  -13.964270     35     6      0     -2.023373      3.650438      3.291886
360      1      0     -1.615230      4.209244  -14.534242     36     6      0     -1.080652      3.839929      2.227387
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37      1      0     -0.546244      7.842478      3.286293
38      1      0      1.089657      7.360747      3.164956
39      1      0     -1.236561      6.194001      1.936674
40      1      0      0.365114      6.374508      1.366702
41      1      0      2.977094      3.632123      3.286293
42      1      0      1.741952      2.456255      3.164956
43      1      0      1.894630      5.054192      1.936674
44      1      0      1.250116      3.576848      1.366702
45      1      0     -2.430850      2.686000      3.286293
46      1      0     -2.831609      4.343598      3.164956
47      1      0     -0.658069      2.912406      1.936674
48      1      0     -1.615230      4.209244      1.366702
49     14      0      4.087813     -2.360100      4.646307
50     17      0      4.087813     -2.360100      6.799607
51      7      0      4.087813     -2.360100      2.623807
52      8      0      5.513607     -3.183283      4.551372
53      6      0      6.025941     -3.577512      3.291886
-----
Xtal, model 4, HF
%chk=C1-Silatrane4.chk
%mem=512MB
%RWF=s1,255MW,s2,255MW,s3,255MW,s4,255MW,s5,255MW,s6,255MW,s7,255MW
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# HF/6-31G(d) Opt(Z-Matrix) IOp(1/8=5) SCF=IntRep Symm=Loose
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Standard orientation:
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Center      Atomic      Atomic      Coordinates (Angstroms)
Number      Number      Type          X          Y          Z
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1           17          0           0.000000    0.000000    2.942956

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54	6	0	5.390476	-2.855836	2.227387	106	8	0	-1.425794	3.897017	-3.399628
55	8	0	2.662019	-3.183283	4.551372	107	6	0	-2.023373	3.650438	-4.659114
56	6	0	2.064440	-3.429862	3.291886	108	6	0	-1.080652	3.839929	-5.723613
57	6	0	3.007162	-3.240371	2.227387	109	1	0	-0.546244	7.842478	-4.664707
58	8	0	4.087813	-0.713735	4.551372	110	1	0	1.089657	7.360747	-4.786044
59	6	0	4.173059	-0.072926	3.291886	111	1	0	-1.236561	6.194001	-6.014326
60	6	0	3.865802	-0.984093	2.227387	112	1	0	0.365114	6.374508	-6.584298
61	1	0	7.064907	-3.448177	3.286293	113	1	0	2.977094	3.632123	-4.664707
62	1	0	5.829765	-4.624045	3.164956	114	1	0	1.741952	2.456255	-4.786044
63	1	0	5.982443	-2.026108	1.936674	115	1	0	1.894630	5.054192	-6.014326
64	1	0	5.337929	-3.503452	1.366702	116	1	0	1.250116	3.576848	-6.584298
65	1	0	1.656964	-4.394300	3.286293	117	1	0	-2.430850	2.686000	-4.664707
66	1	0	1.256204	-2.736702	3.164956	118	1	0	-2.831609	4.343598	-4.786044
67	1	0	3.429744	-4.167894	1.936674	119	1	0	-0.658069	2.912406	-6.014326
68	1	0	2.472583	-2.871056	1.366702	120	1	0	-1.615230	4.209244	-6.584298
69	1	0	3.541569	0.762178	3.286293	121	14	0	-4.087813	-2.360100	-3.304693
70	1	0	5.177471	0.280447	3.164956	122	17	0	-4.087813	-2.360100	-1.151393
71	1	0	2.851252	-0.886299	1.936674	123	7	0	-4.087813	-2.360100	-5.327193
72	1	0	4.452927	-0.705792	1.366702	124	8	0	-5.513607	-3.183283	-3.399628
73	14	0	-4.087813	-2.360100	4.646307	125	6	0	-6.111186	-3.429862	-4.659114
74	17	0	-4.087813	-2.360100	6.799607	126	6	0	-5.168465	-3.240371	-5.723613
75	7	0	-4.087813	-2.360100	2.623807	127	8	0	-4.087813	-0.713735	-3.399628
76	8	0	-5.513607	-3.183283	4.551372	128	6	0	-4.002568	-0.072926	-4.659114
77	6	0	-6.111186	-3.429862	3.291886	129	6	0	-4.309824	-0.984093	-5.723613
78	6	0	-5.168465	-3.240371	2.227387	130	8	0	-2.662019	-3.183283	-3.399628
79	8	0	-4.087813	-0.713735	4.551372	131	6	0	-2.149685	-3.577512	-4.659114
80	6	0	-4.002568	-0.072926	3.291886	132	6	0	-2.785150	-2.855836	-5.723613
81	6	0	-4.309824	-0.984093	2.227387	133	1	0	-6.518663	-4.394300	-4.664707
82	8	0	-2.662019	-3.183283	4.551372	134	1	0	-6.919423	-2.736702	-4.786044
83	6	0	-2.149685	-3.577512	3.291886	135	1	0	-4.745882	-4.167894	-6.014326
84	6	0	-2.785150	-2.855836	2.227387	136	1	0	-5.703043	-2.871056	-6.584298
85	1	0	-6.518663	-4.394300	3.286293	137	1	0	-4.634057	0.762178	-4.664707
86	1	0	-6.919423	-2.736702	3.164956	138	1	0	-2.998156	0.280447	-4.786044
87	1	0	-4.745882	-4.167894	1.936674	139	1	0	-5.324374	-0.886299	-6.014326
88	1	0	-5.703043	-2.871056	1.366702	140	1	0	-3.722699	-0.705792	-6.584298
89	1	0	-4.634057	0.762178	3.286293	141	1	0	-1.110719	-3.448177	-4.664707
90	1	0	-2.998156	0.280447	3.164956	142	1	0	-2.345861	-4.624045	-4.786044
91	1	0	-5.324374	-0.886299	1.936674	143	1	0	-2.193183	-2.026108	-6.014326
92	1	0	-3.722699	-0.705792	1.366702	144	1	0	-2.837698	-3.503452	-6.584298
93	1	0	-1.110719	-3.448177	3.286293	145	14	0	4.087813	-2.360100	-3.304693
94	1	0	-2.345861	-4.624045	3.164956	146	17	0	4.087813	-2.360100	-1.151393
95	1	0	-2.193183	-2.026108	1.936674	147	7	0	4.087813	-2.360100	-5.327193
96	1	0	-2.837698	-3.503452	1.366702	148	8	0	5.513607	-3.183283	-3.399628
97	14	0	0.000000	4.720200	-3.304693	149	6	0	6.025941	-3.577512	-4.659114
98	17	0	0.000000	4.720200	-1.151393	150	6	0	5.390476	-2.855836	-5.723613
99	7	0	0.000000	4.720200	-5.327193	151	8	0	2.662019	-3.183283	-3.399628
100	8	0	0.000000	6.366565	-3.399628	152	6	0	2.064440	-3.429862	-4.659114
101	6	0	0.085246	7.007374	-4.659114	153	6	0	3.007162	-3.240371	-5.723613
102	6	0	-0.222011	6.096207	-5.723613	154	8	0	4.087813	-0.713735	-3.399628
103	8	0	1.425794	3.897017	-3.399628	155	6	0	4.173059	-0.072926	-4.659114
104	6	0	1.938128	3.502788	-4.659114	156	6	0	3.865802	-0.984093	-5.723613
105	6	0	1.302663	4.224464	-5.723613	157	1	0	7.064907	-3.448177	-4.664707

158	1	0	5.829765	-4.624045	-4.786044	210	1	0	-1.089657	-2.640547	-8.761544
159	1	0	5.982443	-2.026108	-6.014326	211	1	0	1.236561	-1.473801	-9.989826
160	1	0	5.337929	-3.503452	-6.584298	212	1	0	-0.365114	-1.654308	-10.559798
161	1	0	1.656964	-4.394300	-4.664707	213	1	0	-2.977094	1.088077	-8.640207
162	1	0	1.256204	-2.736702	-4.786044	214	1	0	-1.741952	2.263945	-8.761544
163	1	0	3.429744	-4.167894	-6.014326	215	1	0	-1.894630	-0.333992	-9.989826
164	1	0	2.472583	-2.871056	-6.584298	216	1	0	-1.250116	1.143352	-10.559798
165	1	0	3.541569	0.762178	-4.664707	217	14	0	8.175600	0.000000	0.670807
166	1	0	5.177471	0.280447	-4.786044	218	14	0	-8.175600	0.000000	0.670807
167	1	0	2.851252	-0.886299	-6.014326	219	14	0	4.087800	-7.080277	0.670807
168	1	0	4.452927	-0.705792	-6.584298	220	14	0	-4.087800	-7.080277	0.670807
169	14	0	0.000000	0.000000	8.621807	221	14	0	4.087800	7.080277	0.670807
170	17	0	0.000000	0.000000	10.775107	222	14	0	-4.087800	7.080277	0.670807
171	7	0	0.000000	0.000000	6.599307	223	17	0	8.175600	0.000000	2.824107
172	8	0	0.000000	-1.646365	8.526872	224	17	0	4.087800	-7.080277	2.824107
173	6	0	-0.085246	-2.287174	7.267386	225	17	0	-4.087800	-7.080277	2.824107
174	6	0	0.222011	-1.376007	6.202887	226	17	0	-8.175600	0.000000	2.824107
175	8	0	-1.425794	0.823183	8.526872	227	17	0	-4.087800	7.080277	2.824107
176	6	0	-1.938128	1.217412	7.267386	228	17	0	4.087800	7.080277	2.824107
177	6	0	-1.302663	0.495736	6.202887	229	7	0	8.175600	0.000000	-1.351693
178	8	0	1.425794	0.823183	8.526872	230	7	0	4.087800	-7.080277	-1.351693
179	6	0	2.023373	1.069762	7.267386	231	7	0	-4.087800	-7.080277	-1.351693
180	6	0	1.080652	0.880271	6.202887	232	7	0	-8.175600	0.000000	-1.351693
181	1	0	0.546244	-3.122278	7.261793	233	7	0	-4.087800	7.080277	-1.351693
182	1	0	-1.089657	-2.640547	7.140456	234	7	0	4.087800	7.080277	-1.351693
183	1	0	1.236561	-1.473801	5.912174	235	8	0	5.513594	-6.257095	0.575872
184	1	0	-0.365114	-1.654308	5.342202	236	8	0	-5.513594	-6.257095	0.575872
185	1	0	-2.977094	1.088077	7.261793	237	8	0	8.175600	-1.646365	0.575872
186	1	0	-1.741952	2.263945	7.140456	238	8	0	-8.175600	-1.646365	0.575872
187	1	0	-1.894630	-0.333992	5.912174	239	8	0	2.662006	7.903460	0.575872
188	1	0	-1.250116	1.143352	5.342202	240	8	0	-2.662006	7.903460	0.575872
189	1	0	2.430850	2.034200	7.261793	241	6	0	8.090354	-2.287174	-0.683614
190	1	0	2.831609	0.376602	7.140456	242	6	0	8.397611	-1.376007	-1.748113
191	1	0	0.658069	1.807794	5.912174	243	8	0	6.749806	0.823183	0.575872
192	1	0	1.615230	0.510956	5.342202	244	6	0	6.237472	1.217412	-0.683614
193	14	0	0.000000	0.000000	-7.280193	245	6	0	6.872937	0.495736	-1.748113
194	17	0	0.000000	0.000000	-5.126893	246	8	0	9.601394	0.823183	0.575872
195	7	0	0.000000	0.000000	-9.302693	247	6	0	10.198973	1.069762	-0.683614
196	8	0	1.425794	0.823183	-7.375128	248	6	0	9.256252	0.880271	-1.748113
197	6	0	2.023373	1.069762	-8.634614	249	1	0	8.721844	-3.122278	-0.689207
198	6	0	1.080652	0.880271	-9.699113	250	1	0	7.085943	-2.640547	-0.810544
199	8	0	0.000000	-1.646365	-7.375128	251	1	0	9.412161	-1.473801	-2.038826
200	6	0	-0.085246	-2.287174	-8.634614	252	1	0	7.810486	-1.654308	-2.608798
201	6	0	0.222011	-1.376007	-9.699113	253	1	0	5.198506	1.088077	-0.689207
202	8	0	-1.425794	0.823183	-7.375128	254	1	0	6.433648	2.263945	-0.810544
203	6	0	-1.938128	1.217412	-8.634614	255	1	0	6.280970	-0.333992	-2.038826
204	6	0	-1.302663	0.495736	-9.699113	256	1	0	6.925484	1.143352	-2.608798
205	1	0	2.430850	2.034200	-8.640207	257	1	0	10.606450	2.034200	-0.689207
206	1	0	2.831609	0.376602	-8.761544	258	1	0	11.007209	0.376602	-0.810544
207	1	0	0.658069	1.807794	-9.989826	259	1	0	8.833669	1.807794	-2.038826
208	1	0	1.615230	0.510956	-10.559798	260	1	0	9.790830	0.510956	-2.608798
209	1	0	0.546244	-3.122278	-8.640207	261	6	0	6.111173	-6.010515	-0.683614

262	6	0	5.168452	-6.200006	-1.748113	314	1	0	-9.917552	2.263945	-0.810544
263	8	0	4.087800	-8.726642	0.575872	315	1	0	-10.070230	-0.333992	-2.038826
264	6	0	4.002554	-9.367451	-0.683614	316	1	0	-9.425716	1.143352	-2.608798
265	6	0	4.309811	-8.456285	-1.748113	317	1	0	-5.744750	2.034200	-0.689207
266	8	0	2.662006	-6.257095	0.575872	318	1	0	-5.343991	0.376602	-0.810544
267	6	0	2.149672	-5.862866	-0.683614	319	1	0	-7.517531	1.807794	-2.038826
268	6	0	2.785137	-6.584541	-1.748113	320	1	0	-6.560370	0.510956	-2.608798
269	1	0	6.518650	-5.046077	-0.689207	321	6	0	-2.064427	8.150039	-0.683614
270	1	0	6.919409	-6.703675	-0.810544	322	6	0	-3.007148	7.960548	-1.748113
271	1	0	4.745869	-5.272484	-2.038826	323	8	0	-4.087800	5.433912	0.575872
272	1	0	5.703030	-6.569322	-2.608798	324	6	0	-4.173046	4.793104	-0.683614
273	1	0	4.634044	-10.202555	-0.689207	325	6	0	-3.865789	5.704270	-1.748113
274	1	0	2.998143	-9.720824	-0.810544	326	8	0	-5.513594	7.903460	0.575872
275	1	0	5.324361	-8.554079	-2.038826	327	6	0	-6.025928	8.297689	-0.683614
276	1	0	3.722686	-8.734585	-2.608798	328	6	0	-5.390463	7.576013	-1.748113
277	1	0	1.110706	-5.992200	-0.689207	329	1	0	-1.656950	9.114477	-0.689207
278	1	0	2.345848	-4.816333	-0.810544	330	1	0	-1.256191	7.456880	-0.810544
279	1	0	2.193170	-7.414270	-2.038826	331	1	0	-3.429731	8.888071	-2.038826
280	1	0	2.837684	-5.936925	-2.608798	332	1	0	-2.472570	7.591233	-2.608798
281	6	0	-6.025928	-5.862866	-0.683614	333	1	0	-3.541556	3.958000	-0.689207
282	6	0	-5.390463	-6.584541	-1.748113	334	1	0	-5.177457	4.439730	-0.810544
283	8	0	-2.662006	-6.257095	0.575872	335	1	0	-2.851239	5.606476	-2.038826
284	6	0	-2.064427	-6.010515	-0.683614	336	1	0	-4.452914	5.425969	-2.608798
285	6	0	-3.007148	-6.200006	-1.748113	337	1	0	-7.064894	8.168355	-0.689207
286	8	0	-4.087800	-8.726642	0.575872	338	1	0	-5.829752	9.344222	-0.810544
287	6	0	-4.173046	-9.367451	-0.683614	339	1	0	-5.982430	6.746285	-2.038826
288	6	0	-3.865789	-8.456285	-1.748113	340	1	0	-5.337916	8.223630	-2.608798
289	1	0	-7.064894	-5.992200	-0.689207	341	6	0	2.149672	8.297689	-0.683614
290	1	0	-5.829752	-4.816333	-0.810544	342	6	0	2.785137	7.576013	-1.748113
291	1	0	-5.982430	-7.414270	-2.038826	343	8	0	5.513594	7.903460	0.575872
292	1	0	-5.337916	-5.936925	-2.608798	344	6	0	6.111173	8.150039	-0.683614
293	1	0	-1.656950	-5.046077	-0.689207	345	6	0	5.168452	7.960548	-1.748113
294	1	0	-1.256191	-6.703675	-0.810544	346	8	0	4.087800	5.433912	0.575872
295	1	0	-3.429731	-5.272484	-2.038826	347	6	0	4.002554	4.793104	-0.683614
296	1	0	-2.472570	-6.569322	-2.608798	348	6	0	4.309811	5.704270	-1.748113
297	1	0	-3.541556	-10.202555	-0.689207	349	1	0	1.110706	8.168355	-0.689207
298	1	0	-5.177457	-9.720824	-0.810544	350	1	0	2.345848	9.344222	-0.810544
299	1	0	-2.851239	-8.554079	-2.038826	351	1	0	2.193170	6.746285	-2.038826
300	1	0	-4.452914	-8.734585	-2.608798	352	1	0	2.837684	8.223630	-2.608798
301	6	0	-8.260846	-2.287174	-0.683614	353	1	0	6.518650	9.114477	-0.689207
302	6	0	-7.953589	-1.376007	-1.748113	354	1	0	6.919409	7.456880	-0.810544
303	8	0	-9.601394	0.823183	0.575872	355	1	0	4.745869	8.888071	-2.038826
304	6	0	-10.113728	1.217412	-0.683614	356	1	0	5.703030	7.591233	-2.608798
305	6	0	-9.478263	0.495736	-1.748113	357	1	0	4.634044	3.958000	-0.689207
306	8	0	-6.749806	0.823183	0.575872	358	1	0	2.998143	4.439730	-0.810544
307	6	0	-6.152227	1.069762	-0.683614	359	1	0	5.324361	5.606476	-2.038826
308	6	0	-7.094948	0.880271	-1.748113	360	1	0	3.722686	5.425969	-2.608798
309	1	0	-7.629356	-3.122278	-0.689207						
310	1	0	-9.265257	-2.640547	-0.810544						
311	1	0	-6.939039	-1.473801	-2.038826						
312	1	0	-8.540714	-1.654308	-2.608798						
313	1	0	-11.152694	1.088077	-0.689207						

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Xtal, model 1, ONIOM

%mem=128MB

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 # ONIOM(HF/6-31G(d):UFF) Opt(Z-Matrix, Newton) MaxDisk=2GB  
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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	17	0	0.000000	0.000000	2.982807
2	14	0	0.000000	0.000000	0.913993
3	7	0	0.000000	0.000000	-1.477577
4	8	0	0.000000	-1.608994	0.603378
5	6	0	-0.257695	-2.237019	-0.613117
6	6	0	0.289677	-1.394495	-1.763174
7	8	0	-1.393430	0.804497	0.603378
8	6	0	-1.808468	1.341680	-0.613117
9	6	0	-1.352506	0.446380	-1.763174
10	8	0	1.393430	0.804497	0.603378
11	6	0	2.066163	0.895339	-0.613117
12	6	0	1.062830	0.948115	-1.763174
13	1	0	0.212742	-3.212042	-0.602057
14	1	0	-1.323923	-2.392355	-0.718184
15	1	0	1.362554	-1.508437	-1.800922
16	1	0	-0.111769	-1.717746	-2.721200
17	1	0	-2.888081	1.421781	-0.602057
18	1	0	-1.409879	2.342729	-0.718184
19	1	0	-1.987622	-0.425788	-1.800922
20	1	0	-1.431727	0.955668	-2.721200
21	1	0	2.675339	1.790261	-0.602057
22	1	0	2.733802	0.049626	-0.718184
23	1	0	0.625068	1.934225	-1.800922
24	1	0	1.543496	0.762078	-2.721200
25	14	0	0.000000	4.720200	4.639302
26	17	0	0.000000	4.720200	6.792602
27	7	0	0.000000	4.720200	2.616802
28	8	0	0.000000	6.366565	4.544367
29	6	0	0.085246	7.007374	3.284882
30	6	0	-0.222011	6.096207	2.220382
31	8	0	1.425794	3.897017	4.544367
32	6	0	1.938128	3.502788	3.284882
33	6	0	1.302663	4.224464	2.220382
34	8	0	-1.425794	3.897017	4.544367
35	6	0	-2.023373	3.650438	3.284882
36	6	0	-1.080652	3.839929	2.220382
37	1	0	-0.546244	7.842478	3.279288
38	1	0	1.089657	7.360747	3.157951
39	1	0	-1.236561	6.194001	1.929669
40	1	0	0.365114	6.374508	1.359697
41	1	0	2.977094	3.632123	3.279288
42	1	0	1.741952	2.456255	3.157951
43	1	0	1.894630	5.054192	1.929669

44	1	0	1.250116	3.576848	1.359697
45	1	0	-2.430850	2.686000	3.279288
46	1	0	-2.831609	4.343598	3.157951
47	1	0	-0.658069	2.912406	1.929669
48	1	0	-1.615230	4.209244	1.359697
49	14	0	4.087813	-2.360100	4.639302
50	17	0	4.087813	-2.360100	6.792602
51	7	0	4.087813	-2.360100	2.616802
52	8	0	5.513607	-3.183283	4.544367
53	6	0	6.025941	-3.577512	3.284882
54	6	0	5.390476	-2.855836	2.220382
55	8	0	2.662019	-3.183283	4.544367
56	6	0	2.064440	-3.429862	3.284882
57	6	0	3.007162	-3.240371	2.220382
58	8	0	4.087813	-0.713735	4.544367
59	6	0	4.173059	-0.072926	3.284882
60	6	0	3.865802	-0.984093	2.220382
61	1	0	7.064907	-3.448177	3.279288
62	1	0	5.829765	-4.624045	3.157951
63	1	0	5.982443	-2.026108	1.929669
64	1	0	5.337929	-3.503452	1.359697
65	1	0	1.656964	-4.394300	3.279288
66	1	0	1.256204	-2.736702	3.157951
67	1	0	3.429744	-4.167894	1.929669
68	1	0	2.472583	-2.871056	1.359697
69	1	0	3.541569	0.762178	3.279288
70	1	0	5.177471	0.280447	3.157951
71	1	0	2.851252	-0.886299	1.929669
72	1	0	4.452927	-0.705792	1.359697
73	14	0	-4.087813	-2.360100	4.639302
74	17	0	-4.087813	-2.360100	6.792602
75	7	0	-4.087813	-2.360100	2.616802
76	8	0	-5.513607	-3.183283	4.544367
77	6	0	-6.111186	-3.429862	3.284882
78	6	0	-5.168465	-3.240371	2.220382
79	8	0	-4.087813	-0.713735	4.544367
80	6	0	-4.002568	-0.072926	3.284882
81	6	0	-4.309824	-0.984093	2.220382
82	8	0	-2.662019	-3.183283	4.544367
83	6	0	-2.149685	-3.577512	3.284882
84	6	0	-2.785150	-2.855836	2.220382
85	1	0	-6.518663	-4.394300	3.279288
86	1	0	-6.919423	-2.736702	3.157951
87	1	0	-4.745882	-4.167894	1.929669
88	1	0	-5.703043	-2.871056	1.359697
89	1	0	-4.634057	0.762178	3.279288
90	1	0	-2.998156	0.280447	3.157951
91	1	0	-5.324374	-0.886299	1.929669
92	1	0	-3.722699	-0.705792	1.359697
93	1	0	-1.110719	-3.448177	3.279288
94	1	0	-2.345861	-4.624045	3.157951
95	1	0	-2.193183	-2.026108	1.929669



96	1	0	-2.837698	-3.503452	1.359697	148	8	0	5.513607	-3.183283	-3.406633
97	14	0	0.000000	4.720200	-3.311698	149	6	0	6.025941	-3.577512	-4.666118
98	17	0	0.000000	4.720200	-1.158398	150	6	0	5.390476	-2.855836	-5.730618
99	7	0	0.000000	4.720200	-5.334198	151	8	0	2.662019	-3.183283	-3.406633
100	8	0	0.000000	6.366565	-3.406633	152	6	0	2.064440	-3.429862	-4.666118
101	6	0	0.085246	7.007374	-4.666118	153	6	0	3.007162	-3.240371	-5.730618
102	6	0	-0.222011	6.096207	-5.730618	154	8	0	4.087813	-0.713735	-3.406633
103	8	0	1.425794	3.897017	-3.406633	155	6	0	4.173059	-0.072926	-4.666118
104	6	0	1.938128	3.502788	-4.666118	156	6	0	3.865802	-0.984093	-5.730618
105	6	0	1.302663	4.224464	-5.730618	157	1	0	7.064907	-3.448177	-4.671712
106	8	0	-1.425794	3.897017	-3.406633	158	1	0	5.829765	-4.624045	-4.793049
107	6	0	-2.023373	3.650438	-4.666118	159	1	0	5.982443	-2.026108	-6.021331
108	6	0	-1.080652	3.839929	-5.730618	160	1	0	5.337929	-3.503452	-6.591303
109	1	0	-0.546244	7.842478	-4.671712	161	1	0	1.656964	-4.394300	-4.671712
110	1	0	1.089657	7.360747	-4.793049	162	1	0	1.256204	-2.736702	-4.793049
111	1	0	-1.236561	6.194001	-6.021331	163	1	0	3.429744	-4.167894	-6.021331
112	1	0	0.365114	6.374508	-6.591303	164	1	0	2.472583	-2.871056	-6.591303
113	1	0	2.977094	3.632123	-4.671712	165	1	0	3.541569	0.762178	-4.671712
114	1	0	1.741952	2.456255	-4.793049	166	1	0	5.177471	0.280447	-4.793049
115	1	0	1.894630	5.054192	-6.021331	167	1	0	2.851252	-0.886299	-6.021331
116	1	0	1.250116	3.576848	-6.591303	168	1	0	4.452927	-0.705792	-6.591303
117	1	0	-2.430850	2.686000	-4.671712						
118	1	0	-2.831609	4.343598	-4.793049						
119	1	0	-0.658069	2.912406	-6.021331						
120	1	0	-1.615230	4.209244	-6.591303						
121	14	0	-4.087813	-2.360100	-3.311698						
122	17	0	-4.087813	-2.360100	-1.158398						
123	7	0	-4.087813	-2.360100	-5.334198						
124	8	0	-5.513607	-3.183283	-3.406633						
125	6	0	-6.111186	-3.429862	-4.666118						
126	6	0	-5.168465	-3.240371	-5.730618						
127	8	0	-4.087813	-0.713735	-3.406633						
128	6	0	-4.002568	-0.072926	-4.666118						
129	6	0	-4.309824	-0.984093	-5.730618	1	17	0	0.000000	0.000000	2.940452
130	8	0	-2.662019	-3.183283	-3.406633	2	14	0	0.000000	0.000000	0.878652
131	6	0	-2.149685	-3.577512	-4.666118	3	7	0	0.000000	0.000000	-1.494198
132	6	0	-2.785150	-2.855836	-5.730618	4	8	0	0.000000	-1.611854	0.579312
133	1	0	-6.518663	-4.394300	-4.671712	5	6	0	-0.254475	-2.240496	-0.636034
134	1	0	-6.919423	-2.736702	-4.793049	6	6	0	0.291719	-1.394944	-1.783090
135	1	0	-4.745882	-4.167894	-6.021331	7	8	0	-1.395907	0.805927	0.579312
136	1	0	-5.703043	-2.871056	-6.591303	8	6	0	-1.813089	1.340630	-0.636034
137	1	0	-4.634057	0.762178	-4.671712	9	6	0	-1.353916	0.444837	-1.783090
138	1	0	-2.998156	0.280447	-4.793049	10	8	0	1.395907	0.805927	0.579312
139	1	0	-5.324374	-0.886299	-6.021331	11	6	0	2.067564	0.899867	-0.636034
140	1	0	-3.722699	-0.705792	-6.591303	12	6	0	1.062198	0.950108	-1.783090
141	1	0	-1.110719	-3.448177	-4.671712	13	1	0	0.218154	-3.214593	-0.626266
142	1	0	-2.345861	-4.624045	-4.793049	14	1	0	-1.320246	-2.398199	-0.743456
143	1	0	-2.193183	-2.026108	-6.021331	15	1	0	1.364681	-1.505932	-1.822174
144	1	0	-2.837698	-3.503452	-6.591303	16	1	0	-0.111540	-1.719844	-2.738888
145	14	0	4.087813	-2.360100	-3.311698	17	1	0	-2.892997	1.418369	-0.626266
146	17	0	4.087813	-2.360100	-1.158398	18	1	0	-1.416778	2.342466	-0.743456
147	7	0	4.087813	-2.360100	-5.334198	19	1	0	-1.986516	-0.428882	-1.822174

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Xtal, model 2, ONIOM

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# ONIOM(HF/6-31G(d):UFF) Opt(Z-Matrix, Newton)

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Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	17	0	0.000000	0.000000	2.940452
2	14	0	0.000000	0.000000	0.878652
3	7	0	0.000000	0.000000	-1.494198
4	8	0	0.000000	-1.611854	0.579312
5	6	0	-0.254475	-2.240496	-0.636034
6	6	0	0.291719	-1.394944	-1.783090
7	8	0	-1.395907	0.805927	0.579312
8	6	0	-1.813089	1.340630	-0.636034
9	6	0	-1.353916	0.444837	-1.783090
10	8	0	1.395907	0.805927	0.579312
11	6	0	2.067564	0.899867	-0.636034
12	6	0	1.062198	0.950108	-1.783090
13	1	0	0.218154	-3.214593	-0.626266
14	1	0	-1.320246	-2.398199	-0.743456
15	1	0	1.364681	-1.505932	-1.822174
16	1	0	-0.111540	-1.719844	-2.738888
17	1	0	-2.892997	1.418369	-0.626266
18	1	0	-1.416778	2.342466	-0.743456
19	1	0	-1.986516	-0.428882	-1.822174

20	1	0	-1.433658	0.956518	-2.738888	72	1	0	4.452927	-0.705792	1.365825
21	1	0	2.674842	1.796224	-0.626266	73	14	0	-4.087813	-2.360100	4.645429
22	1	0	2.737024	0.055733	-0.743456	74	17	0	-4.087813	-2.360100	6.798729
23	1	0	0.621835	1.934814	-1.822174	75	7	0	-4.087813	-2.360100	2.622929
24	1	0	1.545198	0.763325	-2.738888	76	8	0	-5.513607	-3.183283	4.550495
25	14	0	0.000000	4.720200	4.645429	77	6	0	-6.111186	-3.429862	3.291009
26	17	0	0.000000	4.720200	6.798729	78	6	0	-5.168465	-3.240371	2.226510
27	7	0	0.000000	4.720200	2.622929	79	8	0	-4.087813	-0.713735	4.550495
28	8	0	0.000000	6.366565	4.550495	80	6	0	-4.002568	-0.072926	3.291009
29	6	0	0.085246	7.007374	3.291009	81	6	0	-4.309824	-0.984093	2.226510
30	6	0	-0.222011	6.096207	2.226510	82	8	0	-2.662019	-3.183283	4.550495
31	8	0	1.425794	3.897017	4.550495	83	6	0	-2.149685	-3.577512	3.291009
32	6	0	1.938128	3.502788	3.291009	84	6	0	-2.785150	-2.855836	2.226510
33	6	0	1.302663	4.224464	2.226510	85	1	0	-6.518663	-4.394300	3.285415
34	8	0	-1.425794	3.897017	4.550495	86	1	0	-6.919423	-2.736702	3.164078
35	6	0	-2.023373	3.650438	3.291009	87	1	0	-4.745882	-4.167894	1.935797
36	6	0	-1.080652	3.839929	2.226510	88	1	0	-5.703043	-2.871056	1.365825
37	1	0	-0.546244	7.842478	3.285415	89	1	0	-4.634057	0.762178	3.285415
38	1	0	1.089657	7.360747	3.164078	90	1	0	-2.998156	0.280447	3.164078
39	1	0	-1.236561	6.194001	1.935797	91	1	0	-5.324374	-0.886299	1.935797
40	1	0	0.365114	6.374508	1.365825	92	1	0	-3.722699	-0.705792	1.365825
41	1	0	2.977094	3.632123	3.285415	93	1	0	-1.110719	-3.448177	3.285415
42	1	0	1.741952	2.456255	3.164078	94	1	0	-4.624045	3.164078	3.164078
43	1	0	1.894630	5.054192	1.935797	95	1	0	-2.193183	-2.026108	1.935797
44	1	0	1.250116	3.576848	1.365825	96	1	0	-2.837698	-3.503452	1.365825
45	1	0	-2.430850	2.686000	3.285415	97	14	0	0.000000	4.720200	-3.305571
46	1	0	-2.831609	4.343598	3.164078	98	17	0	0.000000	4.720200	-1.152271
47	1	0	-0.658069	2.912406	1.935797	99	7	0	0.000000	4.720200	-5.328071
48	1	0	-1.615230	4.209244	1.365825	100	8	0	0.000000	6.366565	-3.400505
49	14	0	4.087813	-2.360100	4.645429	101	6	0	0.085246	7.007374	-4.659991
50	17	0	4.087813	-2.360100	6.798729	102	6	0	-0.222011	6.096207	-5.724490
51	7	0	4.087813	-2.360100	2.622929	103	8	0	1.425794	3.897017	-3.400505
52	8	0	5.513607	-3.183283	4.550495	104	6	0	1.938128	3.502788	-4.659991
53	6	0	6.025941	-3.577512	3.291009	105	6	0	1.302663	4.224464	-5.724490
54	6	0	5.390476	-2.855836	2.226510	106	8	0	-1.425794	3.897017	-3.400505
55	8	0	2.662019	-3.183283	4.550495	107	6	0	-2.023373	3.650438	-4.659991
56	6	0	2.064440	-3.429862	3.291009	108	6	0	-1.080652	3.839929	-5.724490
57	6	0	3.007162	-3.240371	2.226510	109	1	0	-0.546244	7.842478	-4.665585
58	8	0	4.087813	-0.713735	4.550495	110	1	0	1.089657	7.360747	-4.786922
59	6	0	4.173059	-0.072926	3.291009	111	1	0	-1.236561	6.194001	-6.015203
60	6	0	3.865802	-0.984093	2.226510	112	1	0	0.365114	6.374508	-6.585175
61	1	0	7.064907	-3.448177	3.285415	113	1	0	2.977094	3.632123	-4.665585
62	1	0	5.829765	-4.624045	3.164078	114	1	0	1.741952	2.456255	-4.786922
63	1	0	5.982443	-2.026108	1.935797	115	1	0	1.894630	5.054192	-6.015203
64	1	0	5.337929	-3.503452	1.365825	116	1	0	1.250116	3.576848	-6.585175
65	1	0	1.656964	-4.394300	3.285415	117	1	0	-2.430850	2.686000	-4.665585
66	1	0	1.256204	-2.736702	3.164078	118	1	0	-2.831609	4.343598	-4.786922
67	1	0	3.429744	-4.167894	1.935797	119	1	0	-0.658069	2.912406	-6.015203
68	1	0	2.472583	-2.871056	1.365825	120	1	0	-1.615230	4.209244	-6.585175
69	1	0	3.541569	0.762178	3.285415	121	14	0	-4.087813	-2.360100	-3.305571
70	1	0	5.177471	0.280447	3.164078	122	17	0	-4.087813	-2.360100	-1.152271
71	1	0	2.851252	-0.886299	1.935797	123	7	0	-4.087813	-2.360100	-5.328071

124	8	0	-5.513607	-3.183283	-3.400505	176	6	0	-1.938128	1.217412	7.266509
125	6	0	-6.111186	-3.429862	-4.659991	177	6	0	-1.302663	0.495736	6.202010
126	6	0	-5.168465	-3.240371	-5.724490	178	8	0	1.425794	0.823183	8.525995
127	8	0	-4.087813	-0.713735	-3.400505	179	6	0	2.023373	1.069762	7.266509
128	6	0	-4.002568	-0.072926	-4.659991	180	6	0	1.080652	0.880271	6.202010
129	6	0	-4.309824	-0.984093	-5.724490	181	1	0	0.546244	-3.122278	7.260915
130	8	0	-2.662019	-3.183283	-3.400505	182	1	0	-1.089657	-2.640547	7.139578
131	6	0	-2.149685	-3.577512	-4.659991	183	1	0	1.236561	-1.473801	5.911297
132	6	0	-2.785150	-2.855836	-5.724490	184	1	0	-0.365114	-1.654308	5.341325
133	1	0	-6.518663	-4.394300	-4.665585	185	1	0	-2.977094	1.088077	7.260915
134	1	0	-6.919423	-2.736702	-4.786922	186	1	0	-1.741952	2.263945	7.139578
135	1	0	-4.745882	-4.167894	-6.015203	187	1	0	-1.894630	-0.333992	5.911297
136	1	0	-5.703043	-2.871056	-6.585175	188	1	0	-1.250116	1.143352	5.341325
137	1	0	-4.634057	0.762178	-4.665585	189	1	0	2.430850	2.034200	7.260915
138	1	0	-2.998156	0.280447	-4.786922	190	1	0	2.831609	0.376602	7.139578
139	1	0	-5.324374	-0.886299	-6.015203	191	1	0	0.658069	1.807794	5.911297
140	1	0	-3.722699	-0.705792	-6.585175	192	1	0	1.615230	0.510956	5.341325
141	1	0	-1.110719	-3.448177	-4.665585	193	14	0	0.000000	0.000000	-7.281071
142	1	0	-2.345861	-4.624045	-4.786922	194	17	0	0.000000	0.000000	-5.127771
143	1	0	-2.193183	-2.026108	-6.015203	195	7	0	0.000000	0.000000	-9.303571
144	1	0	-2.837698	-3.503452	-6.585175	196	8	0	1.425794	0.823183	-7.376005
145	14	0	4.087813	-2.360100	-3.305571	197	6	0	2.023373	1.069762	-8.635491
146	17	0	4.087813	-2.360100	-1.152271	198	6	0	1.080652	0.880271	-9.699990
147	7	0	4.087813	-2.360100	-5.328071	199	8	0	0.000000	-1.646365	-7.376005
148	8	0	5.513607	-3.183283	-3.400505	200	6	0	-0.085246	-2.287174	-8.635491
149	6	0	6.025941	-3.577512	-4.659991	201	6	0	0.222011	-1.376007	-9.699990
150	6	0	5.390476	-2.855836	-5.724490	202	8	0	-1.425794	0.823183	-7.376005
151	8	0	2.662019	-3.183283	-3.400505	203	6	0	-1.938128	1.217412	-8.635491
152	6	0	2.064440	-3.429862	-4.659991	204	6	0	-1.302663	0.495736	-9.699990
153	6	0	3.007162	-3.240371	-5.724490	205	1	0	2.430850	2.034200	-8.641085
154	8	0	4.087813	-0.713735	-3.400505	206	1	0	2.831609	0.376602	-8.762422
155	6	0	4.173059	-0.072926	-4.659991	207	1	0	0.658069	1.807794	-9.990703
156	6	0	3.865802	-0.984093	-5.724490	208	1	0	1.615230	0.510956	-10.560675
157	1	0	7.064907	-3.448177	-4.665585	209	1	0	0.546244	-3.122278	-8.641085
158	1	0	5.829765	-4.624045	-4.786922	210	1	0	-1.089657	-2.640547	-8.762422
159	1	0	5.982443	-2.026108	-6.015203	211	1	0	1.236561	-1.473801	-9.990703
160	1	0	5.337929	-3.503452	-6.585175	212	1	0	-0.365114	-1.654308	-10.560675
161	1	0	1.656964	-4.394300	-4.665585	213	1	0	-2.977094	1.088077	-8.641085
162	1	0	1.256204	-2.736702	-4.786922	214	1	0	-1.741952	2.263945	-8.762422
163	1	0	3.429744	-4.167894	-6.015203	215	1	0	-1.894630	-0.333992	-9.990703
164	1	0	2.472583	-2.871056	-6.585175	216	1	0	-1.250116	1.143352	-10.560675
165	1	0	3.541569	0.762178	-4.665585						
166	1	0	5.177471	0.280447	-4.786922						
167	1	0	2.851252	-0.886299	-6.015203						
168	1	0	4.452927	-0.705792	-6.585175						
169	14	0	0.000000	0.000000	8.620929						
170	17	0	0.000000	0.000000	10.774229						
171	7	0	0.000000	0.000000	6.598429						
172	8	0	0.000000	-1.646365	8.525995						
173	6	0	-0.085246	-2.287174	7.266509						
174	6	0	0.222011	-1.376007	6.202010						
175	8	0	-1.425794	0.823183	8.525995						

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**Xtal, model 3, ONIOM**

%mem=128MB

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# ONIOM(HF/6-31G(d):UFF) Opt(Z-Matrix, Newton) MaxDisk=2GB

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Standard orientation:

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Center	Atomic	Atomic	Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z	51	7	0	4.087813	-2.360100	2.624944
1	17	0	0.000000	0.000000	2.941615	52	8	0	5.513607	-3.183283	4.552509
2	14	0	0.000000	0.000000	0.879479	53	6	0	6.025941	-3.577512	3.293023
3	7	0	0.000000	0.000000	-1.490857	54	6	0	5.390476	-2.855836	2.228524
4	8	0	0.000000	-1.612140	0.581247	55	8	0	2.662019	-3.183283	4.552509
5	6	0	-0.247937	-2.242524	-0.634457	56	6	0	2.064440	-3.429862	3.293023
6	6	0	0.295736	-1.393921	-1.780622	57	6	0	3.007162	-3.240371	2.228524
7	8	0	-1.396154	0.806070	0.581247	58	8	0	4.087813	-0.713735	4.552509
8	6	0	-1.818114	1.335982	-0.634457	59	6	0	4.173059	-0.072926	3.293023
9	6	0	-1.355039	0.440846	-1.780622	60	6	0	3.865802	-0.984093	2.228524
10	8	0	1.396154	0.806070	0.581247	61	1	0	7.064907	-3.448177	3.287430
11	6	0	2.066051	0.906542	-0.634457	62	1	0	5.829765	-4.624045	3.166093
12	6	0	1.059303	0.953075	-1.780622	63	1	0	5.982443	-2.026108	1.937811
13	1	0	0.231977	-3.212977	-0.623810	64	1	0	5.337929	-3.503452	1.367839
14	1	0	-1.312390	-2.408299	-0.743831	65	1	0	1.656964	-4.394300	3.287430
15	1	0	1.369055	-1.501465	-1.819103	66	1	0	1.256204	-2.736702	3.166093
16	1	0	-0.105587	-1.719199	-2.737038	67	1	0	3.429744	-4.167894	1.937811
17	1	0	-2.898509	1.405590	-0.623810	68	1	0	2.472583	-2.871056	1.367839
18	1	0	-1.429453	2.340712	-0.743831	69	1	0	3.541569	0.762178	3.287430
19	1	0	-1.984834	-0.434904	-1.819103	70	1	0	5.177471	0.280447	3.166093
20	1	0	-1.436076	0.951040	-2.737038	71	1	0	2.851252	-0.886299	1.937811
21	1	0	2.666531	1.807387	-0.623810	72	1	0	4.452927	-0.705792	1.367839
22	1	0	2.741843	0.067587	-0.743831	73	14	0	-4.087813	-2.360100	4.647444
23	1	0	0.615779	1.936369	-1.819103	74	17	0	-4.087813	-2.360100	6.800744
24	1	0	1.541663	0.768158	-2.737038	75	7	0	-4.087813	-2.360100	2.624944
25	14	0	0.000000	4.720200	4.647444	76	8	0	-5.513607	-3.183283	4.552509
26	17	0	0.000000	4.720200	6.800744	77	6	0	-6.111186	-3.429862	3.293023
27	7	0	0.000000	4.720200	2.624944	78	6	0	-5.168465	-3.240371	2.228524
28	8	0	0.000000	6.366565	4.552509	79	8	0	-4.087813	-0.713735	4.552509
29	6	0	0.085246	7.007374	3.293023	80	6	0	-4.002568	-0.072926	3.293023
30	6	0	-0.222011	6.096207	2.228524	81	6	0	-4.309824	-0.984093	2.228524
31	8	0	1.425794	3.897017	4.552509	82	8	0	-2.662019	-3.183283	4.552509
32	6	0	1.938128	3.502788	3.293023	83	6	0	-2.149685	-3.577512	3.293023
33	6	0	1.302663	4.224464	2.228524	84	6	0	-2.785150	-2.855836	2.228524
34	8	0	-1.425794	3.897017	4.552509	85	1	0	-6.518663	-4.394300	3.287430
35	6	0	-2.023373	3.650438	3.293023	86	1	0	-6.919423	-2.736702	3.166093
36	6	0	-1.080652	3.839929	2.228524	87	1	0	-4.745882	-4.167894	1.937811
37	1	0	-0.546244	7.842478	3.287430	88	1	0	-5.703043	-2.871056	1.367839
38	1	0	1.089657	7.360747	3.166093	89	1	0	-4.634057	0.762178	3.287430
39	1	0	-1.236561	6.194001	1.937811	90	1	0	-2.998156	0.280447	3.166093
40	1	0	0.365114	6.374508	1.367839	91	1	0	-5.324374	-0.886299	1.937811
41	1	0	2.977094	3.632123	3.287430	92	1	0	-3.722699	-0.705792	1.367839
42	1	0	1.741952	2.456255	3.166093	93	1	0	-1.110719	-3.448177	3.287430
43	1	0	1.894630	5.054192	1.937811	94	1	0	-2.345861	-4.624045	3.166093
44	1	0	1.250116	3.576848	1.367839	95	1	0	-2.193183	-2.026108	1.937811
45	1	0	-2.430850	2.686000	3.287430	96	1	0	-2.837698	-3.503452	1.367839
46	1	0	-2.831609	4.343598	3.166093	97	14	0	0.000000	4.720200	-3.303556
47	1	0	-0.658069	2.912406	1.937811	98	17	0	0.000000	4.720200	-1.150256
48	1	0	-1.615230	4.209244	1.367839	99	7	0	0.000000	4.720200	-5.326056
49	14	0	4.087813	-2.360100	4.647444	100	8	0	0.000000	6.366565	-3.398491
50	17	0	4.087813	-2.360100	6.800744	101	6	0	0.085246	7.007374	-4.657977
						102	6	0	-0.222011	6.096207	-5.722476

103	8	0	1.425794	3.897017	-3.398491	155	6	0	4.173059	-0.072926	-4.657977
104	6	0	1.938128	3.502788	-4.657977	156	6	0	3.865802	-0.984093	-5.722476
105	6	0	1.302663	4.224464	-5.722476	157	1	0	7.064907	-3.448177	-4.663570
106	8	0	-1.425794	3.897017	-3.398491	158	1	0	5.829765	-4.624045	-4.784907
107	6	0	-2.023373	3.650438	-4.657977	159	1	0	5.982443	-2.026108	-6.013189
108	6	0	-1.080652	3.839929	-5.722476	160	1	0	5.337929	-3.503452	-6.583161
109	1	0	-0.546244	7.842478	-4.663570	161	1	0	1.656964	-4.394300	-4.663570
110	1	0	1.089657	7.360747	-4.784907	162	1	0	1.256204	-2.736702	-4.784907
111	1	0	-1.236561	6.194001	-6.013189	163	1	0	3.429744	-4.167894	-6.013189
112	1	0	0.365114	6.374508	-6.583161	164	1	0	2.472583	-2.871056	-6.583161
113	1	0	2.977094	3.632123	-4.663570	165	1	0	3.541569	0.762178	-4.663570
114	1	0	1.741952	2.456255	-4.784907	166	1	0	5.177471	0.280447	-4.784907
115	1	0	1.894630	5.054192	-6.013189	167	1	0	2.851252	-0.886299	-6.013189
116	1	0	1.250116	3.576848	-6.583161	168	1	0	4.452927	-0.705792	-6.583161
117	1	0	-2.430850	2.686000	-4.663570	169	14	0	0.000000	0.000000	8.622944
118	1	0	-2.831609	4.343598	-4.784907	170	17	0	0.000000	0.000000	10.776244
119	1	0	-0.658069	2.912406	-6.013189	171	7	0	0.000000	0.000000	6.600444
120	1	0	-1.615230	4.209244	-6.583161	172	8	0	0.000000	-1.646365	8.528009
121	14	0	-4.087813	-2.360100	-3.303556	173	6	0	-0.085246	-2.287174	7.268523
122	17	0	-4.087813	-2.360100	-1.150256	174	6	0	0.222011	-1.376007	6.204024
123	7	0	-4.087813	-2.360100	-5.326056	175	8	0	-1.425794	0.823183	8.528009
124	8	0	-5.513607	-3.183283	-3.398491	176	6	0	-1.938128	1.217412	7.268523
125	6	0	-6.111186	-3.429862	-4.657977	177	6	0	-1.302663	0.495736	6.204024
126	6	0	-5.168465	-3.240371	-5.722476	178	8	0	1.425794	0.823183	8.528009
127	8	0	-4.087813	-0.713735	-3.398491	179	6	0	2.023373	1.069762	7.268523
128	6	0	-4.002568	-0.072926	-4.657977	180	6	0	1.080652	0.880271	6.204024
129	6	0	-4.309824	-0.984093	-5.722476	181	1	0	0.546244	-3.122278	7.262930
130	8	0	-2.662019	-3.183283	-3.398491	182	1	0	-1.089657	-2.640547	7.141593
131	6	0	-2.149685	-3.577512	-4.657977	183	1	0	1.236561	-1.473801	5.913311
132	6	0	-2.785150	-2.855836	-5.722476	184	1	0	-0.365114	-1.654308	5.343339
133	1	0	-6.518663	-4.394300	-4.663570	185	1	0	-2.977094	1.088077	7.262930
134	1	0	-6.919423	-2.736702	-4.784907	186	1	0	-1.741952	2.263945	7.141593
135	1	0	-4.745882	-4.167894	-6.013189	187	1	0	-1.894630	-0.333992	5.913311
136	1	0	-5.703043	-2.871056	-6.583161	188	1	0	-1.250116	1.143352	5.343339
137	1	0	-4.634057	0.762178	-4.663570	189	1	0	2.430850	2.034200	7.262930
138	1	0	-2.998156	0.280447	-4.784907	190	1	0	2.831609	0.376602	7.141593
139	1	0	-5.324374	-0.886299	-6.013189	191	1	0	0.658069	1.807794	5.913311
140	1	0	-3.722699	-0.705792	-6.583161	192	1	0	1.615230	0.510956	5.343339
141	1	0	-1.110719	-3.448177	-4.663570	193	14	0	0.000000	0.000000	-7.279056
142	1	0	-2.345861	-4.624045	-4.784907	194	17	0	0.000000	0.000000	-5.125756
143	1	0	-2.193183	-2.026108	-6.013189	195	7	0	0.000000	0.000000	-9.301556
144	1	0	-2.837698	-3.503452	-6.583161	196	8	0	1.425794	0.823183	-7.373991
145	14	0	4.087813	-2.360100	-3.303556	197	6	0	2.023373	1.069762	-8.633477
146	17	0	4.087813	-2.360100	-1.150256	198	6	0	1.080652	0.880271	-9.697976
147	7	0	4.087813	-2.360100	-5.326056	199	8	0	0.000000	-1.646365	-7.373991
148	8	0	5.513607	-3.183283	-3.398491	200	6	0	-0.085246	-2.287174	-8.633477
149	6	0	6.025941	-3.577512	-4.657977	201	6	0	0.222011	-1.376007	-9.697976
150	6	0	5.390476	-2.855836	-5.722476	202	8	0	-1.425794	0.823183	-7.373991
151	8	0	2.662019	-3.183283	-3.398491	203	6	0	-1.938128	1.217412	-8.633477
152	6	0	2.064440	-3.429862	-4.657977	204	6	0	-1.302663	0.495736	-9.697976
153	6	0	3.007162	-3.240371	-5.722476	205	1	0	2.430850	2.034200	-8.639070
154	8	0	4.087813	-0.713735	-3.398491	206	1	0	2.831609	0.376602	-8.760407

207	1	0	0.658069	1.807794	-9.988689	259	1	0	3.429744	-4.167894	9.888811
208	1	0	1.615230	0.510956	-10.558661	260	1	0	2.472583	-2.871056	9.318839
209	1	0	0.546244	-3.122278	-8.639070	261	1	0	3.541569	0.762178	11.238430
210	1	0	-1.089657	-2.640547	-8.760407	262	1	0	5.177471	0.280447	11.117093
211	1	0	1.236561	-1.473801	-9.988689	263	1	0	2.851252	-0.886299	9.888811
212	1	0	-0.365114	-1.654308	-10.558661	264	1	0	4.452927	-0.705792	9.318839
213	1	0	-2.977094	1.088077	-8.639070	265	14	0	-4.087813	-2.360100	12.598444
214	1	0	-1.741952	2.263945	-8.760407	266	17	0	-4.087813	-2.360100	14.751744
215	1	0	-1.894630	-0.333992	-9.988689	267	7	0	-4.087813	-2.360100	10.575944
216	1	0	-1.250116	1.143352	-10.558661	268	8	0	-5.513607	-3.183283	12.503509
217	14	0	0.000000	4.720200	12.598444	269	6	0	-6.111186	-3.429862	11.244023
218	17	0	0.000000	4.720200	14.751744	270	6	0	-5.168465	-3.240371	10.179524
219	7	0	0.000000	4.720200	10.575944	271	8	0	-4.087813	-0.713735	12.503509
220	8	0	0.000000	6.366565	12.503509	272	6	0	-4.002568	-0.072926	11.244023
221	6	0	0.085246	7.007374	11.244023	273	6	0	-4.309824	-0.984093	10.179524
222	6	0	-0.222011	6.096207	10.179524	274	8	0	-2.662019	-3.183283	12.503509
223	8	0	1.425794	3.897017	12.503509	275	6	0	-2.149685	-3.577512	11.244023
224	6	0	1.938128	3.502788	11.244023	276	6	0	-2.785150	-2.855836	10.179524
225	6	0	1.302663	4.224464	10.179524	277	1	0	-6.518663	-4.394300	11.238430
226	8	0	-1.425794	3.897017	12.503509	278	1	0	-6.919423	-2.736702	11.117093
227	6	0	-2.023373	3.650438	11.244023	279	1	0	-4.745882	-4.167894	9.888811
228	6	0	-1.080652	3.839929	10.179524	280	1	0	-5.703043	-2.871056	9.318839
229	1	0	-0.546244	7.842478	11.238430	281	1	0	-4.634057	0.762178	11.238430
230	1	0	1.089657	7.360747	11.117093	282	1	0	-2.998156	0.280447	11.117093
231	1	0	-1.236561	6.194001	9.888811	283	1	0	-5.324374	-0.886299	9.888811
232	1	0	0.365114	6.374508	9.318839	284	1	0	-3.722699	-0.705792	9.318839
233	1	0	2.977094	3.632123	11.238430	285	1	0	-1.110719	-3.448177	11.238430
234	1	0	1.741952	2.456255	11.117093	286	1	0	-2.345861	-4.624045	11.117093
235	1	0	1.894630	5.054192	9.888811	287	1	0	-2.193183	-2.026108	9.888811
236	1	0	1.250116	3.576848	9.318839	288	1	0	-2.837698	-3.503452	9.318839
237	1	0	-2.430850	2.686000	11.238430	289	14	0	-4.087813	-2.360100	-11.254556
238	1	0	-2.831609	4.343598	11.117093	290	17	0	-4.087813	-2.360100	-9.101256
239	1	0	-0.658069	2.912406	9.888811	291	7	0	-4.087813	-2.360100	-13.277056
240	1	0	-1.615230	4.209244	9.318839	292	8	0	-5.513607	-3.183283	-11.349491
241	14	0	4.087813	-2.360100	12.598444	293	6	0	-6.111186	-3.429862	-12.608977
242	17	0	4.087813	-2.360100	14.751744	294	6	0	-5.168465	-3.240371	-13.673476
243	7	0	4.087813	-2.360100	10.575944	295	8	0	-4.087813	-0.713735	-11.349491
244	8	0	5.513607	-3.183283	12.503509	296	6	0	-4.002568	-0.072926	-12.608977
245	6	0	6.025941	-3.577512	11.244023	297	6	0	-4.309824	-0.984093	-13.673476
246	6	0	5.390476	-2.855836	10.179524	298	8	0	-2.662019	-3.183283	-11.349491
247	8	0	2.662019	-3.183283	12.503509	299	6	0	-2.149685	-3.577512	-12.608977
248	6	0	2.064440	-3.429862	11.244023	300	6	0	-2.785150	-2.855836	-13.673476
249	6	0	3.007162	-3.240371	10.179524	301	1	0	-6.518663	-4.394300	-12.614570
250	8	0	4.087813	-0.713735	12.503509	302	1	0	-6.919423	-2.736702	-12.735907
251	6	0	4.173059	-0.072926	11.244023	303	1	0	-4.745882	-4.167894	-13.964189
252	6	0	3.865802	-0.984093	10.179524	304	1	0	-5.703043	-2.871056	-14.534161
253	1	0	7.064907	-3.448177	11.238430	305	1	0	-4.634057	0.762178	-12.614570
254	1	0	5.829765	-4.624045	11.117093	306	1	0	-2.998156	0.280447	-12.735907
255	1	0	5.982443	-2.026108	9.888811	307	1	0	-5.324374	-0.886299	-13.964189
256	1	0	5.337929	-3.503452	9.318839	308	1	0	-3.722699	-0.705792	-14.534161
257	1	0	1.656964	-4.394300	11.238430	309	1	0	-1.110719	-3.448177	-12.614570
258	1	0	1.256204	-2.736702	11.117093	310	1	0	-2.345861	-4.624045	-12.735907

```

311      1      0      -2.193183  -2.026108  -13.964189
312      1      0      -2.837698  -3.503452  -14.534161
313     14      0       4.087813  -2.360100  -11.254556
314     17      0       4.087813  -2.360100   -9.101256
315      7      0       4.087813  -2.360100  -13.277056
316      8      0       5.513607  -3.183283  -11.349491
317      6      0       6.025941  -3.577512  -12.608977
318      6      0       5.390476  -2.855836  -13.673476
319      8      0       2.662019  -3.183283  -11.349491
320      6      0       2.064440  -3.429862  -12.608977
321      6      0       3.007162  -3.240371  -13.673476
322      8      0       4.087813  -0.713735  -11.349491
323      6      0       4.173059  -0.072926  -12.608977
324      6      0       3.865802  -0.984093  -13.673476
325      1      0       7.064907  -3.448177  -12.614570
326      1      0       5.829765  -4.624045  -12.735907
327      1      0       5.982443  -2.026108  -13.964189
328      1      0       5.337929  -3.503452  -14.534161
329      1      0       1.656964  -4.394300  -12.614570
330      1      0       1.256204  -2.736702  -12.735907
331      1      0       3.429744  -4.167894  -13.964189
332      1      0       2.472583  -2.871056  -14.534161
333      1      0       3.541569  0.762178  -12.614570
334      1      0       5.177471  0.280447  -12.735907
335      1      0       2.851252  -0.886299  -13.964189
336      1      0       4.452927  -0.705792  -14.534161
337     14      0       0.000000  4.720200  -11.254556
338     17      0       0.000000  4.720200   -9.101256
339      7      0       0.000000  4.720200  -13.277056
340      8      0       0.000000  6.366565  -11.349491
341      6      0       0.085246  7.007374  -12.608977
342      6      0      -0.222011  6.096207  -13.673476
343      8      0       1.425794  3.897017  -11.349491
344      6      0       1.938128  3.502788  -12.608977
345      6      0       1.302663  4.224464  -13.673476
346      8      0      -1.425794  3.897017  -11.349491
347      6      0      -2.023373  3.650438  -12.608977
348      6      0      -1.080652  3.839929  -13.673476
349      1      0      -0.546244  7.842478  -12.614570
350      1      0       1.089657  7.360747  -12.735907
351      1      0      -1.236561  6.194001  -13.964189
352      1      0       0.365114  6.374508  -14.534161
353      1      0       2.977094  3.632123  -12.614570
354      1      0       1.741952  2.456255  -12.735907
355      1      0       1.894630  5.054192  -13.964189
356      1      0       1.250116  3.576848  -14.534161
357      1      0      -2.430850  2.686000  -12.614570
358      1      0      -2.831609  4.343598  -12.735907
359      1      0      -0.658069  2.912406  -13.964189
360      1      0      -1.615230  4.209244  -14.534161

```

**Xtal, model 1, DFT**

```

%chk=C1-Silatranel_b3lyp.chk
%mem=256MB

```

```

%rwf=s1,255mw,s2,255mw,s3,255mw,s4,255mw,s5,255mw,s6,255mw,s7,255mw,s8,2
55mw

```

```

# b3lyp/6-31G(d) Opt(Z-Matrix) IOp(1/8=5)

```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	17	0	0.000000	0.000000	2.927891
2	14	0	0.000000	0.000000	0.832264
3	7	0	0.000000	0.000000	-1.393863
4	8	0	0.000000	-1.667969	0.630697
5	6	0	-0.220309	-2.286863	-0.628385
6	6	0	0.345234	-1.390850	-1.733493
7	8	0	-1.444503	0.833984	0.630697
8	6	0	-1.870327	1.334225	-0.628385
9	6	0	-1.377129	0.396443	-1.733493
10	8	0	1.444503	0.833984	0.630697
11	6	0	2.090636	0.952638	-0.628385
12	6	0	1.031895	0.994407	-1.733493
13	1	0	0.292501	-3.254216	-0.635549
14	1	0	-1.291795	-2.466116	-0.769659
15	1	0	1.431969	-1.480383	-1.750209
16	1	0	-0.044464	-1.676876	-2.721445
17	1	0	-2.964485	1.373794	-0.635549
18	1	0	-1.489822	2.351785	-0.769659
19	1	0	-1.998034	-0.499930	-1.750209
20	1	0	-1.429985	0.876945	-2.721445
21	1	0	2.671983	1.880422	-0.635549
22	1	0	2.781617	0.114331	-0.769659
23	1	0	0.566065	1.980313	-1.750209
24	1	0	1.474449	0.799931	-2.721445
25	14	0	0.000000	4.720200	6.403332
26	17	0	0.000000	4.720200	6.793632
27	7	0	0.000000	4.720200	2.617832
28	8	0	0.000000	6.366565	4.545398
29	6	0	0.085246	7.007374	3.285912
30	6	0	-0.222011	6.096207	2.221413
31	8	0	1.425794	3.897017	4.545398
32	6	0	1.938128	3.502788	3.285912
33	6	0	1.302663	4.224464	2.221413
34	8	0	-1.425794	3.897017	4.545398
35	6	0	-2.023373	3.650438	3.285912
36	6	0	-1.080652	3.839929	2.221413
37	1	0	-0.546244	7.842478	3.280319

38	1	0	1.089657	7.360747	3.158981	90	1	0	-2.998156	0.280447	3.158981
39	1	0	-1.236561	6.194001	1.930700	91	1	0	-5.324374	-0.886299	1.930700
40	1	0	0.365114	6.374508	1.360728	92	1	0	-3.722699	-0.705792	1.360728
41	1	0	2.977094	3.632123	3.280319	93	1	0	-1.110719	-3.448177	3.280319
42	1	0	1.741952	2.456255	3.158981	94	1	0	-2.345861	-4.624045	3.158981
43	1	0	1.894630	5.054192	1.930700	95	1	0	-2.193183	-2.026108	1.930700
44	1	0	1.250116	3.576848	1.360728	96	1	0	-2.837698	-3.503452	1.360728
45	1	0	-2.430850	2.686000	3.280319	97	14	0	0.000000	4.720200	-3.310668
46	1	0	-2.831609	4.343598	3.158981	98	17	0	0.000000	4.720200	-1.157368
47	1	0	-0.658069	2.912406	1.930700	99	7	0	0.000000	4.720200	-5.333168
48	1	0	-1.615230	4.209244	1.360728	100	8	0	0.000000	6.366565	-3.405602
49	14	0	4.087813	-2.360100	4.640332	101	6	0	0.085246	7.007374	-4.665088
50	17	0	4.087813	-2.360100	6.793632	102	6	0	-0.222011	6.096207	-5.729587
51	7	0	4.087813	-2.360100	2.617832	103	8	0	1.425794	3.897017	-3.405602
52	8	0	5.513607	-3.183283	4.545398	104	6	0	1.938128	3.502788	-4.665088
53	6	0	6.025941	-3.577512	3.285912	105	6	0	1.302663	4.224464	-5.729587
54	6	0	5.390476	-2.855836	2.221413	106	8	0	-1.425794	3.897017	-3.405602
55	8	0	2.662019	-3.183283	4.545398	107	6	0	-2.023373	3.650438	-4.665088
56	6	0	2.064440	-3.429862	3.285912	108	6	0	-1.080652	3.839929	-5.729587
57	6	0	3.007162	-3.240371	2.221413	109	1	0	-0.546244	7.842478	-4.670681
58	8	0	4.087813	-0.713735	4.545398	110	1	0	1.089657	7.360747	-4.792019
59	6	0	4.173059	-0.072926	3.285912	111	1	0	-1.236561	6.194001	-6.020300
60	6	0	3.865802	-0.984093	2.221413	112	1	0	0.365114	6.374508	-6.590272
61	1	0	7.064907	-3.448177	3.280319	113	1	0	2.977094	3.632123	-4.670681
62	1	0	5.829765	-4.624045	3.158981	114	1	0	1.741952	2.456255	-4.792019
63	1	0	5.982443	-2.026108	1.930700	115	1	0	1.894630	5.054192	-6.020300
64	1	0	5.337929	-3.503452	1.360728	116	1	0	1.250116	3.576848	-6.590272
65	1	0	1.656964	-4.394300	3.280319	117	1	0	-2.430850	2.686000	-4.670681
66	1	0	1.256204	-2.736702	3.158981	118	1	0	-2.831609	4.343598	-4.792019
67	1	0	3.429744	-4.167894	1.930700	119	1	0	-0.658069	2.912406	-6.020300
68	1	0	2.472583	-2.871056	1.360728	120	1	0	-1.615230	4.209244	-6.590272
69	1	0	3.541569	0.762178	3.280319	121	14	0	-4.087813	-2.360100	-3.310668
70	1	0	5.177471	0.280447	3.158981	122	17	0	-4.087813	-2.360100	-1.157368
71	1	0	2.851252	-0.886299	1.930700	123	7	0	-4.087813	-2.360100	-5.333168
72	1	0	4.452927	-0.705792	1.360728	124	8	0	-5.513607	-3.183283	-3.405602
73	14	0	-4.087813	-2.360100	4.640332	125	6	0	-6.111186	-3.429862	-4.665088
74	17	0	-4.087813	-2.360100	6.793632	126	6	0	-5.168465	-3.240371	-5.729587
75	7	0	-4.087813	-2.360100	2.617832	127	8	0	-4.087813	-0.713735	-3.405602
76	8	0	-5.513607	-3.183283	4.545398	128	6	0	-4.002568	-0.072926	-4.665088
77	6	0	-6.111186	-3.429862	3.285912	129	6	0	-4.309824	-0.984093	-5.729587
78	6	0	-5.168465	-3.240371	2.221413	130	8	0	-2.662019	-3.183283	-3.405602
79	8	0	-4.087813	-0.713735	4.545398	131	6	0	-2.149685	-3.577512	-4.665088
80	6	0	-4.002568	-0.072926	3.285912	132	6	0	-2.785150	-2.855836	-5.729587
81	6	0	-4.309824	-0.984093	2.221413	133	1	0	-6.518663	-4.394300	-4.670681
82	8	0	-2.662019	-3.183283	4.545398	134	1	0	-6.919423	-2.736702	-4.792019
83	6	0	-2.149685	-3.577512	3.285912	135	1	0	-4.745882	-4.167894	-6.020300
84	6	0	-2.785150	-2.855836	2.221413	136	1	0	-5.703043	-2.871056	-6.590272
85	1	0	-6.518663	-4.394300	3.280319	137	1	0	-4.634057	0.762178	-4.670681
86	1	0	-6.919423	-2.736702	3.158981	138	1	0	-2.998156	0.280447	-4.792019
87	1	0	-4.745882	-4.167894	1.930700	139	1	0	-5.324374	-0.886299	-6.020300
88	1	0	-5.703043	-2.871056	1.360728	140	1	0	-3.722699	-0.705792	-6.590272
89	1	0	-4.634057	0.762178	3.280319	141	1	0	-1.110719	-3.448177	-4.670681



142	1	0	-2.345861	-4.624045	-4.792019
143	1	0	-2.193183	-2.026108	-6.020300
144	1	0	-2.837698	-3.503452	-6.590272
145	14	0	4.087813	-2.360100	-3.310668
146	17	0	4.087813	-2.360100	-1.157368
147	7	0	4.087813	-2.360100	-5.333168
148	8	0	5.513607	-3.183283	-3.405602
149	6	0	6.025941	-3.577512	-4.665088
150	6	0	5.390476	-2.855836	-5.729587
151	8	0	2.662019	-3.183283	-3.405602
152	6	0	2.064440	-3.429862	-4.665088
153	6	0	3.007162	-3.240371	-5.729587
154	8	0	4.087813	-0.713735	-3.405602
155	6	0	4.173059	-0.072926	-4.665088
156	6	0	3.865802	-0.984093	-5.729587
157	1	0	7.064907	-3.448177	-4.670681
158	1	0	5.829765	-4.624045	-4.792019
159	1	0	5.982443	-2.026108	-6.020300
160	1	0	5.337929	-3.503452	-6.590272
161	1	0	1.656964	-4.394300	-4.670681
162	1	0	1.256204	-2.736702	-4.792019
163	1	0	3.429744	-4.167894	-6.020300
164	1	0	2.472583	-2.871056	-6.590272
165	1	0	3.541569	0.762178	-4.670681
166	1	0	5.177471	0.280447	-4.792019
167	1	0	2.851252	-0.886299	-6.020300
168	1	0	4.452927	-0.705792	-6.590272

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