

Supporting Information for

**Computational study of the spin-state energies and UV-Vis spectra of bis(1,4,7-triazacyclononane) complexes of some first-row transition metal cations†**

**Matija Zlatar,<sup>a</sup> Maja Gruden-Pavlović,<sup>b,\*</sup> Mireia Güell<sup>c</sup> and Marcel Swart<sup>c,d,\*</sup>**

<sup>a</sup> Center for Chemistry, IHTM, University of Belgrade, Studentski trg 12–16, 11000 Belgrade, Serbia

<sup>10</sup> <sup>b</sup> Faculty of Chemistry, University of Belgrade, Studentski trg 12–16, 11000 Belgrade, Serbia; E-mail: gmaja@chem.bg.ac.rs

<sup>c</sup> Institut de Química Computacional and Departament de Química, Universitat de Girona, Campus Montilivi, Facultat de Ciències, 17071 Girona, Spain

<sup>d</sup> Institució Catalana de Recerca i Estudis Avançats (ICREA), Pg. Lluís Companys 23, 08010 Barcelona, Spain. Fax: +34 972 418356; Tel: +34 972 418861; E-mail: marcel.swart@icrea.cat

<sup>15</sup> **Table S1.** M-N bond lengths at different level of theory and comparison with experiment S2

Cartesian coordinates of all species S3-S25

<sup>20</sup>

**Table S1** M-N bond lengths from geometry optimizations at different level of theory (LDA, OPBE and SSB-D) and comparison with experimental data

M <sup>n+</sup>	d <sup>n</sup>	Symm.	Spin state	State	LDA	OPBE	SSB-D	exp.	Ref. code
Cr <sup>3+</sup>	d <sup>3</sup>	D <sub>3</sub>	HS	<sup>4</sup> A <sub>2</sub>	2.076	2.137	2.111		
			LS	<sup>2</sup> A <sub>2</sub>	2.061	2.109	2.095		
Mn <sup>2+</sup>	d <sup>5</sup>	D <sub>3</sub>	HS	<sup>6</sup> A <sub>1</sub>	2.250	2.344	2.313	2.278 <sup>a</sup>	CEXNUP <sup>1</sup>
			IS	<sup>4</sup> E	2.124	2.210	2.192		
		C <sub>2</sub>	LS	<sup>2</sup> E	2.018	2.077	2.079		
			IS	<sup>4</sup> B	2.052/2.310 <sup>c</sup>	2.112/2.443 <sup>c</sup>	2.119/2.373 <sup>c</sup>		
Fe <sup>3+</sup>	d <sup>5</sup>	D <sub>3</sub>	HS	<sup>6</sup> A <sub>1</sub>	2.162	2.233	2.189		
			IS	<sup>4</sup> E	2.075	2.149	2.121		
		C <sub>2</sub>	LS	<sup>2</sup> E	1.981	2.032	2.023	2.005 <sup>a</sup>	DETTUR <sup>2</sup>
			IS	<sup>4</sup> B	2.015/2.205 <sup>c</sup>	2.079/2.283 <sup>c</sup>	2.066/2.225 <sup>c</sup>		
Fe <sup>2+</sup>	d <sup>6</sup>	D <sub>3</sub>	HS	<sup>5</sup> E	2.171	2.258	2.236		
			IS	<sup>3</sup> E	2.084	2.167	2.154		
		C <sub>2</sub>	LS	<sup>1</sup> A <sub>1</sub>	1.975	2.029	2.036	2.034 <sup>a</sup>	DETTOL <sup>2</sup>
			HS	<sup>5</sup> B	2.185 <sup>b</sup>	2.277 <sup>b</sup>	2.249 <sup>b</sup>		
Co <sup>3+</sup>	d <sup>6</sup>	D <sub>3</sub>	HS	<sup>5</sup> A <sub>1</sub>	2.128	2.200	2.164		
			IS	<sup>3</sup> E	1.992	2.114	2.097		
		C <sub>2</sub>	LS	<sup>1</sup> A <sub>1</sub>	1.951	1.997	1.993	1.977 <sup>a</sup>	XACPAS <sup>3</sup>
			IS	<sup>3</sup> B	1.951/2.092 <sup>c</sup>	2.001/2.161 <sup>c</sup>	1.994/2.132 <sup>c</sup>		
Co <sup>2+</sup>	d <sup>7</sup>	D <sub>3</sub>	HS	<sup>4</sup> E	2.126	2.211	2.190		
			LS	<sup>2</sup> E	2.032	2.103	2.102		
		C <sub>2</sub>	HS	<sup>4</sup> B	2.129 <sup>b</sup>	2.215 <sup>b</sup>	2.195 <sup>b</sup>	2.161 <sup>a</sup>	DOTZUH <sup>4</sup>
			LS	<sup>2</sup> A	1.958/2.204 <sup>c</sup>	2.016/2.324 <sup>c</sup>	2.021/2.276 <sup>c</sup>		
Ni <sup>3+</sup>	d <sup>7</sup>	D <sub>3</sub>	HS	<sup>4</sup> E	2.109	2.191	2.150		
			LS	<sup>2</sup> E	2.013	2.078	2.063		
		C <sub>2</sub>	HS	<sup>4</sup> B	2.111 <sup>b</sup>	2.190 <sup>b</sup>	2.149 <sup>b</sup>		
			LS	<sup>2</sup> A	1.952/2.148 <sup>c</sup>	2.007/2.231 <sup>c</sup>	2.002/2.173 <sup>c</sup>	1.971/2.109 <sup>c</sup>	DORTIN <sup>5</sup>

<sup>a</sup> Average of six similar bond lengths.

<sup>b</sup> Average of three pairs of similar bond lengths.

<sup>5</sup> Elongated octahedron – four short and two long bond distances

<sup>d</sup> Compressed octahedron – four long and two short bond lengths

## References

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Cartesian coordinates (Å)

49  
 Cr<sup>3+</sup> ^4A D\_3 LDA

5	Cr	0.000000	0.000000	0.000000
	N	0.025587	-1.573381	1.353695
	N	-1.375382	0.764532	1.353695
	N	1.349795	0.808849	1.353695
	C	1.085392	-1.376493	2.384648
10	C	2.080116	-0.345504	1.925793
	C	0.649382	1.628224	2.384648
	C	-0.740843	1.974185	1.925793
	C	-1.339273	-1.628681	1.925793
	C	-1.734774	-0.251731	2.384648
15	H	1.589945	-2.328759	2.616826
	H	-0.728747	2.753771	1.143506
	H	-1.336512	2.384791	2.761678
	H	-2.242989	1.062796	0.884846
	H	2.749209	-0.745772	1.143506
20	H	0.595598	-1.059298	3.319919
	H	-2.811737	-0.212553	-2.616826
	H	1.221792	2.541312	2.616826
	H	0.201086	-2.473884	0.884846
	H	-1.215178	0.013846	3.319919
25	H	2.733546	-0.034942	2.761678
	H	2.041903	1.411088	0.884846
	H	-1.397034	-2.349849	2.761678
	H	0.619580	1.045452	3.319919
	H	-2.020462	-2.007999	1.143506
30	N	-1.375382	-0.764532	-1.353695
	N	1.349795	-0.808849	-1.353695
	N	0.025587	1.573381	-1.353695
	C	-1.734774	0.251731	-2.384648
	C	-0.740843	-1.974185	-1.925793
35	H	-2.242989	-1.062796	-0.884846
	C	2.080116	0.345504	-1.925793
	C	0.649382	-1.628224	-2.384648
	H	2.041903	-1.411088	-0.884846
	C	-1.339273	1.628681	-1.925793
40	C	1.085392	1.376493	-2.384648
	H	0.201086	2.473884	-0.884846
	H	-2.811737	0.212553	-2.616826
	H	-1.215178	-0.013846	-3.319919
	H	-1.336512	-2.384791	-2.761678
45	H	-0.728747	-2.753771	-1.143506
	H	2.749209	0.745772	-1.143506
	H	2.733546	0.034942	-2.761678
	H	1.221792	-2.541312	-2.616826
	H	0.619580	-1.045452	-3.319919
50	H	-2.020462	2.007999	-1.143506
	H	-1.397034	2.349849	-2.761678
	H	1.589945	2.328759	-2.616826
	H	0.595598	1.059298	-3.319919

55 49  
 Cr<sup>3+</sup> ^2A D\_3 LDA

Cr	0.000000	0.000000	0.000000	
N	-0.040200	1.566100	1.339200	
N	1.376400	-0.748200	1.339200	
60	N	-1.336200	-0.817900	1.339200
	C	-1.099100	1.366500	2.372300
	C	-2.083100	0.325900	1.913400
	C	-0.633900	-1.635100	2.372300
	C	0.759300	-1.967000	1.913400
65	C	1.323800	1.641000	1.913400
	C	1.733000	0.268500	2.372300
	H	-1.610400	2.316000	2.601000
	H	0.756800	-2.747300	1.131800
	H	1.361800	-2.368200	2.749000
70	H	2.246600	-1.038200	0.868400
	H	-2.757600	0.718300	1.131800
	H	-0.606400	1.055600	3.308100

H	2.810900	0.236600	2.601000	
H	-1.200500	-2.552600	2.601000	
75	H	-0.224200	2.464700	0.868400
	H	1.217400	-0.002600	3.308100
	H	-2.731900	0.004800	2.749000
	H	-2.022400	-1.426500	0.868400
	H	1.370100	2.363500	2.749000
80	H	-0.611000	-1.053000	3.308100
	H	2.000800	2.029000	1.131800
	N	1.376400	0.748200	-1.339200
	N	-1.336200	0.817900	-1.339200
	N	-0.040200	-1.566100	-1.339200
85	C	1.733000	-0.268500	-2.372300
	C	0.759300	1.967000	-1.913400
	H	2.246600	1.038200	-0.868400
	C	-2.083100	-0.325900	-1.913400
	C	-0.633900	1.635100	-2.372300
90	H	-2.022400	1.426500	-0.868400
	C	1.323800	-1.641000	-1.913400
	C	-1.099100	-1.366500	-2.372300
	H	-0.224200	-2.464700	-0.868400
	H	2.810900	-0.236600	-2.601000
95	H	1.217400	0.002600	-3.308100
	H	1.361800	2.368200	-2.749000
	H	0.756800	2.747300	-1.131800
	H	-2.757600	-0.718300	-1.131800
	H	-2.731900	-0.004800	-2.749000
100	H	-1.200500	2.552600	-2.601000
	H	-0.611000	1.053000	-3.308100
	H	2.000800	-2.029000	-1.131800
	H	1.370100	-2.363500	-2.749000
	H	-1.610400	-2.316000	-2.601000
105	H	-0.606400	-1.055600	-3.308100

49  
 Cr<sup>3+</sup> ^2A D\_3 OPBE

Cr	0.000000	0.000000	0.000000	
110	N	0.040600	-1.577900	1.399700
	N	-1.386800	0.753800	1.399700
	N	1.346200	0.824100	1.399700
	C	1.120400	-1.390600	2.429300
	C	2.096600	-0.320900	1.989000
115	C	0.644100	1.665600	2.429300
	C	-0.770400	1.976200	1.989000
	C	-1.326200	-1.655300	1.989000
	C	-1.764500	-0.275000	2.429300
	H	1.646600	-2.336300	2.603500
120	H	-0.792100	2.762800	1.226700
	H	-1.363500	2.351600	2.834000
	H	-2.253500	1.054200	0.954300
	H	2.788700	-0.695400	1.226700
	H	0.649700	-1.126400	3.380200
125	H	-2.846600	-0.257800	2.603500
	H	1.200000	2.594200	2.603500
	H	0.213700	-2.478700	0.954300
	H	-1.300300	0.000600	3.380200
	H	2.718300	0.005000	2.834000
130	H	2.039700	1.424400	0.954300
	H	-1.354800	-2.356600	2.834000
	H	0.650700	1.125800	3.380200
	H	-1.996600	-2.067400	1.226700
	N	-1.386800	-0.753800	-1.399700
135	N	1.346200	-0.824100	-1.399700
	N	0.040600	1.577900	-1.399700
	C	-1.764500	0.275000	-2.429300
	C	-0.770400	-1.976200	-1.989000
	H	-2.253500	-1.054200	-0.954300
140	C	2.096600	0.320900	-1.989000
	C	0.644100	-1.665600	-2.429300
	H	2.039700	-1.424400	-0.954300
	C	-1.326200	1.655300	-1.989000
	C	1.120400	1.390600	-2.429300
145	H	0.213700	2.478700	-0.954300

H	-2.846600	0.257800	-2.603500	C	-0.656971	-1.641007	2.408460
H	-1.300300	-0.000600	-3.380200	75 C	0.744966	-1.977004	1.950719
H	-1.363500	-2.351600	-2.834000	C	1.339653	1.633661	1.950719
H	-0.792100	-2.762800	-1.226700	C	1.749640	0.251550	2.408460
5 H	2.788700	0.695400	-1.226700	H	-1.608663	2.327151	2.609756
H	2.718300	-0.005000	-2.834000	H	0.731773	-2.732521	1.164998
H	1.200000	-2.594200	-2.603500	80 H	1.323364	-2.387462	2.780401
H	0.650700	-1.125800	-3.380200	H	2.249161	-1.075906	0.946549
H	-1.996600	2.067400	-1.226700	H	-2.732319	0.732527	1.164998
10 H	-1.354800	2.356600	-2.834000	H	-0.624771	1.085522	3.341670
H	1.646600	2.336300	-2.603500	H	2.819704	0.229568	2.609756
H	0.649700	1.126400	-3.380200	85 H	-1.211041	-2.556719	2.609756
				H	-0.192819	2.485784	0.946549
49				H	1.252475	-0.001693	3.341670
15 Cr <sup>3+</sup> ^4A D_3 OPBE				H	-2.729285	0.047664	2.780401
Cr	0.000000	0.000000	0.000000	H	-2.056342	-1.409878	0.946549
N	0.031900	-1.580700	1.438000	90 H	1.405921	2.339798	2.780401
N	-1.384900	0.762800	1.438000	H	-0.627704	-1.083829	3.341670
N	1.353000	0.818000	1.438000	H	2.000547	1.999994	1.164998
20 C	1.111600	-1.396100	2.465100	N	1.390293	0.771165	-1.388060
C	2.094300	-0.333300	2.022300	N	-1.362995	0.818447	-1.388060
C	0.653200	1.660700	2.465100	95 N	-0.027298	-1.589612	-1.388060
C	-0.758500	1.980400	2.022300	C	1.749640	-0.251550	-2.408460
C	-1.335800	-1.647100	2.022300	C	0.744966	1.977004	-1.950719
25 C	-1.764900	-0.264600	2.465100	H	2.249161	1.075906	-0.946549
H	1.633300	-2.344000	2.641400	C	-2.084619	-0.343343	-1.950719
H	-0.771900	2.763900	1.256300	100 C	-0.656971	1.641007	-2.408460
H	-1.348600	2.365300	2.865100	H	-2.056342	1.409878	-0.946549
H	-2.248600	1.066500	0.989700	C	1.339653	-1.633661	-1.950719
30 H	2.779600	-0.713500	1.256300	C	-1.092669	-1.389457	-2.408460
H	0.643900	-1.126800	3.416100	H	-0.192819	-2.485784	-0.946549
H	-2.846600	-0.242500	2.641400	105 H	2.819704	-0.229568	-2.609756
H	1.213300	2.586500	2.641400	H	1.252475	0.001693	-3.341670
H	0.200600	-2.480600	0.989700	H	1.323364	2.387462	-2.780401
35 H	-1.297800	0.005800	3.416100	H	0.731773	2.732521	-1.164998
H	2.722700	-0.014700	2.865100	H	-2.732319	-0.732527	-1.164998
H	2.047900	1.414000	0.989700	110 H	-2.729285	-0.047664	-2.780401
H	-1.374100	-2.350500	2.865100	H	-1.211041	2.556719	-2.609756
H	0.653900	1.121100	3.416100	H	-0.627704	1.083829	-3.341670
40 H	-2.007700	-2.050400	1.256300	H	2.000547	-1.999994	-1.164998
N	-1.384900	-0.762800	-1.438000	H	1.405921	-2.339798	-2.780401
N	1.353000	-0.818000	-1.438000	115 H	-1.608663	-2.327151	-2.609756
N	0.031900	1.580700	-1.438000	H	-0.624771	-1.085522	-3.341670
C	-1.764900	0.264600	-2.465100				
45 C	-0.758500	-1.980400	-2.022300	49			
H	-2.248600	-1.066500	-0.989700	Cr <sup>3+</sup> ^2A D_3 SSB-D			
C	2.094300	0.333300	-2.022300	120 Cr	0.000000000	0.000000000	0.000000000
C	0.653200	-1.660700	-2.465100	N	0.040555789	-1.588299186	1.365819071
H	2.047900	-1.414000	-0.989700	N	-1.395785338	0.759027249	1.365819071
50 C	-1.335800	1.647100	-2.022300	N	1.355229549	0.829271937	1.365819071
C	1.111600	1.396100	-2.465100	C	1.105736918	-1.380848718	2.387134034
H	0.200600	2.480600	-0.989700	125 C	2.088335530	-0.324693149	1.931778558
H	-2.846600	0.242500	-2.641400	C	0.642981609	1.648020620	2.387134034
H	-1.297800	-0.005800	-3.416100	C	-0.762975249	1.970898196	1.931778558
55 H	-1.348600	-2.365300	-2.865100	C	-1.325360281	-1.646205046	1.931778558
H	-0.771900	-2.763900	-1.256300	C	-1.748718528	-0.267171902	2.387134034
H	2.779600	0.713500	-1.256300	130 H	1.629395118	-2.314656398	2.586330885
H	2.722700	0.014700	-2.865100	H	-0.760803070	2.729104037	1.148746296
H	1.213300	-2.586500	-2.641400	H	-1.344955436	2.371109037	2.763917808
60 H	0.653900	-1.121100	-3.416100	H	-2.258189198	1.057724616	0.926504477
H	-2.007700	2.050400	-1.256300	H	2.743874961	-0.705677232	1.148746296
H	-1.374100	2.350500	-2.865100	135 H	0.634409770	-1.082804587	3.320528201
H	1.633300	2.344000	-2.641400	H	-2.819248801	-0.253769366	2.586330885
H	0.643900	1.126800	-3.416100	H	1.189853683	2.568425764	2.586330885
65				H	0.213078211	-2.484511520	0.926504477
49				H	-1.254941164	-0.008012683	3.320528201
Cr <sup>3+</sup> ^4A D_3 SSB-D				140 H	2.725918380	-0.020788944	2.763917808
Cr	0.000000	0.000000	0.000000	H	2.045110986	1.426786904	0.926504477
N	-0.027298	1.589612	1.388060	H	-1.380962943	-2.350320093	2.763917808
70 N	1.390293	-0.771165	1.388060	H	0.620531395	1.090817270	3.320528201
N	-1.362995	-0.818447	1.388060	H	-1.983071891	-2.023426805	1.148746296
C	-1.092669	1.389457	2.408460	145 N	-1.395785338	-0.759027249	-1.365819071
C	-2.084619	0.343343	1.950719	N	1.355229549	-0.829271937	-1.365819071

N	0.040555789	1.588299186	-1.365819071	H	0.617400	1.041200	-3.251600
C	-1.748718528	0.267171902	-2.387134034	75			
C	-0.762975249	-1.970898196	-1.931778558		49		
H	-2.258189198	-1.057724616	-0.926504477		Mn <sup>2+</sup> ^6A_1 D_3 LDA		
5 C	2.088335530	0.324693149	-1.931778558		Mn	0.000000	0.000000
C	0.642981609	-1.648020620	-2.387134034		N	-1.513900	-0.622900
H	2.045110986	-1.426786904	-0.926504477	80	N	1.296400	-0.999700
C	-1.325360281	1.646205046	-1.931778558		N	0.217500	1.622600
C	1.105736918	1.380848718	-2.387134034		C	-1.692500	0.438200
10 H	0.213078211	2.484511520	-0.926504477		C	-1.141400	1.764700
H	-2.819248801	0.253769366	-2.586330885		C	1.225700	1.246600
H	-1.254941164	0.008012683	-3.320528201	85	C	2.099000	0.106100
H	-1.344955436	-2.371109037	-2.763917808		C	-0.957600	-1.870800
H	-0.760803070	-2.729104037	-1.148746296		C	0.466700	-1.684800
15 H	2.743874961	0.705677232	-1.148746296		H	-2.753700	0.565500
H	2.725918380	0.020788944	-2.763917808		H	2.766400	0.449200
H	1.189853683	-2.568425764	-2.586330885	90	H	2.751400	-0.214400
H	0.620531395	-1.090817270	-3.320528201		H	1.936900	-1.677400
H	-1.983071891	2.023426805	-1.148746296		H	-1.772200	2.171200
20 H	-1.380962943	2.350320093	-2.763917808		H	-1.189300	0.128100
H	1.629395118	2.314656398	-2.586330885		H	0.887100	-2.667500
H	0.634409770	1.082804587	-3.320528201	95	H	1.866600	2.102000
					H	-2.421100	-0.838800
					H	0.483700	-1.094000
					H	-1.190000	2.489900
					H	0.484200	2.516100
					100 H	-1.561300	-2.275600
					H	0.705600	0.965900
					H	-0.994200	-2.620400
					N	0.217500	-1.622600
					N	-1.513900	0.622900
					105 N	1.296400	0.999700
					C	1.225700	-1.246600
					C	-1.141400	-1.764700
					H	0.484200	-2.516100
					C	-0.957600	1.870800
					110 C	-1.692500	-0.438200
					H	-2.421100	0.838800
					C	2.099000	-0.106100
					C	0.466700	1.684800
					H	1.936900	1.677400
					115 H	1.866600	-2.102000
					H	0.705600	-0.965900
					H	-1.190000	-2.489900
					H	-1.772200	-2.171200
					H	-0.994200	2.620400
					120 H	-1.561300	2.275600
					H	-2.753700	-0.565500
					H	-1.189300	-0.128100
					H	2.766400	-0.449200
					H	2.751400	0.214400
					125 H	0.887100	2.667500
					H	0.483700	1.094000
					49		
					Mn <sup>2+</sup> ^2A_C_2 LDA		
					130 Mn	0.000000	0.000000
					N	-1.294700	-1.548800
					N	-1.281900	0.731800
					N	-1.285900	0.793700
					C	-2.323900	-1.376500
					135 C	-1.870800	-0.345100
					C	-2.304900	1.611900
					C	-1.847000	1.943300
					C	-1.882000	-1.635800
					C	-2.326100	-0.260600
					140 H	-2.556300	-2.328800
					H	-1.058700	2.717000
					H	-2.686100	2.358000
					H	-0.810200	1.028600
					H	-1.091400	-0.750600
					145 H	-3.261200	-1.055100
					H	-2.555500	-0.227400
49							
25 Mn <sup>2+</sup> ^2E_D_3 LDA							
Mn	0.000000	0.000000	0.000000				
N	-1.362000	-0.754200	1.284500				
N	1.334200	-0.802500	1.284500				
N	0.027900	1.556600	1.284500				
30 C	-1.729100	0.249000	2.315000				
C	-1.324600	1.625800	1.863700				
C	1.080200	1.372900	2.315000				
C	2.070300	0.334200	1.863700				
C	-0.745700	-1.960000	1.863700				
35 C	0.648900	-1.622000	2.315000				
H	-2.806200	0.216300	2.546800				
H	2.739700	0.734200	1.081900				
H	2.717300	0.026900	2.706600				
H	2.026800	-1.402300	0.813100				
40 H	-2.005700	2.005500	1.081900				
H	-1.210400	-0.014100	3.251600				
H	1.215800	-2.538400	2.546800				
H	1.590400	2.322100	2.546800				
H	-2.227900	-1.054100	0.813100				
45 H	0.617400	-1.041200	3.251600				
H	-1.382000	2.339800	2.706600				
H	0.201000	2.456400	0.813100				
H	-1.335300	-2.366700	2.706600				
H	0.593000	1.055300	3.251600				
50 H	-0.734000	-2.739700	1.081900				
N	0.027900	-1.556600	-1.284500				
N	-1.362000	0.754200	-1.284500				
N	1.334200	0.802500	-1.284500				
C	1.080200	-1.372900	-2.315000				
55 C	-1.324600	-1.625800	-1.863700				
H	0.201000	-2.456400	-0.813100				
C	-0.745700	1.960000	-1.863700				
C	-1.729100	-0.249000	-2.315000				
H	-2.227900	1.054100	-0.813100				
60 C	2.070300	-0.334200	-1.863700				
C	0.648900	1.622000	-2.315000				
H	2.026800	1.402300	-0.813100				
H	1.590400	-2.322100	-2.546800				
H	0.593000	-1.055300	-3.251600				
65 H	-1.382000	-2.339800	-2.706600				
H	-2.005700	-2.005500	-1.081900				
H	-0.734000	2.739700	-1.081900				
H	-1.335300	2.366700	-2.706600				
H	-2.806200	-0.216300	-2.546800				
70 H	-1.210400	0.014100	-3.251600				
H	2.739700	-0.734200	-1.081900				
H	2.717300	-0.026900	-2.706600				
H	1.215800	2.538400	-2.546800				

H	-2.537600	2.533600	1.204600	H	1.296600	-0.014900	-3.346200
H	-0.812700	-2.442300	0.201600	75 H	1.334000	-2.351100	-2.812300
H	-3.260400	0.012700	-1.216800	H	0.764300	-2.756800	-1.199000
H	-2.712900	-0.037000	2.724100	H	-2.769600	0.716500	-1.199000
5 H	-0.823300	1.394500	2.046400	H	-2.703100	0.020300	-2.812300
H	-2.728000	-2.347100	-1.369700	H	-1.221500	-2.577200	-2.568800
H	-3.243300	1.034300	0.612100	80 H	-0.661200	-1.115500	-3.346200
H	-1.102800	-2.022200	-2.002200	H	2.005300	2.040300	-1.199000
N	1.281900	-0.731800	-1.371500	H	1.369100	2.330800	-2.812300
10 N	1.285900	-0.793700	1.348700	H	-1.621200	2.346500	-2.568800
N	1.294700	1.548800	0.025300	H	-0.635400	1.130300	-3.346200
C	2.326100	0.260600	-1.734400	85			
C	1.847000	-1.943300	-0.750100	49			
H	0.810200	-1.028600	-2.237900	Mn <sup>2+</sup> ^6A_1 D_3 OPBE			
15 C	1.870800	0.345100	2.076300	Mn	0.000000	0.000000	0.000000
C	2.304900	-1.611900	0.646400	N	-0.190200	1.638500	-1.665900
H	0.823300	-1.394500	2.046400	90 N	1.514100	-0.654500	-1.665900
C	1.882000	1.635800	-1.322200	N	-1.323800	-0.984000	-1.665900
C	2.323900	1.376500	1.080500	C	-1.227700	1.293500	-2.666800
20 H	0.812700	2.442300	0.201600	C	-2.109900	0.136000	-2.219500
H	2.555500	0.227400	-2.811700	C	-0.506400	-1.710000	-2.666800
H	3.260400	-0.012700	-1.216800	95 C	0.937100	-1.895200	-2.219500
H	2.686100	-2.358000	-1.339100	C	1.172800	1.759200	-2.219500
H	1.058700	-2.717000	-0.739200	C	1.734100	0.416500	-2.666800
25 H	1.091400	0.750600	2.744900	H	-1.869800	2.157400	-2.876600
H	2.712900	0.037000	2.724100	H	0.992000	-2.656000	-1.430800
H	2.537600	-2.533600	1.204600	100 H	1.522400	-2.283100	-3.066400
H	3.243300	-1.034300	0.612100	H	2.418000	-0.903200	-1.274200
H	1.102800	2.022200	-2.002200	H	-2.796100	0.468900	-1.430800
30 H	2.728000	2.347100	-1.369700	H	-0.743000	1.054500	-3.618200
H	2.556300	2.328800	1.584800	H	2.803200	0.540600	-2.876600
H	3.261200	1.055100	0.597100	105 H	-0.933400	-2.698000	-2.876600
49				H	-0.426800	2.545600	-1.274200
35 Mn <sup>2+</sup> ^2E D_3 OPBE				H	1.284700	0.116200	-3.618200
Mn	0.000000	0.000000	0.000000	H	-2.738400	-0.176900	-3.066400
N	-0.025600	-1.565700	1.364900	H	-1.991200	-1.642500	-1.274200
N	1.368700	0.760700	1.364900	110 H	1.216000	2.460000	-3.066400
N	-1.343100	0.805000	1.364900	H	-0.541700	-1.170700	-3.618200
40 C	-1.098300	-1.399200	2.392200	H	1.804100	2.187100	-1.430800
C	-2.082000	-0.332400	1.960400	N	1.514100	0.654500	1.665900
C	-0.662600	1.650700	2.392200	N	-1.323800	0.984000	1.665900
C	0.753100	1.969300	1.960400	115 N	-0.190200	-1.638500	1.665900
C	1.328900	-1.636900	1.960400	C	1.734100	-0.416500	2.666800
45 C	1.760900	-0.251500	2.392200	C	0.937100	1.895200	2.219500
H	-1.621200	-2.346500	2.568800	H	2.418000	0.903200	1.274200
H	0.764300	2.756800	1.199000	C	-2.109900	-0.136000	2.219500
H	1.334000	2.351100	2.812300	120 C	-0.506400	1.710000	2.666800
H	2.227900	1.071300	0.916800	H	-1.991200	1.642500	1.274200
50 H	-2.769600	-0.716500	1.199000	C	1.172800	-1.759200	2.219500
H	-0.635400	-1.130300	3.346200	C	-1.227700	-1.293500	2.666800
H	2.842700	-0.230800	2.568800	H	-0.426800	-2.545600	1.274200
H	-1.221500	2.577200	2.568800	125 H	2.803200	-0.540600	2.876600
H	-0.186200	-2.465100	0.916800	H	1.284700	-0.116200	3.618200
55 H	1.296600	0.014900	3.346200	H	1.522400	2.283100	3.066400
H	-2.703100	-0.020300	2.812300	H	0.992000	2.656000	1.430800
H	-2.041700	1.393800	0.916800	H	-2.796100	-0.468900	1.430800
H	1.369100	-2.330800	2.812300	130 H	-2.738400	0.176900	3.066400
H	-0.661200	1.115500	3.346200	H	-0.933400	2.698000	2.876600
60 H	2.005300	-2.040300	1.199000	H	-0.541700	1.170700	3.618200
N	1.368700	-0.760700	-1.364900	H	1.804100	-2.187100	1.430800
N	-1.343100	-0.805000	-1.364900	H	1.216000	-2.460000	3.066400
N	-0.025600	1.565700	-1.364900	135 H	-1.869800	-2.157400	2.876600
C	1.760900	0.251500	-2.392200	H	-0.743000	-1.054500	3.618200
65 C	0.753100	-1.969300	-1.960400	49			
H	2.227900	-1.071300	-0.916800	Mn <sup>2+</sup> ^2A_ C_2 SSB-D			
C	-2.082000	0.332400	-1.960400	140 Mn	0.000000	0.000000	-0.002800
C	-0.662600	-1.650700	-2.392200	N	-1.403300	-1.533200	-0.022900
H	-2.041700	-1.393800	-0.916800	N	-1.352400	0.763500	1.380000
70 C	1.328900	1.636900	-1.960400	N	-1.359100	0.817900	-1.360000
C	-1.098300	1.399200	-2.392200	C	-2.427800	-1.363300	-1.096800
H	-0.186200	2.465100	-0.916800	145 C	-1.979900	-0.311400	-2.088400
H	2.842700	0.230800	-2.568800	C	-2.361000	1.678200	-0.660700

C	-1.915600	1.984700	0.755900	C	1.744757728	0.245114681	-2.373592846
C	-2.004400	-1.612400	1.328100	75 C	0.745633822	-1.965319182	-1.923956724
C	-2.406800	-0.222500	1.769100	H	2.238172867	-1.076200243	-0.917343098
H	-2.620200	-2.311700	-1.612200	C	-2.074833249	0.336921760	-1.923956724
5 H	-1.134800	2.753500	0.764200	C	-0.660103323	-1.633561856	-2.373592846
H	-2.756200	2.391000	1.336000	H	-2.051103183	-1.400214440	-0.917343098
H	-0.900600	1.066500	2.239600	80 C	1.329199428	1.628397423	-1.923956724
H	-1.228700	-0.713100	-2.776800	C	-1.084654405	1.388447175	-2.373592846
H	-3.377200	-1.075600	-0.635900	H	-0.187069684	2.476414682	-0.917343098
10 H	-2.578900	-0.200400	2.851400	H	2.814564630	0.229000134	-2.577346304
H	-2.524900	2.612300	-1.210900	H	1.249065066	-0.004057343	-3.309156337
H	-0.956000	-2.432200	-0.187500	85 H	1.314875206	-2.374667206	-2.762000098
H	-3.353500	0.068800	1.308400	H	0.730348819	-2.721924446	-1.140083377
H	-2.828300	0.014100	-2.707800	H	-2.722430127	0.728461592	-1.140083377
15 H	-0.912000	1.400000	-2.064500	H	-2.713959729	0.048618272	-2.762000098
H	-2.869700	-2.290300	1.360300	H	-1.208962381	-2.551984537	-2.577346304
H	-3.325200	1.161700	-0.654500	90 H	-0.628046295	-1.079693406	-3.309156337
H	-1.251000	-2.034400	2.001600	H	1.992081308	1.993462854	-1.140083377
N	1.352400	-0.763500	1.380000	H	1.399084524	2.326048934	-2.762000098
20 N	1.359100	-0.817900	-1.360000	H	-1.605602249	2.322984403	-2.577346304
N	1.403300	1.533200	-0.022900	H	-0.621018771	1.083750750	-3.309156337
C	2.406800	0.222500	1.769100	95			
C	1.915600	-1.984700	0.755900	49			
H	0.900600	-1.066500	2.239600	Mn <sup>2+</sup> ^6A_1 D_3 SSB-D			
25 C	1.979900	0.311400	-2.088400	Mn	0.000000000	0.000000000	0.000000000
C	2.361000	-1.678200	-0.860700	N	-0.270065245	-1.625807828	1.623012041
H	0.912000	-1.400000	-2.064500	100 N	1.543023503	0.579020551	1.623012041
C	2.004400	1.612400	1.328100	N	-1.272958259	1.046787277	1.623012041
C	2.427800	1.363300	-1.096800	C	-1.273140495	-1.219704896	2.620253128
30 H	0.956000	2.432200	-0.187500	C	-2.104614997	-0.035818520	2.159355850
H	2.578900	0.200400	2.851400	C	-0.419725178	1.712424460	2.620253128
H	3.353500	-0.068800	1.308400	105 C	1.021287750	1.840559312	2.159355850
H	2.756200	-2.391000	1.336000	C	1.083327247	-1.804740792	2.159355850
H	1.134800	-2.753500	0.764200	C	1.692865673	-0.492719563	2.620253128
35 H	1.228700	0.713100	-2.776800	H	-1.948975747	-2.041792648	2.852990324
H	2.828300	-0.014100	-2.707800	H	1.089992036	2.576910295	1.357019348
H	2.524900	-2.612300	-1.210900	110 H	1.619565159	2.214782236	2.994041483
H	3.325200	-1.161700	-0.654500	H	2.454123496	0.779360405	1.239882279
H	1.251000	2.034400	2.001600	H	-2.776665797	-0.344494354	1.357019348
40 H	2.869700	2.290300	1.360300	H	-0.770655202	-0.972566110	3.553181798
H	2.620200	2.311700	-1.612200	H	2.742732176	-0.666966184	2.852990324
H	3.377200	1.075600	-0.635900	115 H	-0.793756429	2.708758832	2.852990324
49				H	-0.552115838	-2.515013495	1.239882279
45 Mn <sup>2+</sup> ^2E D_3 SSB-D				H	1.227594559	-0.181123927	3.553181798
Mn	0.000000000	0.000000000	0.000000000	H	-2.727840260	0.295193453	2.994041483
N	-0.026152096	-1.578215754	1.353389783	H	-1.902007658	1.735653089	1.239882279
N	1.379850984	0.766459497	1.353389783	120 H	1.108275101	-2.509975689	2.994041483
N	-1.353698888	0.811756257	1.353389783	H	-0.456939357	1.153690037	3.553181798
50 C	-1.084654405	-1.388447175	2.373592846	H	1.686673761	-2.232415940	1.357019348
C	-2.074833249	-0.336921760	1.923956724	N	1.543023503	-0.579020551	-1.623012041
C	-0.660103323	1.633561856	2.373592846	N	-1.272958259	-1.046787277	-1.623012041
C	0.745633822	1.965319182	1.923956724	125 N	-0.270065245	1.625807828	-1.623012041
C	1.329199428	-1.628397423	1.923956724	C	1.692865673	0.492719563	-2.620253128
55 C	1.744757728	-0.245114681	2.373592846	C	1.021287750	-1.840559312	-2.159355850
H	-1.605602249	-2.322984403	2.577346304	H	2.454123496	-0.779360405	-1.239882279
H	0.730348819	2.721924446	1.140083377	C	-2.104614997	0.035818520	-2.159355850
H	1.314875206	2.374667206	2.762000098	130 C	-0.419725178	-1.712424460	-2.620253128
H	2.238172867	1.076200243	0.917343098	H	-1.902007658	-1.735653089	-1.239882279
60 H	-2.722430127	-0.728461592	1.140083377	C	1.083327247	1.804740792	-2.159355850
H	-0.621018771	-1.083750750	3.309156337	C	-1.273140495	1.219704896	-2.620253128
H	2.814564630	-0.229000134	2.577346304	H	-0.552115838	2.515013495	-1.239882279
H	-1.208962381	2.551984537	2.577346304	135 H	2.742732176	0.666966184	-2.852990324
H	-0.187069684	-2.476414682	0.917343098	H	1.227594559	0.181123927	-3.553181798
65 H	1.249065066	0.004057343	3.309156337	H	1.619565159	-2.214782236	-2.994041483
H	-2.713959729	-0.048618272	2.762000098	H	1.089992036	-2.576910295	-1.357019348
H	-2.051103183	1.400214440	0.917343098	H	-2.776665797	0.344494354	-1.357019348
H	1.399084524	-2.326048934	2.762000098	140 H	-2.727840260	-0.295193453	-2.994041483
H	-0.628046295	1.079693406	3.309156337	H	-0.793756429	-2.708758832	-2.852990324
70 H	1.992081308	-1.993462854	1.140083377	H	-0.456939357	-1.153690037	-1.357019348
N	1.379850984	-0.766459497	-1.353389783	H	1.686673761	2.232415940	-1.357019348
N	-1.353698888	-0.811756257	-1.353389783	145 H	1.108275101	2.509975689	-2.994041483
N	-0.026152096	1.578215754	-1.353389783	H	-1.948975747	2.041792648	-2.852990324
				H	-0.770655202	0.972566110	-3.553181798

49			H	-0.601996	1.059994	-3.222861
Mn <sup>2+</sup> ^2A_C_2 SSB-D			75 H	1.366028	-2.342832	-2.672694
Mn	0.000000000	0.000000000	H	2.204667	-1.023507	-0.746543
N	1.390822107	1.549038402	H	-2.711966	-0.011599	-2.672694
N	1.337999596	-0.769223406	H	1.218980	-0.008653	-3.222861
N	1.346767735	-0.823550797	H	-2.770651	0.716182	-1.065459
C	2.409408260	1.353098151	80 N	-1.316551	0.797204	1.247160
C	1.943325460	0.317966933	N	-0.032124	-1.538769	1.247160
C	2.340332715	-1.661734738	N	1.348675	0.741564	1.247160
10 C	1.875866861	-1.980656073	C	-0.637919	1.629125	2.284495
C	1.962928562	1.605830500	C	-2.078362	-0.328097	1.833096
C	2.383317479	0.216900621	85 H	-1.988716	1.397543	0.746543
H	2.632301919	2.287419655	C	1.323321	-1.635866	1.833096
H	1.072465847	-2.717066188	C	-1.091904	-1.367016	2.284495
15 H	2.701218474	-2.414532559	H	-0.215950	-2.421051	0.746543
H	0.895231643	-1.071545591	C	0.755041	1.963963	1.833096
H	1.169627548	0.728866826	90 C	1.729823	-0.262108	2.284495
H	3.338102371	1.028119109	H	2.204667	1.023507	0.746543
H	2.581450085	0.198108136	H	-1.220380	2.539903	2.500524
20 H	2.530218700	-2.588073609	H	-0.616984	1.051341	3.222861
H	0.957322409	2.447577161	H	-2.711966	0.011599	2.672694
H	3.314993797	-0.055171704	95 H	-2.770651	-0.716182	1.065459
H	2.777706901	0.016944868	H	2.005557	-2.041363	1.065459
H	0.910976343	-1.403842315	H	1.345938	-2.354431	2.672694
25 H	2.813677039	2.288665008	H	-1.589431	-2.326832	2.500524
H	3.287119933	-1.127823788	H	-0.601996	-1.059994	3.222861
H	1.184227710	1.988552779	100 H	0.765093	2.757545	1.065459
N	-1.337999596	0.769223406	H	1.366028	2.342832	2.672694
N	-1.346767735	0.823550797	H	2.809811	-0.213072	2.500524
30 N	-1.390822107	-1.549038402	H	1.218980	0.008653	3.222861
C	-2.383317479	-0.216900621				
C	-1.875866861	1.980656073				
H	-0.895231643	1.071545591	105 49			
C	-1.943325460	-0.317966933	Fe <sup>3+</sup> ^6A_1 D_3 LDA			
35 C	-2.340332715	1.661734738	Fe	0.000000	0.000000	0.000000
H	-0.910976343	1.403842315	N	-0.568972	-1.492907	-1.456769
C	-1.962928562	-1.605830500	N	-1.008409	1.239198	-1.456769
C	-2.409408260	-1.353098151	110 N	1.577382	0.253709	-1.456769
H	-0.957322409	-2.447577161	C	0.491546	-1.674657	-2.476347
40 H	-2.581450085	-0.198108136	C	1.796284	-1.100254	-1.993931
H	-3.314993797	0.055171704	C	1.204523	1.263020	-2.476347
H	-2.701218474	2.414532559	C	0.054705	2.105754	-1.993931
H	-1.072465847	2.717066188	115 C	-1.850990	-1.005501	-1.993931
H	-1.169627548	-0.728866826	C	-1.696068	0.411637	-2.476347
45 H	-2.777706901	-0.016944868	H	0.617853	-2.741728	-2.723687
H	-2.530218700	2.588073609	H	0.381901	2.785844	-1.186044
H	-3.287119933	1.127823788	H	-0.319437	2.749009	-2.812135
H	-1.184227710	-1.988552779	120 H	-1.714847	1.834481	-1.003711
H	-2.813677039	-2.288665008	H	2.221661	-1.723658	-1.186044
50 H	-2.632301919	-2.287419655	H	0.165676	-1.187034	-3.409294
H	-3.338102371	-1.028119109	H	-2.683332	0.835787	-2.723687
			H	2.065479	1.905940	-2.723687
			125 H	-0.731284	-2.402342	-1.003711
			H	-1.110840	0.450037	-3.409294
			H	2.540430	-1.097864	-2.812135
49			H	2.446131	0.567861	-1.003711
Fe <sup>3+</sup> ^2E D_3 LDA			H	-2.220993	-1.651145	-2.812135
55 Fe	0.000000	0.000000	130 H	0.945163	0.736997	-3.409294
N	-1.316551	-0.797204	H	-2.603563	-1.062186	-1.186044
N	-0.032124	1.538769	N	-0.568972	1.492907	1.456769
N	1.348675	-0.741564	N	-1.008409	-1.239198	1.456769
C	-0.637919	-1.629125	N	1.577382	-0.253709	1.456769
60 C	0.755041	-1.963963	135 C	0.491546	1.674657	2.476347
C	1.729823	0.262108	C	-1.850990	1.005501	1.993931
C	1.323321	1.635866	H	-0.731284	2.402342	1.003711
C	-2.078362	0.328097	C	0.054705	-2.105754	1.993931
C	-1.091904	1.367016	C	-1.696068	-0.411637	2.476347
65 H	-1.220380	-2.539903	140 H	-1.714847	-1.834481	1.003711
H	2.005557	2.041363	C	1.796284	1.100254	1.993931
H	1.345938	2.354431	C	1.204523	-1.263020	2.476347
H	-0.215950	2.421051	H	2.446131	-0.567861	1.003711
H	0.765093	-2.757545	H	0.617853	2.741728	2.723687
70 H	-0.616984	-1.051341	145 H	0.165676	1.187034	3.409294
H	-1.589431	2.326832	H	-2.220993	1.651145	2.812135
H	2.809811	0.213072				
H	-1.988716	-1.397543				

H	-2.603563	1.062186	1.186044	C	-1.699401	0.531153	-2.559195
H	0.381901	-2.785844	1.186044	75 H	0.458430	-2.814292	-2.751951
H	-0.319437	-2.749009	2.812135	H	0.535787	2.786770	-1.299606
H	-2.683332	-0.835787	2.723687	H	-0.146492	2.753833	-2.920240
5 H	-1.110840	-0.450037	3.409294	H	-1.584707	1.966675	-1.117825
H	2.221661	1.723658	1.186044	H	2.145520	-1.857390	-1.299606
H	2.540430	1.097864	2.812135	80 H	0.098395	-1.279640	-3.508281
H	2.065479	-1.905940	2.723687	H	-2.666463	1.010134	-2.751951
H	0.945163	-0.736997	3.409294	H	2.208033	1.804158	-2.751951
10				H	-0.910837	-2.355734	-1.117825
49				H	-1.157398	0.554607	-3.508281
Fe <sup>3+</sup> ^2A_ C_2 LDA				85 H	2.458135	-1.250051	-2.920240
Fe	0.000000	0.000000	-0.008500	H	2.495544	0.389059	-1.117825
N	-1.244300	-0.722200	1.355400	H	-2.311644	-1.503782	-2.920240
15 N	-1.251400	-0.790800	-1.330200	H	1.059003	0.725033	-3.508281
N	-1.259200	1.531500	-0.031300	H	-2.681307	-0.929380	-1.299606
C	-2.290000	0.272300	1.735600	90 N	-0.670256	1.462411	1.543335
C	-1.844300	1.643900	1.321200	N	-0.931357	-1.311664	1.543335
C	-2.295900	1.367800	-1.091000	N	1.601613	-0.150747	1.543335
20 C	-1.844100	0.335700	-2.083300	C	0.389708	1.737301	2.559195
C	-1.820700	-1.949800	0.757800	C	-1.924052	0.892884	2.093012
C	-2.280000	-1.621800	-0.635600	95 H	-0.910837	2.355734	1.117825
H	-2.502000	0.223400	2.816300	C	0.188765	-2.112720	2.093012
H	-1.078900	0.729200	-2.775200	C	-1.699401	-0.531153	2.559195
25 H	-2.684200	-0.004100	-2.716400	H	-1.584707	-1.966675	1.117825
H	-0.757000	-1.391500	-2.006500	C	1.735286	1.219835	2.093012
H	-1.074500	2.052700	1.999100	100 C	1.309693	-1.206148	2.559195
H	-3.227900	-0.005700	1.227800	H	2.495544	-0.389059	1.117825
H	-2.497200	-2.537400	-1.210100	H	0.458430	2.814292	2.751951
30 H	-2.514800	2.329600	-1.583400	H	0.098395	1.279640	3.508281
H	-0.740800	-1.003500	2.209500	H	-2.311644	1.503782	2.920240
H	-3.219800	-1.046500	-0.611900	105 H	-2.681307	0.929380	1.299606
H	-2.684600	2.361600	1.341200	H	0.535787	-2.786770	1.299606
H	-0.750100	2.408000	-0.220500	H	-0.146492	-2.753833	2.920240
35 H	-2.656100	-2.335200	1.370600	H	-2.666463	-1.010134	2.751951
H	-3.233600	1.056800	-0.602300	H	-1.157398	-0.554607	3.508281
H	-1.047100	-2.737900	0.767400	110 H	2.145520	1.857390	1.299606
N	1.259200	-1.531500	-0.031300	H	2.458135	1.250051	2.920240
N	1.244300	0.722200	1.355400	H	2.208033	-1.804158	2.751951
40 N	1.251400	0.790800	-1.330200	H	1.059003	-0.725033	3.508281
C	2.295900	-1.367800	-1.091000	115			
C	1.844300	-1.643900	1.321200	49			
H	0.750100	-2.408000	-0.220500	Fe <sup>3+</sup> ^2E D_3 OPBE			
C	1.820700	1.949800	0.757800	Fe	0.000000	0.000000	0.000000
45 C	2.290000	-0.272300	1.735600	N	1.316100	-0.749600	-1.353900
H	0.740800	1.003500	2.209500	C	1.914400	-1.975400	-0.758100
C	1.844100	-0.335700	-2.083300	120 C	2.349800	0.263100	-1.762000
C	2.280000	1.621800	-0.635600	H	0.835900	-1.041900	-2.203600
H	0.757000	1.391500	-2.006500	H	1.163000	-2.771800	-0.786200
50 H	2.514800	-2.329600	-1.583400	H	2.760500	-2.333400	-1.360200
H	3.233600	-1.056800	-0.602300	H	2.510400	0.224300	-2.845600
H	2.684600	-2.361600	1.341200	125 H	3.303100	-0.009900	-1.301500
H	1.074500	-2.052700	1.999100	N	1.316100	-0.797700	1.326100
H	1.047100	2.737900	0.767400	N	1.316100	1.547300	0.027800
55 H	2.656100	2.335200	1.370600	N	-1.316100	0.797700	1.326100
H	2.502000	-0.223400	2.816300	N	-1.316100	-1.547300	0.027800
H	3.227900	0.005700	1.227800	130 N	-1.316100	0.749600	-1.353900
H	1.078900	-0.729200	-2.775200	C	2.349800	-1.657500	0.653100
H	2.684200	0.004100	-2.716400	C	1.914400	1.644300	-1.331700
60 H	2.497200	2.537400	-1.210100	C	1.914400	0.331200	2.089800
H	3.219800	1.046500	-0.611900	H	0.835900	-1.387500	2.004200
49				135 C	2.349800	1.394300	1.108900
Fe <sup>3+</sup> ^6A_1 D_3 OPBE				H	0.835900	2.429400	0.199500
65 Fe	0.000000	0.000000	0.000000	C	-1.914400	-0.331200	2.089800
N	-0.670256	-1.462411	-1.543335	C	-2.349800	1.657500	0.653100
N	-0.931357	1.311664	-1.543335	H	-0.835900	1.387500	2.004200
N	1.601613	0.150747	-1.543335	140 C	-1.914400	-1.644300	-1.331700
C	0.389708	-1.737301	-2.559195	C	-2.349800	-1.394300	1.108900
70 C	1.735286	-1.219835	-2.093012	H	-0.835900	-2.429400	0.199500
C	1.309693	1.206148	-2.559195	C	-1.914400	1.975400	-0.758100
C	0.188765	2.112720	-2.093012	C	-2.349800	-0.263100	-1.762000
C	-1.924052	-0.892884	-2.093012	145 H	-0.835900	1.041900	-2.203600
				H	2.510400	-2.576600	1.228600

H	3.303100	-1.122100	0.659400
H	1.163000	2.066800	-2.007300
H	2.760500	2.344700	-1.340700
H	1.163000	0.705000	2.793500
5 H	2.760500	-0.011300	2.700900
H	2.510400	2.352200	1.617100
H	3.303100	1.132100	0.642100
H	-1.163000	-0.705000	2.793500
H	-2.760500	0.011300	2.700900
10 H	-2.510400	2.576600	1.228600
H	-3.303100	1.122100	0.659400
H	-1.163000	-2.066800	-2.007300
H	-2.760500	-2.344700	-1.340700
H	-2.510400	-2.352200	1.617100
15 H	-3.303100	-1.132100	0.642100
H	-1.163000	2.771800	-0.786200
H	-2.760500	2.333400	-1.360200
H	-2.510400	-0.224300	-2.845600
H	-3.303100	0.009900	-1.301500
20			
49			
Fe <sup>3+</sup> ^2A_C_2 OPBE			
Fe	0.000000	0.000000	0.003600
N	-1.303400	0.745200	-1.366400
25 N	-1.308600	0.808000	1.339200
N	-1.349100	-1.519700	0.027800
C	-2.358100	-0.245900	-1.771800
C	-1.947300	-1.629300	-1.328800
C	-2.380600	-1.361100	1.108300
30 C	-1.930200	-0.311100	2.095800
C	-1.875100	1.982800	-0.765100
C	-2.321500	1.679100	0.647700
H	-2.512700	-0.209600	-2.856300
H	-1.187800	-0.700800	2.800100
35 H	-2.772600	0.044200	2.704700
H	-0.828400	1.392600	2.021600
H	-1.200200	-2.068200	-1.998400
H	-3.307700	0.048700	-1.317000
H	-2.470600	2.606200	1.213300
40 H	-2.557500	-2.319500	1.610100
H	-0.819300	1.030200	-2.216100
H	-3.283900	1.160600	0.651900
H	-2.803700	-2.317000	-1.331800
H	-0.869000	-2.400600	0.207900
45 H	-2.712900	2.359600	-1.367400
H	-3.328900	-1.081200	0.641800
H	-1.107700	2.764000	-0.793400
N	1.349100	1.519700	0.027800
N	1.303400	-0.745200	-1.366400
50 N	1.308600	-0.808000	1.339200
C	2.380600	1.361100	1.108300
C	1.947300	1.629300	-1.328800
H	0.869000	2.400600	0.207900
C	1.875100	-1.982800	-0.765100
55 C	2.358100	0.245900	-1.771800
H	0.819300	-1.030200	-2.216100
C	1.930200	0.311100	2.095800
C	2.321500	-1.679100	0.647700
H	0.828400	-1.392600	2.021600
60 H	2.557500	2.319500	1.610100
H	3.328900	1.081200	0.641800
H	2.803700	2.317000	-1.331800
H	1.200200	2.068200	-1.998400
H	1.107700	-2.764000	-0.793400
65 H	2.712900	-2.359600	-1.367400
H	2.512700	0.209600	-2.856300
H	3.307700	-0.048700	-1.317000
H	1.187800	0.700800	2.800100
H	2.772600	-0.044200	2.704700
70 H	2.470600	-2.606200	1.213300
H	3.283900	-1.160600	0.651900

49			
75 Fe <sup>3+</sup> ^6A_1 D_3 SSB-D			
Fe	0.000000000	0.000000000	0.000000000
N	1.582152584	0.299407432	-1.483673558
C	1.832148444	-1.049272873	-2.022479681
C	1.185309149	1.307892373	-2.494853986
80 H	2.440910344	0.618359034	-1.054562788
H	2.275728486	-1.642381648	-1.221021419
H	2.553076458	-1.024804250	-2.842016317
H	2.014173486	1.982515679	-2.704272222
H	0.956561933	0.799007819	-3.427864258
85 N	-0.531781850	-1.519888046	-1.483673558
N	-1.050370734	1.220480615	-1.483673558
N	-0.531781850	1.519888046	1.483673558
N	-1.050370734	-1.220480615	1.483673558
N	1.582152584	-0.299407432	1.483673558
90 C	0.540013446	-1.680454021	-2.494853986
C	-0.007377259	2.111323532	-2.022479681
C	-1.824771185	-1.062050659	-2.022479681
H	-0.684940540	-2.423069883	-1.054562788
C	-1.725322595	0.372561648	-2.494853986
95 H	-1.755969804	1.804710849	-1.054562788
C	-1.824771185	1.062050659	2.022479681
C	0.540013446	1.680454021	2.494853986
H	-0.684940540	2.423069883	1.054562788
C	-0.007377259	-2.111323532	2.022479681
100 C	-1.725322595	-0.372561648	2.494853986
H	-1.755969804	-1.804710849	1.054562788
C	1.832148444	1.049272873	2.022479681
C	1.185309149	-1.307892373	2.494853986
H	2.440910344	-0.618359034	1.054562788
105 H	0.709822199	-2.735583246	-2.704272222
H	0.213680103	-1.227910843	-3.427864258
H	0.284479987	2.792029505	-1.221021419
H	-0.389031715	2.723431195	-2.842016317
H	-2.560208473	-1.149647857	-1.221021419
110 H	-2.164044743	-1.698626945	-2.842016317
H	-2.723995685	0.753067567	-2.704272222
H	-1.170242035	0.428903025	-3.427864258
H	-2.560208473	1.149647857	1.221021419
H	-2.164044743	1.698626945	2.842016317
115 H	0.709822199	2.735583246	2.704272222
H	0.213680103	1.227910843	3.427864258
H	0.284479987	-2.792029505	1.221021419
H	-0.389031715	-2.723431195	2.842016317
H	-2.723995685	-0.753067567	2.704272222
120 H	-1.170242035	-0.428903025	3.427864258
H	2.275728486	1.642381648	1.221021419
H	2.553076458	1.024804250	2.842016317
H	2.014173486	-1.982515679	2.704272222
H	0.956561933	-0.799007819	3.427864258
125			
49			
Fe <sup>3+</sup> ^2E D_3 SSB-D			
Fe	0.0000000	0.0000000	0.0000000
N	-1.367916	-0.747407	1.289136
130 C	-0.762585	-1.966890	1.863380
C	-1.746577	0.266165	2.313418
H	-2.215962	-1.033534	0.814988
H	-0.772457	-2.734468	1.090635
H	-1.355163	-2.346811	2.697588
135 H	-2.819549	0.237679	2.497677
H	-1.259741	0.007462	3.250302
N	1.331232	-0.810947	1.289136
N	0.036685	1.558354	1.289136
N	1.331232	0.810947	-1.289136
140 N	0.036685	-1.558354	-1.289136
N	-1.367916	0.747407	-1.289136
C	0.642783	-1.645662	2.313418
C	-1.322085	1.643863	1.863380
C	2.084669	0.323027	1.863380
145 H	2.003048	-1.402312	0.814988
C	1.103794	1.379497	2.313418



C	-1.078103	1.373916	-2.276747	H	-0.974152	1.459432	2.108974
H	-1.228630	-2.532274	-2.499135	75 C	2.245047	1.310411	-1.306163
H	2.007047	2.012047	-1.053695	C	2.177404	1.806806	1.104836
H	1.369662	2.337628	-2.673179	H	2.712877	0.039743	0.211985
5 H	-0.200141	2.420750	-0.747002	C	-1.109229	2.593200	-0.707473
H	0.738961	-2.744177	-1.053695	C	1.119522	2.237711	-1.698889
H	-0.621254	-1.044467	-3.216420	80 H	-0.644131	1.335250	-2.240273
H	-1.578699	2.330162	-2.499135	H	-1.393405	3.471853	1.231406
H	2.807329	0.202112	-2.499135	H	0.259872	3.558065	0.647438
10 H	-1.996360	-1.383702	-0.747002	H	1.107768	2.612336	2.783627
H	-0.593908	1.060255	-3.216420	H	1.134270	0.840356	2.726848
H	1.339615	-2.354976	-2.673179	85 H	2.282271	0.443959	-1.989292
H	2.196502	-1.037048	-0.747002	H	3.209468	1.842974	-1.413056
H	-2.709276	0.017347	-2.673179	H	3.137109	1.708696	1.638348
15 H	1.215161	-0.015788	-3.216420	H	2.207374	2.801601	0.629479
H	-2.746007	0.732129	-1.053695	H	-2.103993	2.114449	-0.670288
N	-1.318417	0.787508	1.242263	90 H	-1.232917	3.538378	-1.268830
N	-0.022794	-1.535536	1.242263	H	1.203020	2.486513	-2.769445
N	1.341210	0.748029	1.242263	H	1.217805	3.197631	-1.165013
20 C	-0.650794	1.620623	2.276747				
C	-2.068320	-0.334516	1.829627	49			
H	-1.996360	1.383702	0.747002	95 Fe <sup>2+</sup> ^5E D_3 OPBE			
C	1.323860	-1.623960	1.829627	Fe	0.000000	0.000000	0.000000
C	-1.078103	-1.373916	2.276747	N	-1.366360	-0.910271	-1.549677
25 H	-0.200141	-2.420750	0.747002	N	-0.105137	1.638438	-1.549677
C	0.744460	1.958476	1.829627	N	1.471497	-0.728167	-1.549677
C	1.728898	-0.246707	2.276747	100 C	-0.592573	-1.682467	-2.552706
H	2.196502	1.037048	0.747002	C	0.840954	-1.938690	-2.112080
H	-1.228630	2.532274	2.499135	C	1.753346	0.328050	-2.552706
30 H	-0.621254	1.044467	3.216420	C	1.258478	1.697632	-2.112080
H	-2.709276	-0.017347	2.673179	C	-2.099431	0.241058	-2.112080
H	-2.746007	-0.732129	1.053695	105 C	-1.160773	1.354417	-2.552706
H	2.007047	-2.012047	1.053695	H	-1.073058	-2.647372	-2.753973
H	1.369662	-2.337628	2.673179	H	1.913451	2.104964	-1.332451
35 H	-1.578699	-2.330162	2.499135	H	1.321329	2.389759	-2.964812
H	-0.593908	-1.060255	3.216420	H	-0.294477	2.553744	-1.151476
H	0.738961	2.744177	1.053695	110 H	0.866227	-2.709580	-1.332451
H	1.339615	2.354976	2.673179	H	-0.605971	-1.143844	-3.505304
H	2.807329	-0.202112	2.499135	H	-1.756162	2.252982	-2.753973
40 H	1.215161	0.015788	3.216420	H	2.829220	0.394390	-2.753973
				H	-2.064369	-1.531897	-1.151476
49				115 H	-0.687612	1.096709	-3.505304
Fe <sup>2+</sup> ^5B C_2 LDA				H	1.408928	-2.339184	-2.964812
Fe	0.000000	0.000000	0.027541	H	2.358846	-1.021848	-1.151476
45 N	0.251077	-1.672332	1.414291	H	-2.730256	-0.050575	-2.964812
N	-2.035673	-0.791569	0.047513	H	1.293584	0.047135	-3.505304
N	0.196569	-1.661616	-1.377667	120 H	-2.779678	0.604615	-1.332451
C	0.623101	-2.898687	0.690159	N	-1.366360	0.910271	1.549677
C	1.109229	-2.593200	-0.707473	N	-0.105137	-1.638438	1.549677
50 C	-1.119522	-2.237711	-1.698889	N	1.471497	0.728167	1.549677
C	-2.245047	-1.310411	-1.306163	C	-0.592573	1.682467	2.552706
C	-1.042949	-1.744744	2.099745	125 C	-2.099431	-0.241058	2.112080
C	-2.177404	-1.806806	1.104836	H	-2.064369	1.531897	1.151476
H	1.393405	-3.471853	1.231406	C	1.258478	-1.697632	2.112080
55 H	-2.282271	-0.443959	-1.989292	C	-1.160773	-1.354417	2.552706
H	-3.209468	-1.842974	-1.413056	H	-0.294477	-2.553744	1.151476
H	-2.712877	-0.039743	0.211985	130 C	0.840954	1.938690	2.112080
H	2.103993	-2.114449	-0.670288	C	1.753346	-0.328050	2.552706
H	-0.259872	-3.558065	0.647438	H	2.358846	1.021848	1.151476
60 H	-3.137109	-1.708696	1.638348	H	-1.073058	2.647372	2.753973
H	-1.203020	-2.486513	-2.769445	H	-0.605971	1.143844	3.505304
H	0.974152	-1.459432	2.108974	135 H	-2.730256	0.050575	2.964812
H	-2.207374	-2.801601	0.629479	H	-2.779678	-0.604615	1.332451
H	1.232917	-3.538378	-1.268830	H	1.913451	-2.104964	1.332451
65 H	0.644131	-1.335250	-2.240273	H	1.321329	-2.389759	2.964812
H	-1.107768	-2.612336	2.783627	H	-1.756162	-2.252982	2.753973
H	-1.217805	-3.197631	-1.165013	140 H	-0.687612	-1.096709	3.505304
H	-1.134270	-0.840356	2.726848	H	0.866227	2.709580	1.332451
N	-0.251077	1.672332	1.414291	H	1.408928	2.339184	2.964812
70 N	2.035673	0.791569	0.047513	H	2.829220	-0.394390	2.753973
N	-0.196569	1.661616	-1.377667	H	1.293584	-0.047135	3.505304
C	-0.623101	2.898687	0.690159				
C	1.042949	1.744744	2.099745	145			

49  
 Fe<sup>2+</sup> ^1A\_1 D\_3 OPBE

Fe	0.000000	0.000000	0.000000
N	-1.329702	-0.790700	-1.313255
5 N	-0.019915	1.546906	-1.313255
N	1.349617	-0.756206	-1.313255
C	-0.666308	-1.649739	-2.342765
C	0.750069	-1.968038	-1.916350
C	1.761870	0.247830	-2.342765
10 C	1.329336	1.633598	-1.916350
C	-2.079405	0.334440	-1.916350
C	-1.095562	1.401909	-2.342765
H	-1.234505	-2.572450	-2.508428
H	2.007577	2.046522	-1.162076
15 H	1.358524	2.324947	-2.770732
H	-0.182216	2.433497	-0.842366
H	0.768552	-2.761873	-1.162076
H	-0.668315	-1.119456	-3.299588
H	-1.610554	2.355338	-2.508428
20 H	2.845060	0.217111	-2.508428
H	-2.016362	-1.374552	-0.842366
H	-0.635320	1.138505	-3.299588
H	1.334201	-2.338989	-2.770732
H	2.198578	-1.058945	-0.842366
25 H	-2.692725	0.014043	-2.770732
H	1.303635	-0.019050	-3.299588
H	-2.776128	0.715351	-1.162076
N	-1.329702	0.790700	1.313255
N	-0.019915	-1.546906	1.313255
30 N	1.349617	0.756206	1.313255
C	-0.666308	1.649739	2.342765
C	-2.079405	-0.334440	1.916350
H	-2.016362	1.374552	0.842366
C	1.329336	-1.633598	1.916350
35 C	-1.095562	-1.401909	2.342765
H	-0.182216	-2.433497	0.842366
C	0.750069	1.968038	1.916350
C	1.761870	-0.247830	2.342765
H	2.198578	1.058945	0.842366
40 H	-1.234505	2.572450	2.508428
H	-0.668315	1.119456	3.299588
H	-2.692725	-0.014043	2.770732
H	-2.776128	-0.715351	1.162076
H	2.007577	-2.046522	1.162076
45 H	1.358524	-2.324947	2.770732
H	-1.610554	-2.355338	2.508428
H	-0.635320	-1.138505	3.299588
H	0.768552	2.761873	1.162076
H	1.334201	2.338989	2.770732
50 H	2.845060	-0.217111	2.508428
H	1.303635	0.019050	3.299588

49  
 Fe<sup>2+</sup> ^5B C\_2 OPBE

55 Fe	0.000000	0.000000	0.043749
N	0.249722	-1.812534	1.398767
N	-2.088876	-0.898074	0.101423
N	0.124077	-1.750101	-1.414138
C	0.625302	-3.032946	0.643262
60 C	1.047942	-2.712001	-0.783152
C	-1.211870	-2.310940	-1.732140
C	-2.338713	-1.404350	-1.260860
C	-1.033908	-1.914221	2.120149
C	-2.215954	-1.927487	1.162161
65 H	1.441458	-3.567029	1.143981
H	-2.423166	-0.531794	-1.919112
H	-3.292133	-1.947972	-1.337879
H	-2.783990	-0.179855	0.282611
H	2.045407	-2.256190	-0.789862
70 H	-0.221207	-3.726128	0.641146
H	-3.138484	-1.785960	1.737736
H	-1.318447	-2.479522	-2.810360
H	0.969930	-1.645457	2.095501

H	-2.312284	-2.911930	0.694366
75 H	1.129052	-3.648066	-1.354841
H	0.554370	-1.454555	-2.285472
H	-1.079955	-2.806715	2.761351
H	-1.302528	-3.299384	-1.271697
H	-1.098225	-1.047356	2.788535
80 N	-0.249722	1.812534	1.398767
N	2.088876	0.898074	0.101423
N	-0.124077	1.750101	-1.414138
C	-0.625302	3.032946	0.643262
C	1.033908	1.914221	2.120149
85 H	-0.969930	1.645457	2.095501
C	2.338713	1.404350	-1.260860
C	2.215954	1.927487	1.162161
H	2.783990	0.179855	0.282611
C	-1.047942	2.712001	-0.783152
90 C	1.211870	2.310940	-1.732140
H	-0.554370	1.454555	-2.285472
H	-1.441458	3.567029	1.143981
H	0.221207	3.726128	0.641146
H	1.079955	2.806715	2.761351
95 H	1.098225	1.047356	2.788535
H	2.423166	0.531794	-1.919112
H	3.292133	1.947972	-1.337879
H	3.138484	1.785960	1.737736
H	2.312284	2.911930	0.694366
100 H	-2.045407	2.256190	-0.789862
H	-1.129052	3.648066	-1.354841
H	1.318447	2.479522	-2.810360
H	1.302528	3.299384	-1.271697

105 49  
 Fe<sup>2+</sup> ^5E D\_3 SSB-D

Fe	0.000000000	0.000000000	0.000000000
N	1.497829299	-0.672499091	-1.518182675
N	-1.331315947	-0.960908678	-1.518182675
110 N	-0.166513353	1.633407769	-1.518182675
C	1.722219400	0.386473464	-2.516745967
C	1.193480509	1.734562881	-2.059487189
C	-1.195805538	1.298249019	-2.516745967
C	-2.098915773	0.166302999	-2.059487189
115 C	0.905435265	-1.900865880	-2.059487189
C	-0.526413862	-1.684722483	-2.516745967
H	2.782530585	0.491529101	-2.743100717
H	-2.756887215	0.512358760	-1.261239103
H	-2.734452894	-0.132441860	-2.896703097
120 H	-1.999230461	-1.607026597	-1.126035165
H	1.822159310	2.131354984	-1.261239103
H	1.242063523	0.102695668	-3.450852858
H	-0.965588604	-2.655506724	-2.743100717
H	-1.816941981	2.163977623	-2.743100717
125 H	2.391341088	-0.927871069	-1.126035165
H	-0.532094704	-1.127006398	-3.450852858
H	1.252528432	2.434326602	-2.896703097
H	-0.392110627	2.534897666	-1.126035165
H	1.481924463	-2.301884742	-2.896703097
130 H	-0.709968819	1.024310730	-3.450852858
H	0.934727905	-2.643713744	-1.261239103
N	-0.166513353	-1.633407769	1.518182675
N	1.497829299	0.672499091	1.518182675
N	-1.331315947	0.960908678	1.518182675
135 C	-1.195805538	-1.298249019	2.516745967
C	1.193480509	-1.734562881	2.059487189
C	-0.392110627	-2.534897666	1.126035165
C	0.905435265	1.900865880	2.059487189
C	1.722219400	-0.386473464	2.516745967
140 H	2.391341088	0.927871069	1.126035165
C	-2.098915773	-0.166302999	2.059487189
C	-0.526413862	1.684722483	2.516745967
H	-1.999230461	1.607026597	1.126035165
H	-1.816941981	-2.163977623	2.743100717
145 H	-0.709968819	-1.024310730	3.450852858
H	1.252528432	-2.434326602	2.896703097

H	1.822159310	-2.131354984	1.261239103
H	0.934727905	2.643713744	1.261239103
H	1.481924463	2.301884742	2.896703097
H	2.782530585	-0.491529101	2.743100717
5 H	1.242063523	-0.102695668	3.450852858
H	-2.756887215	-0.512358760	1.261239103
H	-2.734452894	0.132441860	2.896703097
H	-0.965588604	2.655506724	2.743100717
H	-0.532094704	1.127006398	3.450852858

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Fe<sup>2+</sup> ^1A\_1 D\_3 SSB-D

Fe	0.000000000	0.000000000	0.000000000
N	-0.016345400	-1.561806640	1.306357864
15 N	1.360736926	0.766747788	1.306357864
N	-1.344391526	0.795058852	1.306357864
C	-1.078102262	-1.393781027	2.328673094
C	-2.072230642	-0.345375937	1.882925116
C	-0.667998646	1.630554460	2.328673094
20 C	0.737010986	1.967292347	1.882925116
C	1.335219656	-1.621916410	1.882925116
C	1.746100907	-0.236773433	2.328673094
H	-1.588360364	-2.335803231	2.524223394
H	0.724771638	2.728163342	1.103502082
25 H	1.308740805	2.370565558	2.722061403
H	2.209949591	1.071130409	0.849947145
H	-2.725044579	-0.736411020	1.103502082
H	-0.617783043	-1.091065219	3.266572420
H	2.817045118	-0.207658810	2.524223394
30 H	-1.228684755	2.543462041	2.524223394
H	-0.177348650	-2.449437692	0.849947145
H	1.253781719	0.010516800	3.266572420
H	-2.707340397	-0.051879995	2.722061403
H	-2.032600941	1.378307282	0.849947145
35 H	1.398599592	-2.318685563	2.722061403
H	-0.635998675	1.080548419	3.266572420
H	2.000272941	-1.991752322	1.103502082
N	1.360736926	-0.766747788	-1.306357864
N	-1.344391526	-0.795058852	-1.306357864
40 N	-0.016345400	1.561806640	-1.306357864
C	1.746100907	0.236773433	-2.328673094
C	0.737010986	-1.967292347	-1.882925116
H	2.209949591	-1.071130409	-0.849947145
C	-2.072230642	0.345375937	-1.882925116
45 C	-0.667998646	-1.630554460	-2.328673094
H	-2.032600941	-1.378307282	-0.849947145
C	1.335219656	1.621916410	-1.882925116
C	-1.078102262	1.393781027	-2.328673094
H	-0.177348650	2.449437692	-0.849947145
50 H	2.817045118	0.207658810	-2.524223394
H	1.253781719	-0.010516800	-3.266572420
H	1.308740805	-2.370565558	-2.722061403
H	0.724771638	-2.728163342	-1.103502082
H	-2.725044579	0.736411020	-1.103502082
55 H	-2.707340397	0.051879995	-2.722061403
H	-1.228684755	-2.543462041	-2.524223394
H	-0.635998675	-1.080548419	-3.266572420
H	2.000272941	1.991752322	-1.103502082
H	1.398599592	2.318685563	-2.722061403
60 H	-1.588360364	2.335803231	-2.524223394
H	-0.617783043	1.091065219	-3.266572420

49

Fe<sup>2+</sup> ^5B\_C\_2 SSB-D

65 Fe	0.000000000	0.000000000	0.103686655
N	1.600591416	0.916369765	1.375427934
N	1.554872471	-1.632610027	0.145351116
N	1.491644163	0.710110379	-1.427616568
C	2.572205790	1.670403277	0.564694405
70 C	2.057302770	1.927870354	-0.839837941
C	2.481152086	-0.334995255	-1.737966594
C	2.049246520	-1.699893302	-1.232912402
C	2.167001028	-0.228599301	2.097346123

C	2.591411239	-1.334196927	1.148162153
75 H	2.814272711	2.624760950	1.030380894
H	1.229690277	-2.081626553	-1.842342774
H	2.887426928	-2.393056918	-1.343297886
H	1.158579744	-2.534043951	0.363027896
H	1.256286082	2.667966272	-0.813602078
80 H	3.504075784	1.111083937	0.516717431
H	2.837221915	-2.218138695	1.735335523
H	2.659412268	-0.400656980	-2.810611241
H	1.215519447	1.542598079	2.066175407
H	3.508967974	-1.047381999	0.638550432
85 H	2.867409661	2.345887555	-1.442500507
H	1.032859619	0.977990746	-2.284620784
H	3.023570540	0.054878744	2.714132856
H	3.435706692	-0.065131189	-1.291285977
H	1.388948385	-0.592726466	2.769350262
90 N	-1.600591416	-0.916369765	1.375427934
N	-1.554872471	1.632610027	0.145351116
N	-1.491644163	-0.710110379	-1.427616568
C	-2.572205790	-1.670403277	0.564694405
C	-2.167001028	0.228599301	2.097346123
95 H	-1.215519447	-1.542598079	2.066175407
C	-2.049246520	1.699893302	-1.232912402
C	-2.591411239	1.334196927	1.148162153
H	-1.158579744	2.534043951	0.363027896
C	-2.057302770	-1.927870354	-0.839837941
100 C	-2.481152086	0.334995255	-1.737966594
H	-1.032859619	-0.977990746	-2.284620784
H	-2.814272711	-2.624760950	1.030380894
H	-3.504075784	-1.111083937	0.516717431
H	-3.023570540	-0.054878744	2.714132856
105 H	-1.388948385	0.592726466	2.769350262
H	-1.229690277	2.081626553	-1.842342774
H	-2.887426928	2.393056918	-1.343297886
H	-2.837221915	2.218138695	1.735335523
H	-3.508967974	1.047381999	0.638550432
110 H	-1.256286082	-2.667966272	-0.813602078
H	-2.867409661	-2.345887555	-1.442500507
H	-2.659412268	0.400656980	-2.810611241
H	-3.435706692	0.065131189	-1.291285977

115 49

Co<sup>3+</sup> ^5A\_1 D\_3 LDA

Co	0.000000	0.000000	0.000000
N	1.006887	-1.237375	-1.408508
N	-1.575041	-0.253302	-1.408508
120 N	0.568155	1.490677	-1.408508
C	1.694033	-0.410822	-2.425500
C	1.849461	1.004717	-1.938993
C	-0.491234	1.672487	-2.425500
C	-1.794840	1.099322	-1.938993
125 C	-0.054620	-2.104038	-1.938993
C	-1.202799	-1.261665	-2.425500
H	2.681410	-0.836865	-2.671111
H	-2.218929	1.722600	-1.130235
H	-2.543105	1.097383	-2.754528
130 H	-2.436234	-0.569123	-0.942523
H	2.601280	1.060349	-1.130235
H	1.110363	-0.445922	-3.359501
H	-2.065451	-1.903737	-2.671111
H	-0.615959	2.740602	-2.671111
135 H	1.710992	-1.825279	-0.942523
H	-0.941361	-0.738641	-3.359501
H	2.221914	1.653702	-2.754528
H	0.725242	2.394402	-0.942523
H	0.321191	-2.751085	-2.754528
140 H	-0.169002	1.184564	-3.359501
H	-0.382351	-2.782949	-1.130235
N	-1.575041	0.253302	1.408508
N	0.568155	-1.490677	1.408508
N	1.006887	1.237375	1.408508
145 C	-1.202799	1.261665	2.425500
C	-1.794840	-1.099322	1.938993

H	-2.436234	0.569123	0.942523
C	1.849461	-1.004717	1.938993
C	-0.491234	-1.672487	2.425500
H	0.725242	-2.394402	0.942523
5 C	-0.054620	2.104038	1.938993
C	1.694033	0.410822	2.425500
H	1.710992	1.825279	0.942523
H	-2.065451	1.903737	2.671111
H	-0.941361	0.738641	3.359501
10 H	-2.543105	-1.097383	2.754528
H	-2.218929	-1.722600	1.130235
H	2.601280	-1.060349	1.130235
H	2.221914	-1.653702	2.754528
H	-0.615959	-2.740602	2.671111
15 H	-0.169002	-1.184564	3.359501
H	-0.382351	2.782949	1.130235
H	0.321191	2.751085	2.754528
H	2.681410	0.836865	2.671111
H	1.110363	0.445922	3.359501
20			
49			
Co <sup>3+</sup> ^1A_1 D_3 LDA			
Co	0.000000	0.000000	0.000000
N	-1.329612	0.745889	-1.216816
25 N	1.310765	0.778533	-1.216816
N	0.018847	-1.524422	-1.216816
C	-1.731007	-0.250199	-2.254643
C	-1.331975	-1.626474	-1.807099
C	1.082182	-1.373996	-2.254643
30 C	2.074555	-0.340287	-1.807099
C	-0.742580	1.966761	-1.807099
C	0.648825	1.624195	-2.254643
H	-2.812080	-0.187059	-2.461493
H	2.772773	-0.729246	-1.045307
35 H	2.703735	0.002278	-2.648949
H	1.974328	1.370813	-0.696428
H	-2.017932	-2.036669	-1.045307
H	-1.223729	0.016903	-3.196043
H	1.244042	2.528862	-2.461493
40 H	1.568038	-2.341803	-2.461493
H	-2.174323	1.024412	-0.696428
H	0.626503	1.051329	-3.196043
H	-1.349895	-2.342642	-2.648949
H	0.199995	-2.395225	-0.696428
45 H	-1.353840	2.340364	-2.648949
H	0.597226	-1.068232	-3.196043
H	-0.754841	2.765915	-1.045307
N	0.018847	1.524422	1.216816
N	-1.329612	-0.745889	1.216816
50 N	1.310765	-0.778533	1.216816
C	1.082182	1.373996	2.254643
C	-1.331975	1.626474	1.807099
H	0.199995	2.395225	0.696428
C	-0.742580	-1.966761	1.807099
55 C	-1.731007	0.250199	2.254643
H	-2.174323	-1.024412	0.696428
C	2.074555	0.340287	1.807099
C	0.648825	-1.624195	2.254643
H	1.974328	-1.370813	0.696428
60 H	1.568038	2.341803	2.461493
H	0.597226	1.068232	3.196043
H	-1.349895	2.342642	2.648949
H	-2.017932	2.036669	1.045307
H	-0.754841	-2.765915	1.045307
65 H	-1.353840	-2.340364	2.648949
H	-2.812080	0.187059	2.461493
H	-1.223729	-0.016903	3.196043
H	2.772773	0.729246	1.045307
H	2.703735	-0.002278	2.648949
70 H	1.244042	-2.528862	2.461493
H	0.626503	-1.051329	3.196043

49			
75 Co <sup>3+</sup> ^5A_1 D_3 SSB-D			
Co	0.000000000	0.000000000	0.000000000
N	1.061824212	-1.211907054	-1.435615749
N	-1.580454402	-0.313613215	-1.435615749
N	0.518630189	1.525520269	-1.435615749
80 C	1.728161715	-0.356689598	-2.443307211
C	1.814690980	1.077238696	-1.966636129
C	-0.555178605	1.674976746	-2.443307211
C	-1.840261566	1.032949141	-1.966636129
C	0.025570586	-2.110187837	-1.966636129
85 C	-1.172983110	-1.318287149	-2.443307211
H	2.730989044	-0.728050201	-2.650708691
H	-2.285587095	1.620989546	-1.162586767
H	-2.565572489	1.005139206	-2.783123886
H	-2.430106483	-0.641092290	-0.995456731
90 H	2.546611674	1.168881714	-1.162586767
H	1.175114216	-0.415459535	-3.377362913
H	-1.996004491	-2.001080789	-2.650708691
H	-0.734984552	2.729130990	-2.650708691
H	1.770255451	-1.783987803	-0.995456731
95 H	-0.947355619	-0.809948996	-0.377362913
H	2.153262331	1.719281348	-2.783123886
H	0.659851032	2.425080093	-0.995456731
H	0.412310158	-2.724420554	-2.783123886
H	-0.227758597	1.225408531	-3.377362913
100 H	-0.261024579	-2.789871260	-1.162586767
N	-1.580454402	0.313613215	1.435615749
N	0.518630189	-1.525520269	1.435615749
N	1.061824212	1.211907054	1.435615749
C	-1.172983110	1.318287149	2.443307211
105 C	-1.840261566	-1.032949141	1.966636129
H	-2.430106483	0.641092290	0.995456731
C	1.814690980	-1.077238696	1.966636129
C	-0.555178605	-1.674976746	2.443307211
H	0.659851032	-2.425080093	0.995456731
110 C	0.025570586	2.110187837	1.966636129
C	1.728161715	0.356689598	2.443307211
H	1.770255451	1.783987803	0.995456731
H	-1.996004491	2.001080789	2.650708691
H	-0.947355619	0.809948996	3.377362913
115 H	-2.565572489	-1.005139206	2.783123886
H	-2.285587095	-1.620989546	1.162586767
H	2.546611674	-1.168881714	1.162586767
H	2.153262331	-1.719281348	2.783123886
H	-0.734984552	-2.729130990	2.650708691
120 H	-0.227758597	-1.225408531	3.377362913
H	-0.261024579	2.789871260	1.162586767
H	0.412310158	2.724420554	2.783123886
H	2.730989044	0.728050201	2.650708691
H	1.175114216	0.415459535	3.377362913
125			
49			
Co <sup>3+</sup> ^1A_1 D_3 SSB-D			
Co	0.000000	0.000000	0.000000
N	-0.028666	1.544501	-1.259792
130 N	1.351910	-0.747425	-1.259792
N	-1.323244	-0.797076	-1.259792
C	-1.098445	1.381747	-2.284683
C	-2.081759	0.327456	-1.839705
C	-0.647405	-1.642155	-2.284683
135 C	0.757295	-1.966584	-1.839705
C	1.324465	1.639129	-1.839705
C	1.745850	0.260408	-2.284683
H	-1.601387	2.331272	-2.459705
H	0.774006	-2.741522	-1.075382
140 H	1.351628	-2.334969	-2.677380
H	2.191711	-1.027849	-0.769731
H	-2.761231	0.700453	-1.075382
H	-0.632844	1.092335	-3.223015
H	2.819634	0.221206	-2.459705
145 H	-1.218247	-2.552478	-2.459705
H	-0.205713	2.412002	-0.769731

H	1.262412	0.001891	-3.223015	H	-0.518436853	2.786469489	1.248784619
H	-2.697957	-0.003059	-2.677380	75 H	-2.153934938	-1.842214230	1.248784619
H	-1.985999	-1.384153	-0.769731	H	-2.469060265	-1.235140675	2.868046983
H	1.346329	2.338029	-2.677380	H	-2.193196832	1.816826831	2.708075987
5 H	-0.629568	-1.094226	-3.223015	H	-1.047755703	0.731667049	3.462830558
H	1.987225	2.041070	-1.075382	H	2.672371791	-0.944255259	1.248784619
N	1.351910	0.747425	1.259792	80 H	2.304193334	-1.520698576	2.868046983
N	-1.323244	0.797076	1.259792	H	-0.476819773	-2.807777588	2.708075987
N	-0.028666	-1.544501	1.259792	H	-0.109764400	-1.273216581	3.462830558
10 C	1.745850	-0.260408	2.284683				
C	0.757295	1.966584	1.839705	49			
H	2.191711	1.027849	0.769731	85 Co <sup>3+</sup> ^1A_1 D_3 OPBE			
C	-2.081759	-0.327456	1.839705	Co	0.000000000	0.000000000	0.000000000
C	-0.647405	1.642155	2.284683	N	-1.337278357	0.750626855	-1.279268494
15 H	-1.985999	1.384153	0.769731	N	1.318701104	0.782803601	-1.279268494
C	1.324465	-1.639129	1.839705	N	0.018577253	-1.533430457	-1.279268494
C	-1.098445	-1.381747	2.284683	90 C	-1.762172022	-0.255302916	-2.313170244
H	-0.205713	-2.412002	0.769731	C	-1.336475549	-1.638001019	-1.881125672
H	2.819634	-0.221206	2.459705	C	1.102184822	-1.398434279	-2.313170244
20 H	1.262412	-0.001891	3.223015	C	2.086788268	-0.338421267	-1.881125672
H	1.351628	2.334969	2.677380	C	-0.750312719	1.976422286	-1.881125672
H	0.774006	2.741522	1.075382	95 C	0.659987200	1.653737195	-2.313170244
H	-2.761231	-0.700453	1.075382	H	-2.846602807	-0.205513427	-2.465665614
H	-2.697957	0.003059	2.677380	H	2.796327272	-0.711844529	-1.135360088
25 H	-1.218247	2.552478	2.459705	H	2.692790847	0.008225751	-2.729181428
H	-0.629568	1.094226	3.223015	H	1.987292786	1.366917155	-0.780446569
H	1.987225	-2.041070	1.075382	100 H	-2.014639082	-2.065768190	-1.135360088
H	1.346329	-2.338029	2.677380	H	-1.305200360	0.015856493	-3.268633278
H	-1.601387	-2.331272	2.459705	H	1.245321555	2.567987058	-2.465665614
30 H	-0.632844	-1.092335	3.223015	H	1.601281252	-2.362473632	-2.465665614
				H	-2.177431374	1.037587460	-0.780446569
49				105 H	0.666332306	1.122408423	-3.268633278
Co <sup>3+</sup> ^5A_1 D_3 OPBE				H	-1.339271714	-2.336138156	-2.729181428
Co	0.000000000	0.000000000	0.000000000	H	0.190138587	-2.404504615	-0.780446569
35 N	-1.601456871	-0.161499500	-1.500663212	H	-1.353519133	2.327912405	-1.279181428
N	0.660865766	1.467652083	-1.500663212	H	0.638868055	-1.138264915	-3.268633278
N	0.940591105	-1.306152583	-1.500663212	110 H	-0.781688190	2.777612719	-1.135360088
C	-1.298567792	-1.213115869	-2.513993567	N	0.018577253	1.533430457	1.279268494
C	-0.174526065	-2.112455012	-2.043169358	N	-1.337278357	-0.750626855	-1.279268494
40 C	1.699873057	-0.518034762	-2.513993567	N	1.318701104	-0.782803601	1.279268494
C	1.916702738	0.905083500	-2.043169358	C	1.102184822	1.398434279	2.313170244
C	-1.742176672	1.207371512	-2.043169358	115 C	-1.336475549	1.638001019	1.881125672
C	-0.401305264	1.731150631	-2.513993567	H	0.190138587	2.404504615	0.780446569
H	-2.193196832	-1.816826831	-2.708075987	C	-0.750312719	-1.976422286	1.881125672
45 H	2.672371791	0.944255259	-1.248784619	C	-1.762172022	0.255302916	2.313170244
H	2.304193334	1.520698576	-2.868046983	H	-2.177431374	-1.037587460	0.780446569
H	0.890131227	2.359414332	-1.066978885	120 C	2.086788268	0.338421267	1.881125672
H	-0.518436853	-2.786469489	-1.248784619	C	0.659987200	-1.653737195	2.313170244
H	-1.047755703	-0.731667049	-3.462830558	H	1.987292786	-1.366917155	0.780446569
50 H	-0.476819773	2.807777588	-2.708075987	H	1.601281252	2.362473632	2.465665614
H	2.670016606	-0.990950757	-2.708075987	H	0.638868055	1.138264915	3.268633278
H	-2.488378363	-0.408830911	-1.066978885	125 H	-1.339271714	2.336138156	2.729181428
H	-0.109764400	1.273216581	-3.462830558	H	-2.014639082	2.065768190	1.135360088
H	0.164866931	-2.755839251	-2.868046983	H	-0.781688190	-2.777612719	1.135360088
55 H	1.598247136	-1.950583421	-1.066978885	H	-1.353519133	-2.327912405	2.729181428
H	-2.469060265	1.235140675	-2.868046983	H	-2.846602807	0.205513427	2.465665614
H	1.157520103	-0.541549532	-3.462830558	130 H	-1.305200360	-0.015856493	3.268633278
H	-2.153934938	1.842214230	-1.248784619	H	2.796327272	0.711844529	1.135360088
N	0.940591105	1.306152583	1.500663212	H	2.692790847	-0.008225751	2.729181428
60 N	-1.601456871	0.161499500	1.500663212	H	1.245321555	-2.567987058	2.465665614
N	0.660865766	-1.467652083	1.500663212	H	0.666332306	-1.122408423	3.268633278
C	1.699873057	0.518034762	2.513993567	135			
C	-0.174526065	2.112455012	2.043169358	49			
H	1.598247136	1.950583421	1.066978885	Co <sup>2+</sup> ^2E D_3 LDA			
65 C	-1.742176672	-1.207371512	2.043169358	Co	0.0000000	0.0000000	0.0000000
C	-1.298567792	1.213115869	2.513993567	N	0.018700	-1.565100	1.296100
H	-2.488378363	0.408830911	1.066978885	140 N	-1.364800	0.766300	1.296100
C	1.916702738	-0.905083500	2.043169358	N	1.346000	0.798800	1.296100
C	-0.401305264	-1.731150631	2.513993567	C	1.072100	-1.380400	2.316400
70 H	0.890131227	-2.359414332	1.066978885	C	2.068700	-0.344000	1.864800
H	2.670016606	0.990950757	2.708075987	C	0.659400	1.618700	2.316400
H	1.157520103	0.541549532	3.462830558	145 C	-0.736400	1.963500	1.864800
H	0.164866931	2.755839251	2.868046983	C	-1.332300	-1.619500	1.864800

C	-1.731500	-0.238200	2.316400
H	1.581800	-2.328900	2.551600
H	-0.718400	2.739600	1.079800
H	-1.316100	2.383900	2.708100
5 H	-2.216000	1.059000	0.801500
H	2.731800	-0.747600	1.079800
H	0.590700	-1.058600	3.254800
H	-2.807800	-0.205400	2.551600
H	1.226000	2.534400	2.551600
10 H	0.190900	-2.448600	0.801500
H	-1.212100	0.017700	3.254800
H	2.722500	-0.052200	2.708100
H	2.025100	1.389600	0.801500
H	-1.406500	-2.331700	2.708100
15 H	0.621400	1.040800	3.254800
H	-2.013300	-1.992000	1.079800
N	-1.364800	-0.766300	-1.296100
N	1.346000	-0.798800	-1.296100
N	0.018700	1.565100	-1.296100
20 C	-1.731500	0.238200	-2.316400
C	-0.736400	-1.963500	-1.864800
H	-2.216000	-1.059000	-0.801500
C	2.068700	0.344000	-1.864800
C	0.659400	-1.618700	-2.316400
25 H	2.025100	-1.389600	-0.801500
C	-1.332300	1.619500	-1.864800
C	1.072100	1.380400	-2.316400
H	0.190900	2.448600	-0.801500
H	-2.807800	0.205400	-2.551600
30 H	-1.212100	-0.017700	-3.254800
H	-1.316100	-2.383900	-2.708100
H	-0.718400	-2.739600	-1.079800
H	2.731800	0.747600	-1.079800
H	2.722500	0.052200	-2.708100
35 H	1.226000	-2.534400	-2.551600
H	0.621400	-1.040800	-3.254800
H	-2.013300	1.992000	-1.079800
H	-1.406500	2.331700	-2.708100
H	1.581800	2.328900	-2.551600
40 H	0.590700	1.058600	-3.254800
49			
Co <sup>2+</sup> ^2A_C_2 LDA			
Co	0.000000	0.000000	-0.005100
45 N	-1.390800	1.710000	0.035800
N	-1.249400	-0.695800	-1.333800
N	-1.268100	-0.715200	1.313900
C	-2.390600	1.436800	1.073300
C	-1.879700	0.402600	2.048400
50 C	-2.278300	-1.580400	0.652700
C	-1.815500	-1.917800	-0.736700
C	-1.907700	1.690300	-1.327900
C	-2.295900	0.285900	-1.712300
H	-2.680500	2.348900	1.620700
55 H	-1.018800	-2.679500	-0.717500
H	-2.645500	-2.328400	-1.341200
H	-0.748000	-0.975500	-2.187500
H	-1.107000	0.835700	2.708100
H	-3.316700	1.078100	0.592700
60 H	-2.519700	0.230900	-2.790300
H	-2.476200	-2.491700	1.239500
H	-0.957800	2.622400	0.209800
H	-3.228000	0.001200	-1.197000
H	-2.696800	0.060000	2.709800
65 H	-0.747400	-1.288400	1.990100
H	-2.781700	2.355200	-1.472300
H	-3.231400	-1.027500	0.618100
H	-1.115000	2.076800	-1.994000
N	1.249400	0.695800	-1.333800
70 N	1.268100	0.715200	1.313900
N	1.390800	-1.710000	0.035800
C	2.295900	-0.285900	-1.712300
C	1.815500	1.917800	-0.736700

H	0.748000	0.975500	-2.187500
75 C	1.879700	-0.402600	2.048400
C	2.278300	1.580400	0.652700
H	0.747400	1.288400	1.990100
C	1.907700	-1.690300	-1.327900
C	2.390600	-1.436800	1.073300
80 H	0.957800	-2.622400	0.209800
H	2.519700	-0.230900	-2.790300
H	3.228000	-0.001200	-1.197000
H	2.645500	2.328400	-1.341200
H	1.018800	2.679500	-0.717500
85 H	1.107000	-0.835700	2.708100
H	2.696800	-0.060000	2.709800
H	2.476200	2.491700	1.239500
H	3.231400	1.027500	0.618100
H	1.115000	-2.076800	-1.994000
90 H	2.781700	-2.355200	-1.472300
H	2.680500	-2.348900	1.620700
H	3.316700	-1.078100	0.592700
49			
95 Co <sup>2+</sup> ^4E_D_3 LDA			
Co	0.000000	0.000000	0.000000
N	0.040500	-1.606500	-1.392000
N	-1.411500	0.768200	-1.392000
N	1.371000	0.838300	-1.392000
100 C	1.087000	-1.369500	-2.400500
C	2.075000	-0.324000	-1.941400
C	0.642600	1.626100	-2.400500
C	-0.756900	1.959000	-1.941400
C	-1.318100	-1.635000	-1.941400
105 C	-1.729500	-0.256600	-2.400500
H	1.622400	-2.298600	-2.655600
H	-0.731400	2.722500	-1.143900
H	-1.325500	2.399400	-2.782100
H	-2.277400	1.064300	-0.929000
110 H	2.723400	-0.727800	-1.143900
H	0.600300	-1.043100	-3.334800
H	-2.801900	-0.255800	-2.655600
H	1.179500	2.554400	-2.655600
H	0.217000	-2.504400	-0.929000
115 H	-1.203500	0.001700	-3.334800
H	2.740700	-0.051800	-2.782100
H	2.060400	1.440200	-0.929000
H	-1.415200	-2.347600	-2.782100
H	0.603200	1.041500	-3.334800
120 H	-1.992000	-1.994700	-1.143900
N	-1.411500	-0.768200	1.392000
N	1.371000	-0.838300	1.392000
N	0.040500	1.606500	1.392000
C	-1.729500	0.256600	2.400500
125 C	-0.756900	-1.959000	1.941400
H	-2.277400	-1.064300	0.929000
C	2.075000	0.324000	1.941400
C	0.642600	-1.626100	2.400500
H	2.060400	-1.440200	0.929000
130 C	-1.318100	1.635000	1.941400
C	1.087000	1.369500	2.400500
H	0.217000	2.504400	0.929000
H	-2.801900	0.255800	2.655600
H	-1.203500	-0.001700	3.334800
135 H	-1.325500	-2.399400	2.782100
H	-0.731400	-2.722500	1.143900
H	2.723400	0.727800	1.143900
H	2.740700	0.051800	2.782100
H	1.179500	-2.554400	2.655600
140 H	0.603200	-1.041500	3.334800
H	-1.992000	1.994700	1.143900
H	-1.415200	2.347600	2.782100
H	1.622400	2.298600	2.655600
H	0.600300	1.043100	3.334800
145			

49  
 Co<sup>2+</sup> ^4B C\_2 LDA

Co	0.000000	0.000000	0.025400
N	-1.291400	1.691100	0.063700
5 N	-1.432600	-0.638900	-1.416500
N	-1.460900	-0.761200	1.373500
C	-2.318300	1.512600	1.102700
C	-1.934300	0.431100	2.083600
C	-2.510700	-1.466200	0.618100
10 C	-2.057600	-1.804800	-0.782900
C	-1.831500	1.785900	-1.294000
C	-2.375400	0.447300	-1.729400
H	-2.517500	2.451000	1.646000
H	-1.306800	-2.614900	-0.761100
15 H	-2.916500	-2.187000	-1.365900
H	-0.976900	-0.950900	-2.280500
H	-1.113800	0.774900	2.737700
H	-3.268700	1.251500	0.608000
H	-2.621400	0.474700	-2.803500
20 H	-2.832900	-2.385200	1.134500
H	-0.763400	2.548600	0.258900
H	-3.327900	0.240800	-1.213400
H	-2.794400	0.210100	2.743500
H	-1.053400	-1.402600	2.062200
25 H	-2.623000	2.554000	-1.381800
H	-3.403400	-0.820000	0.579600
H	-1.007800	2.102500	-1.957700
N	1.432600	0.638900	-1.416500
N	1.460900	0.761200	1.373500
30 N	1.291400	-1.691100	0.063700
C	2.375400	-0.447300	-1.729400
C	2.057600	1.804800	-0.782900
H	0.976900	0.950900	-2.280500
C	1.934300	-0.431100	2.083600
35 C	2.510700	1.466200	0.618100
H	1.053400	1.402600	2.062200
C	1.831500	-1.785900	-1.294000
C	2.318300	-1.512600	1.102700
H	0.763400	-2.548600	0.258900
40 H	2.621400	-0.474700	-2.803500
H	3.327900	-0.240800	-1.213400
H	2.916500	2.187000	-1.365900
H	1.306800	2.614900	-0.761100
H	1.113800	-0.774900	2.737700
45 H	2.794400	-0.210100	2.743500
H	2.832900	2.385200	1.134500
H	3.403400	0.820000	0.579600
H	1.007800	-2.102500	-1.957700
H	2.623000	-2.554000	-1.381800
50 H	2.517500	-2.451000	1.646000
H	3.268700	-1.251500	0.608000

H	-1.302319	0.019477	3.361557
75 H	2.708016	-0.043617	2.826968
H	2.048936	1.387397	0.924791
H	-1.391782	-2.323402	2.826968
H	0.668027	1.118103	3.361557
H	-2.011276	-2.028307	1.208698
80 N	-1.376536	-0.773083	-1.388903
N	1.357778	-0.805573	-1.388903
N	0.018758	1.578657	-1.388903
C	-1.764479	0.242698	-2.405174
C	-0.745780	-1.972045	-1.973602
85 H	-2.225989	-1.080732	-0.924791
C	2.080731	0.340159	-1.973602
C	0.672057	-1.649433	-2.405174
H	2.048936	-1.387397	-0.924791
C	-1.334952	1.631886	-1.973602
90 C	1.092422	1.406735	-2.405174
H	0.177053	2.468129	-0.924791
H	-2.846457	0.226610	-2.581870
H	-1.302319	-0.019477	-3.361557
H	-1.316234	-2.367019	-2.826968
95 H	-0.750927	-2.755969	-1.208698
H	2.762203	0.727663	-1.208698
H	2.708016	0.043617	-2.826968
H	1.226978	-2.578409	-2.581870
H	0.668027	-1.118103	-3.361557
100 H	-2.011276	2.028307	-1.208698
H	-1.391782	2.323402	-2.826968
H	1.619479	2.351799	-2.581870
H	0.634292	1.137580	-3.361557

105 49  
 Co<sup>2+</sup> ^2A C\_2 OPBE

Co	0.000000	0.000000	0.000298
N	-1.319349	1.477478	0.006634
N	-1.447313	-0.837760	-1.399352
110 N	-1.419293	-0.887299	1.375756
C	-2.346257	1.352740	1.090476
C	-1.959616	0.283141	2.089007
C	-2.451357	-1.691455	0.678270
C	-2.040781	-2.016224	-0.750599
115 C	-1.930920	1.571212	-1.341857
C	-2.434669	0.206705	-1.767011
H	-2.485647	2.314793	1.597178
H	-1.290637	-2.815605	-0.765044
H	-2.911885	-2.405005	-1.298232
120 H	-0.996787	-1.154455	-2.251906
H	-1.181503	0.646243	2.768314
H	-3.307842	1.113965	0.627754
H	-2.636907	0.205850	-2.844782
H	-2.651765	-2.625226	1.217004
125 H	-0.827903	2.353755	0.162880
H	-3.391880	-0.017527	-1.286749
H	-2.828523	0.032821	2.716169
H	-0.980271	-1.483745	2.070420
H	-2.743433	2.311192	-1.362370
130 H	-3.397062	-1.140877	0.682368
H	-1.159876	1.932760	-2.029130
N	1.447313	0.837760	-1.399352
N	1.419293	0.887299	1.375756
N	1.319349	-1.477478	0.006634
135 C	2.434669	-0.206705	-1.767011
C	2.040781	2.016224	-0.750599
C	0.996787	1.154455	-2.251906
C	1.959616	-0.283141	2.089007
C	2.451357	1.691455	0.678270
140 H	0.980271	1.483745	2.070420
C	1.930920	-1.571212	-1.341857
C	2.346257	-1.352740	1.090476
H	0.827903	-2.353755	0.162880
H	2.636907	-0.205850	-2.844782
145 H	3.391880	0.017527	-1.286749
H	2.911885	2.405005	-1.298232

H	1.290637	2.815605	-0.765044	C	-2.517158	0.289327	-1.770142
H	1.181503	-0.646243	2.768314	75 H	-2.738947	2.271875	1.696317
H	2.828523	-0.032821	2.716169	H	-1.267311	-2.716874	-0.827139
H	2.651765	2.625226	1.217004	H	-2.897587	-2.366346	-1.386317
5 H	3.397062	1.140877	0.682368	H	-1.062051	-1.031950	-2.313369
H	1.159876	-1.932760	-2.029130	H	-1.323757	0.647247	2.774269
H	2.743433	-2.311192	-1.362370	80 H	-3.485137	1.082962	0.659033
H	2.485647	-2.314793	1.597178	H	-2.702132	0.326435	-2.850257
H	3.307842	-1.113965	0.627754	H	-2.692007	-2.642258	1.112261
10				H	-1.096496	2.502522	0.254095
49				H	-3.471465	0.003864	-1.316835
Co <sup>2+</sup> ^4E D_3 OPBE				85 H	-2.947634	-0.029761	2.720024
Co	0.000000	0.000000	0.000000	H	-1.092002	-1.486928	2.072579
N	0.069100	-1.617900	-1.505400	H	-2.952453	2.353769	-1.349721
15 N	-1.435700	0.749100	-1.505400	H	-3.464022	-1.157393	0.616334
N	1.366600	0.868800	-1.505400	H	-1.319690	2.078672	-1.947460
C	1.132000	-1.376300	-2.512100	90 N	1.499302	0.739612	-1.444719
C	2.093100	-0.283300	-2.072100	N	1.511724	0.882017	1.372871
C	0.625800	1.668500	-2.512100	N	1.527828	-1.601632	0.068773
20 C	-0.801200	1.954300	-2.072100	C	2.517158	-0.289327	-1.770142
C	-1.291900	-1.671000	-2.072100	C	2.054018	1.953115	-0.813956
C	-1.757900	-0.292300	-2.512100	95 H	1.062051	1.031950	-2.313369
H	1.699600	-2.293500	-2.709200	C	2.093497	-0.266288	2.093178
H	-0.813700	2.726100	-1.294000	C	2.504574	1.683676	0.613899
25 H	-1.368700	2.360000	-2.922400	H	1.092002	1.486928	2.072579
H	-2.306600	1.046400	-1.075900	C	2.094632	-1.667752	-1.290297
H	2.767700	-0.658400	-1.294000	100 C	2.535448	-1.355492	1.129402
H	0.665500	-1.109600	-3.465100	H	1.096496	-2.502522	0.254095
H	-2.836000	-0.325200	-2.709200	H	2.702132	-0.326435	-2.850257
30 H	1.136400	2.618600	-2.709200	H	3.471465	-0.003864	-1.316835
H	0.247100	-2.520800	-1.075900	H	2.897587	2.366346	-1.386317
H	-1.293700	-0.021600	-3.465100	105 H	1.267311	2.716874	-0.827139
H	2.728200	0.005300	-2.922400	H	1.323757	-0.647247	2.774269
H	2.059500	1.474400	-1.075900	H	2.947634	0.029761	2.720024
35 H	-1.359500	-2.365300	-2.922400	H	2.692007	2.642258	1.112261
H	0.628200	1.131200	-3.465100	H	3.464022	1.157393	0.616334
H	-1.954000	-2.067700	-1.294000	110 H	1.319690	-2.078672	-1.947460
N	-1.435700	-0.749100	1.505400	H	2.952453	-2.353769	-1.349721
N	1.366600	-0.868800	1.505400	H	2.738947	-2.271875	1.696317
40 N	0.069100	1.617900	1.505400	H	3.485137	-1.082962	0.659033
C	-1.757900	0.292300	2.512100	115			
C	-0.801200	-1.954300	2.072100	49			
H	-2.306600	-1.046400	1.075900	Co <sup>2+</sup> ^2E D_3 SSB-D			
C	2.093100	0.283300	2.072100	Co	0.000000	0.000000	0.000000
45 C	0.625800	-1.668500	2.512100	N	-0.017800	-1.589700	-1.375200
H	2.059500	-1.474400	1.075900	N	1.385600	0.779500	-1.375200
C	-1.291900	1.671000	2.072100	120 N	-1.367900	0.810300	-1.375200
C	1.132000	1.376300	2.512100	C	-1.076800	-1.395300	-2.386000
H	0.247100	2.520800	1.075900	C	-2.073400	-0.347200	-1.935200
50 H	-2.836000	0.325200	2.709200	C	-0.670000	1.630200	-2.386000
H	-1.293700	0.021600	3.465100	C	0.736000	1.969300	-1.935200
H	-1.368700	-2.360000	2.922400	125 C	1.337400	-1.622000	-1.935200
H	-0.813700	-2.726100	1.294000	C	1.746800	-0.234900	-2.386000
H	2.767700	0.658400	1.294000	H	-1.599100	-2.328500	-2.593100
55 H	2.728200	-0.005300	2.922400	H	0.713000	2.721400	-1.147400
H	1.136400	-2.618600	2.709200	H	1.295400	2.392700	-2.773100
H	0.628200	-1.131200	3.465100	130 H	2.235100	1.086300	-0.924700
H	-1.954000	2.067700	1.294000	H	-2.713300	-0.743200	-1.147400
H	-1.359500	2.365300	2.922400	H	-0.617500	-1.087000	-3.322700
60 H	1.699600	2.293500	2.709200	H	2.816100	-0.220600	-2.593100
H	0.665500	1.109600	3.465100	H	-1.217000	2.549100	-2.593100
49				135 H	-0.176700	-2.478800	-0.924700
Co <sup>2+</sup> ^4B C_2 OPBE				H	1.250100	0.008700	-3.322700
65 Co	0.000000	0.000000	0.011521	H	-2.719800	-0.074500	-2.773100
N	-1.527828	1.601632	0.068773	H	-2.058400	1.392500	-0.924700
N	-1.499302	-0.739612	-1.444719	H	1.424400	-2.318200	-2.773100
N	-1.511724	-0.882017	1.372871	140 H	-0.632600	1.078300	-3.322700
C	-2.535448	1.355492	1.129402	H	2.000300	-1.978100	-1.147400
70 C	-2.093497	0.266288	2.093178	N	1.385600	-0.779500	1.375200
C	-2.504574	-1.683676	0.613899	N	-1.367900	-0.810300	1.375200
C	-2.054018	-1.953115	-0.813956	N	-0.017800	1.589700	1.375200
C	-2.094632	1.667752	-1.290297	145 C	1.746800	0.234900	2.386000
				C	0.736000	-1.969300	1.935200

H	2.235100	-1.086300	0.924700
C	-2.073400	0.347200	1.935200
C	-0.670000	-1.630200	2.386000
H	-2.058400	-1.392500	0.924700
5 C	1.337400	1.622000	1.935200
C	-1.076800	1.395300	2.386000
H	-0.176700	2.478800	0.924700
H	2.816100	0.220600	2.593100
H	1.250100	-0.008700	3.322700
10 H	1.295400	-2.392700	2.773100
H	0.713000	-2.721400	1.147400
H	-2.713300	0.743200	1.147400
H	-2.719800	0.074500	2.773100
H	-1.217000	-2.549100	2.593100
15 H	-0.632600	-1.078300	3.322700
H	2.000300	1.978100	1.147400
H	1.424400	2.318200	2.773100
H	-1.599100	2.328500	2.593100
H	-0.617500	1.087000	3.322700

20	49		
Co <sup>2+</sup> ^4E D_3 SSB-D			
Co	0.000000000	0.000000000	0.000000000
N	0.087799750	1.620143467	1.471648780
25 N	-1.446985275	-0.734034919	1.471648780
N	1.359185525	-0.886108547	1.471648780
C	1.133880452	1.351722102	2.473763736
C	2.087971873	0.263245748	2.017697365
C	0.603685453	-1.657830328	2.473763736
30 C	-0.816008431	-1.939859559	2.017697365
C	-1.271963442	1.676613810	2.017697365
C	-1.737565905	0.306108226	2.473763736
H	1.706710991	2.251658121	2.693783267
H	-0.813247596	-2.683893072	1.220594642
35 H	-1.380303009	-2.360380811	2.853664649
H	-2.318469723	-1.018738660	1.051061420
H	2.730943380	0.637653458	1.220594642
H	0.662342741	1.057460556	3.408928435
H	-2.803348629	0.352226014	2.693783267
40 H	1.096637638	-2.603884136	2.693783267
H	0.276981302	2.517223008	1.051061420
H	-1.246959076	0.044875362	3.408928435
H	2.734301249	-0.015187066	2.853664649
H	2.041488421	-1.498484348	1.051061420
45 H	-1.353998240	2.375567876	2.853664649
H	0.584616335	-1.102335918	3.408928435
H	-1.917695784	2.046239614	1.220594642
N	-1.446985275	0.734034919	-1.471648780
N	1.359185525	0.886108547	-1.471648780
50 N	0.087799750	-1.620143467	-1.471648780
C	-1.737565905	-0.306108226	-2.473763736
C	-0.816008431	1.939859559	-2.017697365
H	-2.318469723	1.018738660	-1.051061420
C	2.087971873	-0.263245748	-2.017697365
55 C	0.603685453	1.657830328	-2.473763736
H	2.041488421	1.498484348	-1.051061420
C	-1.271963442	-1.676613810	-2.017697365
C	1.133880452	-1.351722102	-2.473763736
H	0.276981302	-2.517223008	-1.051061420
60 H	-2.803348629	-0.352226014	-2.693783267
H	-1.246959076	-0.044875362	-3.408928435
H	-1.380303009	2.360380811	-2.853664649
H	-0.813247596	2.683893072	-1.220594642
H	2.730943380	-0.637653458	-1.220594642
65 H	2.734301249	0.015187066	-2.853664649
H	1.096637638	2.603884136	-2.693783267
H	0.584616335	1.102335918	-3.408928435
H	-1.917695784	-2.046239614	-1.220594642
H	-1.353998240	-2.375567876	-2.853664649
70 H	1.706710991	-2.251658121	-2.693783267
H	0.662342741	-1.057460556	-3.408928435

49			
75 Co <sup>2+</sup> ^4B C_2 SSB-D			
Co	0.000000000	0.000000000	0.035740276
N	1.494280156	-1.607654543	0.106978474
N	1.451636427	0.710390915	-1.450099312
N	1.489832817	0.908163008	1.364179698
80 C	2.507103468	-1.324537271	1.137527451
C	2.055925704	-0.233368680	2.090543670
C	2.471099148	1.675596880	0.576315264
C	1.988043889	1.931630363	-0.840112320
C	2.025663589	-1.686308850	-1.256402426
85 C	2.462293220	-0.318702379	-1.746508322
H	2.743438053	-2.218043506	1.714068751
H	1.178787590	2.663121374	-0.833293760
H	2.807681448	2.360115944	-1.421951851
H	1.010577616	0.979684390	-2.316110638
90 H	1.271445602	-0.609162313	2.748070913
H	3.432948074	-1.025866647	0.650687930
H	2.665325566	-0.373357163	-2.815225111
H	2.690230180	2.631862357	1.049430088
H	1.073997544	-2.500729888	0.315580628
95 H	3.402148226	-0.041741434	-1.273844733
H	2.899743411	0.056176320	2.721578892
H	1.084726850	1.525497111	2.051366448
H	2.866397316	-2.379704647	-1.336935016
H	3.411072793	1.128687910	0.549182385
100 H	1.223792536	-2.072021709	-1.886401899
N	-1.451636427	-0.710390915	-1.450099312
N	-1.489832817	-0.908163008	1.364179698
N	-1.494280156	1.607654543	0.106978474
C	-2.462293220	0.318702379	-1.746508322
105 C	-1.988043889	-1.931630363	-0.840112320
H	-1.010577616	-0.979684390	-2.316110638
C	-2.055925704	0.233368680	2.090543670
C	-2.471099148	-1.675596880	0.576315264
H	-1.084726850	-1.525497111	2.051366448
110 C	-2.025663589	1.686308850	-1.256402426
C	-2.507103468	1.324537271	1.137527451
H	-1.073997544	2.500729888	0.315580628
H	-2.665325566	0.373357163	-2.815225111
H	-3.402148226	0.041741434	-1.273844733
115 H	-2.807681448	-2.360115944	-1.421951851
H	-1.178787590	-2.663121374	-0.833293760
H	-1.271445602	0.609162313	2.748070913
H	-2.899743411	-0.056176320	2.721578892
H	-2.690230180	-2.631862357	1.049430088
120 H	-3.411072793	-1.128687910	0.549182385
H	-1.223792536	2.072021709	-1.886401899
H	-2.866397316	2.379704647	-1.336935016
H	-2.743438053	2.218043506	1.714068751
H	-3.432948074	1.025866647	0.650687930

125	49		
Co <sup>2+</sup> ^2A C_2 SSB-D			
Co	0.000000000	0.000000000	0.002497274
N	-1.667101149	-1.549625582	-0.028025618
130 N	-1.226324448	0.855573273	1.352759885
N	-1.247700575	0.864880976	-1.341715295
C	-2.617669361	-1.162348402	-1.074813499
C	-1.983247962	-0.190924719	-2.053366004
C	-2.132845644	1.847654944	-0.6711171788
135 C	-1.630123387	2.125250981	0.726694276
C	-2.171226783	-1.448591411	1.337442707
C	-2.374787149	-0.000422872	1.734490739
H	-2.979435444	-2.027566848	-1.629516381
H	-0.745670696	2.758524899	0.696082334
140 H	-2.394811890	2.643768083	1.309556124
H	-0.729727342	1.093718527	2.200274917
H	-1.263614875	-0.709456896	-2.686382467
H	-3.497090402	-0.708399001	-0.621815401
H	-2.555110342	0.059160457	2.806999692
145 H	-2.191201246	2.773892451	-1.240598058
H	-1.388571772	-2.505667604	-0.182137606

H	-3.268695811	0.386768832	1.251444797	H	-0.738100	-2.757500	-1.071900
H	-2.749451291	0.226074985	-2.710666845	75 H	2.757100	0.739600	-1.071900
H	-0.706924486	1.364695779	-2.033685929	H	2.722300	0.027100	-2.685700
H	-3.115204105	-1.980166313	1.490133944	H	1.232100	-2.535000	-2.522500
5 H	-3.140785380	1.441530362	-0.633875459	H	0.621000	-1.048400	-3.240700
H	-1.432547445	-1.920387888	1.986437238	H	-2.019000	2.018000	-1.071900
N	1.226324448	-0.855573273	1.352759885	80 H	-1.384700	2.344000	-2.685700
N	1.247700575	-0.864880976	-1.341715295	H	1.579300	2.334600	-2.522500
N	1.667101149	1.549625582	-0.028025618	H	0.597500	1.062000	-3.240700
10 C	2.374787149	0.000422872	1.734490739				
C	1.630123387	-2.125250981	0.726694276	49			
H	0.729727342	-1.093718527	2.200274917	85 Ni <sup>3+</sup> ^2A C_2 LDA			
C	1.983247962	0.190924719	-2.053366004	Ni	0.000000	0.000000	-0.004400
C	2.132845644	-1.847654944	-0.6711171788	N	-1.236700	-0.705500	-1.332800
15 H	0.706924486	-1.364695779	-2.033685929	N	-1.252800	-0.725600	1.311100
C	2.171226783	1.448591411	1.337442707	N	-1.348100	1.671800	0.033400
C	2.617669361	1.162348402	-1.074813499	90 C	-2.281100	0.285600	-1.717000
H	1.388571772	2.505667604	-0.182137606	C	-1.880800	1.684200	-1.331900
H	2.555110342	-0.059160457	2.806999692	C	-2.357700	1.425800	1.080800
20 H	3.268695811	-0.386768832	1.251444797	C	-1.855600	0.393400	2.058000
H	2.394811890	-2.643768083	1.309556124	C	-1.802900	-1.935400	-0.736800
H	0.745670696	-2.758524899	0.696082334	95 C	-2.270400	-1.591700	0.645200
H	1.263614875	0.709456896	-2.686382467	H	-2.489000	0.219600	-2.798200
H	2.749451291	-0.226074985	-2.710666845	H	-1.092600	0.809700	2.739600
25 H	2.191201246	-2.773892451	-1.240598058	H	-2.675200	0.033300	2.707400
H	3.140785380	-1.441530362	-0.633875459	H	-0.710100	-1.302200	1.970300
H	1.432547445	1.920387888	1.986437238	100 H	-1.104000	2.091100	-2.004200
H	3.115204105	1.980166313	1.490133944	H	-3.216000	-0.000600	-1.208600
H	2.979435444	2.027566848	-1.629516381	H	-2.466000	-2.495400	1.246100
30 H	3.497090402	0.708399001	-0.621815401	H	-2.621100	2.355000	1.613300
				H	-0.714400	-0.977100	-2.178600
49				105 H	-3.219100	-1.031700	0.614000
Ni <sup>3+</sup> ^2E D_3 LDA				H	-2.750500	2.360600	-1.436200
Ni	0.000000	0.000000	0.000000	H	-0.882200	2.569700	0.214100
35 N	0.019800	-1.556700	1.276700	H	-2.627200	-2.331700	-1.358600
N	-1.358100	0.761200	1.276700	H	-3.290500	1.085400	0.601200
N	1.338200	0.795500	1.276700	110 H	-1.016800	-2.708400	-0.729400
C	1.080800	-1.376000	2.301100	N	1.348100	-1.671800	0.033400
C	2.076100	-0.344600	1.845900	N	1.236700	0.705500	-1.332800
40 C	0.651300	1.624000	2.301100	N	1.252800	0.725600	1.311100
C	-0.739600	1.970300	1.845900	C	2.357700	-1.425800	1.080800
C	-1.336500	-1.625600	1.845900	115 C	1.880800	-1.684200	-1.331900
C	-1.732100	-0.247900	2.301100	H	0.882200	-2.569700	0.214100
H	1.579300	-2.334600	2.522500	C	1.802900	1.935400	-0.736800
45 H	-0.738100	2.757500	1.071900	C	2.281100	-0.285600	-1.717000
H	-1.337700	2.371200	2.685700	H	0.714400	0.977100	-2.178600
H	-2.203000	1.041400	0.760000	120 C	1.855600	-0.393400	2.058000
H	2.757100	-0.739600	1.071900	C	2.270400	1.591700	0.645200
H	0.597500	-1.062000	3.240700	H	0.710100	1.302200	1.970300
50 H	-2.811500	-0.200500	2.522500	H	2.621100	-2.355000	1.613300
H	1.232100	2.535000	2.522500	H	3.290500	-1.085400	0.601200
H	0.199700	-2.428600	0.760000	125 H	2.750500	-2.360600	-1.436200
H	-1.218500	0.013600	3.240700	H	1.104000	-2.091100	-2.004200
H	2.722300	-0.027100	2.685700	H	1.016800	2.708400	-0.729400
55 H	2.003400	1.387200	0.760000	H	2.627200	2.331700	-1.358600
H	-1.384700	-2.344000	2.685700	H	2.489000	-0.219600	-2.798200
H	0.621000	1.048400	3.240700	130 H	3.216000	0.000600	-1.208600
H	-2.019000	-2.018000	1.071900	H	1.092600	-0.809700	2.739600
N	-1.358100	-0.761200	-1.276700	H	2.675200	-0.033300	2.707400
60 N	1.338200	-0.795500	-1.276700	H	2.466000	2.495400	1.246100
N	0.019800	1.556700	-1.276700	H	3.219100	1.031700	0.614000
C	-1.732100	0.247900	-2.301100	135			
C	-0.739600	-1.970300	-1.845900	49			
H	-2.203000	-1.041400	-0.760000	Ni <sup>3+</sup> ^2E D_3 OPBE			
65 C	2.076100	0.344600	-1.845900	Ni	0.000000	0.000000	0.000000
C	0.651300	-1.624000	-2.301100	N	-1.371300	-0.763100	-1.362800
H	2.003400	-1.387200	-0.760000	140 N	1.346500	-0.806000	-1.362800
C	-1.336500	1.625600	-1.845900	N	0.024700	1.569100	-1.362800
C	1.080800	1.376000	-2.301100	C	-1.763700	0.258600	-2.382700
70 H	0.199700	2.428600	-0.760000	C	-1.335900	1.642100	-1.943400
H	-2.811500	0.200500	-2.522500	C	1.105800	1.398100	-2.382700
H	-1.218500	-0.013600	-3.240700	145 C	2.090000	0.335900	-1.943400
H	-1.337700	-2.371200	-2.685700	C	-0.754100	-1.977900	-1.943400

C	0.657900	-1.656700	-2.382700
H	-2.847200	0.229500	-2.548700
H	2.784100	0.713300	-1.185300
H	2.712100	0.012900	-2.790300
5 H	2.018800	-1.391900	-0.872000
H	-2.009800	2.054500	-1.185300
H	-1.302500	-0.008300	-3.337300
H	1.224800	-2.580500	-2.548700
H	1.622400	2.351000	-2.548700
10 H	-2.214900	-1.052400	-0.872000
H	0.658400	-1.123900	-3.337300
H	-1.367200	2.342200	-2.790300
H	0.196000	2.444300	-0.872000
H	-1.344800	-2.355200	-2.790300
15 H	0.644100	1.132100	-3.337300
H	-0.774300	-2.767800	-1.185300
N	0.024700	-1.569100	1.362800
N	-1.371300	0.763100	1.362800
N	1.346500	0.806000	1.362800
20 C	1.105800	-1.398100	2.382700
C	-1.335900	-1.642100	1.943400
H	0.196000	-2.444300	0.872000
C	-0.754100	1.977900	1.943400
C	-1.763700	-0.258600	2.382700
25 H	-2.214900	1.052400	0.872000
C	2.090000	-0.335900	1.943400
C	0.657900	1.656700	2.382700
H	2.018800	1.391900	0.872000
H	1.622400	-2.351000	2.548700
30 H	0.644100	-1.132100	3.337300
H	-1.367200	-2.342200	2.790300
H	-2.009800	-2.054500	1.185300
H	-0.774300	2.767800	1.185300
H	-1.344800	2.355200	2.790300
35 H	-2.847200	-0.229500	2.548700
H	-1.302500	0.008300	3.337300
H	2.784100	-0.713300	1.185300
H	2.712100	-0.012900	2.790300
H	1.224800	2.580500	2.548700
40 H	0.658400	1.123900	3.337300
49			
Ni <sup>3+</sup> ^2A C_2 OPBE			
Ni	0.000000	0.000000	-0.007100
45 N	-1.254400	-0.800500	-1.345600
N	-1.269700	-0.828000	1.318300
N	-1.581500	1.573600	0.036700
C	-2.379400	0.108600	-1.749000
C	-2.129900	1.543200	-1.330500
50 C	-2.560200	1.253200	1.106000
C	-1.975400	0.238400	2.070700
C	-1.721900	-2.081400	-0.749700
C	-2.202800	-1.799400	0.651000
H	-2.524600	0.048300	-2.834400
55 H	-1.260600	0.701000	2.759800
H	-2.763100	-0.197900	2.701200
H	-0.706900	-1.352900	1.985300
H	-1.416100	2.041100	-1.996400
H	-3.298700	-0.270800	-1.295400
60 H	-2.268100	-2.722200	1.239500
H	-2.847400	2.157000	1.656500
H	-0.733700	-1.035700	-2.189100
H	-3.205300	-1.364100	0.647100
H	-3.066500	2.113300	-1.414700
65 H	-1.219400	2.508600	0.206500
H	-2.515000	-2.528400	-1.365300
H	-3.481800	0.875400	0.654000
H	-0.886200	-2.786700	-0.760100
N	1.581500	-1.573600	0.036700
70 N	1.254400	0.800500	-1.345600
N	1.269700	0.828000	1.318300
C	2.560200	-1.253200	1.106000
C	2.129900	-1.543200	-1.330500

H	1.219400	-2.508600	0.206500
75 C	1.721900	2.081400	-0.749700
C	2.379400	-0.108600	-1.749000
H	0.733700	1.035700	-2.189100
C	1.975400	-0.238400	2.070700
C	2.202800	1.799400	0.651000
80 H	0.706900	1.352900	1.985300
H	2.847400	-2.157000	1.656500
H	3.481800	-0.875400	0.654000
H	3.066500	-2.113300	-1.414700
H	1.416100	-2.041100	-1.996400
85 H	0.886200	2.786700	-0.760100
H	2.515000	2.528400	-1.365300
H	2.524600	-0.048300	-2.834400
H	3.298700	0.270800	-1.295400
H	1.260600	-0.701000	2.759800
90 H	2.763100	0.197900	2.701200
H	2.268100	2.722200	1.239500
H	3.205300	1.364100	0.647100

49			
95 Ni <sup>3+</sup> ^2E D_3 SSB-D			
Ni	0.000000000	0.000000000	0.000000000
N	0.028123588	1.578213723	-1.328353014
N	-1.380834971	-0.764751120	-1.328353014
N	1.352711383	-0.813462604	-1.328353014
100 C	1.094817934	1.385538446	-2.341219217
C	2.083250454	0.335307445	-1.886950381
C	0.652502525	-1.640909367	-2.341219217
C	-0.751240462	-1.971801538	-1.886950381
C	-1.332009992	1.636494094	-1.886950381
105 C	-1.747320460	0.255370921	-2.341219217
H	1.610211823	2.326102674	-2.532632958
H	-0.750462035	-2.733276017	-1.108191382
H	-1.332208566	-2.371304479	-2.721208506
H	-2.222692264	-1.050916137	-0.845511189
110 H	2.742317484	0.716718822	-1.108191382
H	0.631164575	1.086100294	-3.277897615
H	-2.819569919	0.231433007	-2.532632958
H	1.209358096	-2.557535681	-2.532632958
H	0.201226061	2.450366034	-0.845511189
115 H	-1.256172733	0.003554409	-3.277897615
H	2.719714202	0.031925778	-2.721208506
H	2.021466204	-1.399449897	-0.845511189
H	-1.387505636	2.339378701	-2.721208506
H	0.625008158	-1.089654703	-3.277897615
120 H	-1.991855449	2.016557195	-1.108191382
N	-1.380834971	0.764751120	1.328353014
N	1.352711383	0.813462604	1.328353014
N	0.028123588	-1.578213723	1.328353014
C	-1.747320460	-0.255370921	2.341219217
125 C	-0.751240462	1.971801538	1.886950381
H	-2.222692264	1.050916137	0.845511189
C	2.083250454	-0.335307445	1.886950381
C	0.652502525	1.640909367	2.341219217
H	2.021466204	1.399449897	0.845511189
130 C	-1.332009992	-1.636494094	1.886950381
C	1.094817934	-1.385538446	2.341219217
H	0.201226061	-2.450366034	0.845511189
H	-2.819569919	-0.231433007	2.532632958
H	-1.256172733	-0.003554409	3.277897615
135 H	-1.332208566	2.371304479	2.721208506
H	-0.750462035	2.733276017	1.108191382
H	2.742317484	-0.716718822	1.108191382
H	2.719714202	-0.031925778	2.721208506
H	1.209358096	2.557535681	2.532632958
140 H	0.625008158	1.089654703	3.277897615
H	-1.991855449	-2.016557195	1.108191382
H	-1.387505636	-2.339378701	2.721208506
H	1.610211823	-2.326102674	2.532632958
H	0.631164575	-1.086100294	3.277897615
145 49			
Ni <sup>3+</sup> ^2A C_2 OPBE			

Ni	0.000000000	0.000000000	0.000035566	H	1.856100	1.661900	-0.894200
N	1.575299182	-1.496298281	0.043563766	75 H	-1.133100	-2.520900	-2.730500
N	1.184349265	0.860429612	-1.354976989	H	0.467500	1.109600	-3.328400
N	1.206918518	0.896896958	1.331678305	H	-1.750400	-2.204700	-1.103900
5 C	2.544729841	-1.138559548	1.096308026	N	-1.480300	-0.592000	1.380300
C	1.929054255	-0.153242409	2.069774631	N	1.252800	-0.986000	1.380300
C	2.101638023	1.871494794	0.646201276	80 N	0.227500	1.577900	1.380300
C	1.592071357	2.143243953	-0.745701850	C	-1.686200	0.463800	2.393100
C	2.098437916	-1.450863353	-1.325231038	C	-0.973700	-1.865300	1.910400
10 C	2.324295302	-0.013398023	-1.741043956	H	-2.367300	-0.776500	0.894200
H	2.876184729	-2.022572756	1.639588237	C	2.102200	0.089400	1.910400
H	0.718699383	2.791710108	-0.732893743	85 C	0.441400	-1.692100	2.393100
H	2.353883580	2.635222919	-1.354229792	H	1.856100	-1.661900	0.894200
H	0.656710012	1.077048967	-2.192048314	C	-1.128500	1.775900	1.910400
15 H	1.214802145	-0.640822126	2.732465419	C	1.244700	1.228400	2.393100
H	3.432621120	-0.710307717	0.636976624	H	0.511200	2.438400	0.894200
H	2.482297328	0.044180429	-2.817530570	90 H	-2.756300	0.572600	2.637500
H	2.164605950	2.794084618	1.221945467	H	-1.194700	0.149900	3.328400
H	1.247246899	-2.435772162	0.216881395	H	-1.616600	-2.241700	2.730500
20 H	3.223044045	0.374613719	-1.269052611	H	-1.034100	-2.618200	1.103900
H	2.700689322	0.286073369	2.705622308	H	2.784500	0.413600	1.103900
H	0.635734240	1.405680820	1.995061111	95 H	2.749700	-0.279200	2.730500
H	3.034179568	-2.004403085	-1.431337328	H	0.882200	-2.673400	2.637500
H	3.102651386	1.449371964	0.613113014	H	0.467500	-1.109600	3.328400
25 H	1.369944528	-1.941037633	-1.971543570	H	-1.750400	2.204700	1.103900
N	-1.184349265	-0.860429612	-1.354976989	H	-1.133100	2.520900	2.730500
N	-1.206918518	-0.896896958	1.331678305	100 H	1.874100	2.100700	2.637500
N	-1.575299182	1.496298281	0.043563766	H	0.727200	0.959700	3.328400
C	-2.324295302	0.013398023	-1.741043956				
30 C	-1.592071357	-2.143243953	-0.745701850	49			
H	-0.656710012	-1.077048967	-2.192048314	Ni <sup>3+</sup> ^4B C_2 LDA			
C	-1.929054255	0.153242409	2.069774631	105 Ni	0.000000	0.000000	0.228400
C	-2.101638023	-1.871494794	0.646201276	N	1.360900	-1.578300	0.280000
H	-0.635734240	-1.405680820	1.995061111	N	1.291400	0.622600	-1.381000
35 C	-2.098437916	1.450863353	-1.325231038	N	1.488100	1.013600	1.294500
C	-2.544729841	1.138559548	1.096308026	C	2.433400	-1.238500	1.242000
H	-1.247246899	2.435772162	0.216881395	110 C	2.014400	-0.081600	2.114000
H	-2.482297328	-0.044180429	-2.817530570	C	2.470000	1.700300	0.433000
H	-3.223044045	-0.374613719	-1.269052611	C	1.883400	1.891200	-0.934700
40 H	-2.353883580	-2.635222919	-1.354229792	C	1.830100	-1.763900	-1.101500
H	-0.718699383	-2.791710108	-0.732893743	C	2.271200	-0.441600	-1.671600
H	-1.214802145	0.640822126	2.732465419	115 H	2.692200	-2.104700	1.873200
H	-2.700689322	-0.286073369	2.705622308	H	1.087000	2.656300	-0.922800
H	-2.164605950	-2.794084618	1.221945467	H	2.647500	2.247800	-1.652600
45 H	-3.102651386	-1.449371964	0.613113014	H	0.720300	0.811000	-2.214400
H	-1.369944528	1.941037633	-1.971543570	H	1.226000	-0.381900	2.830300
H	-3.034179568	2.004403085	-1.431337328	120 H	3.350200	-0.994500	0.680400
H	-2.876184729	2.022572756	1.639588237	H	2.440300	-0.532600	-2.758700
H	-3.432621120	0.710307717	0.636976624	H	2.769000	2.668000	0.870300
50				H	0.917700	-2.456400	0.578300
49				H	3.241100	-0.141700	-1.243100
Ni <sup>3+</sup> ^4E D_3 LDA				125 H	2.867900	0.259000	2.736600
Ni	0.000000	0.000000	0.000000	H	1.028300	1.700300	1.908100
N	0.227500	-1.577900	-1.380300	H	2.661400	-2.491300	-1.156600
55 N	-1.480300	0.592000	-1.380300	H	3.385800	1.088500	0.393100
N	1.252800	0.986000	-1.380300	H	1.000900	-2.202100	-1.684700
C	1.244700	-1.228400	-2.393100	130 N	-1.291400	-0.622600	-1.381000
C	2.102200	-0.089400	-1.910400	N	-1.488100	-1.013600	1.294500
C	0.441400	1.692100	-2.393100	N	-1.360900	1.578300	0.280000
60 C	-0.973700	1.865300	-1.910400	C	-2.271200	0.441600	-1.671600
C	-1.128500	-1.775900	-1.910400	C	-1.883400	-1.891200	-0.934700
C	-1.686200	-0.463800	-2.393100	135 H	-0.720300	-0.811000	-2.214400
H	1.874100	-2.100700	-2.637500	C	-2.014400	0.081600	2.114000
H	-1.034100	2.618200	-1.103900	C	-2.470000	-1.700300	0.433000
65 H	-1.616600	2.241700	-2.730500	H	-1.028300	-1.700300	1.908100
H	-2.367300	0.776500	-0.894200	C	-1.830100	1.763900	-1.101500
H	2.784500	-0.413600	-1.103900	140 C	-2.433400	1.238500	1.242000
H	0.727200	-0.959700	-3.328400	H	-0.917700	2.456400	0.578300
H	-2.756300	-0.572600	-2.637500	H	-2.440300	0.532600	-2.758700
70 H	0.882200	2.673400	-2.637500	H	-3.241100	0.141700	-1.243100
H	0.511200	-2.438400	-0.894200	H	-2.647500	-2.247800	-1.652600
H	-1.194700	-0.149900	-3.328400	145 H	-1.087000	-2.656300	-0.922800
H	2.749700	0.279200	-2.730500	H	-1.226000	0.381900	2.830300

H	-2.867900	-0.259000	2.736600
H	-2.769000	-2.668000	0.870300
H	-3.385800	-1.088500	0.393100
H	-1.000900	2.202100	-1.684700
5 H	-2.661400	2.491300	-1.156600
H	-2.692200	2.104700	1.873200
H	-3.350200	0.994500	0.680400

49

Ni <sup>3+</sup> ^4E D_3 OPBE			
Ni	0.000000	0.000000	0.000000
N	0.276500	-1.583600	-1.488400
N	-1.509700	0.552300	-1.488400
N	1.233200	1.031300	-1.488400
15 C	1.306000	-1.213100	-2.497300
C	2.117300	-0.020300	-2.033900
C	0.397600	1.737500	-2.497300
C	-1.041100	1.843800	-2.033900
C	-1.076200	-1.823500	-2.033900
20 C	-1.703500	-0.524500	-2.497300
H	1.975500	-2.061100	-2.685200
H	-1.149300	2.599400	-1.247700
H	-1.681900	2.175300	-2.865300
H	-2.400500	0.723700	-1.026600
25 H	2.825700	-0.304400	-1.247700
H	0.809500	-1.004100	-3.448600
H	-2.772800	-0.680300	-2.685200
H	0.797200	2.741400	-2.685200
H	0.573500	-2.440700	-1.026600
30 H	-1.274300	-0.199000	-3.448600
H	2.724800	0.369000	-2.865300
H	1.827000	1.717100	-1.026600
H	-1.042900	-2.544200	-2.865300
H	0.464800	1.203100	-3.448600
35 H	-1.676500	-2.295000	-1.247700
N	-1.509700	-0.552300	1.488400
N	1.233200	-1.031300	1.488400
N	0.276500	1.583600	1.488400
C	-1.703500	0.524500	2.497300
40 C	-1.041100	-1.843800	2.033900
H	-2.400500	-0.723700	1.026600
C	2.117300	0.020300	2.033900
C	0.397600	-1.737500	2.497300
H	1.827000	-1.717100	1.026600
45 C	-1.076200	1.823500	2.033900
C	1.306000	1.213100	2.497300
H	0.573500	2.440700	1.026600
H	-2.772800	0.680300	2.685200
H	-1.274300	0.199000	3.448600
50 H	-1.681900	-2.175300	2.865300
H	-1.149300	-2.599400	1.247700
H	2.825700	0.304400	1.247700
H	2.724800	-0.369000	2.865300
H	0.797200	-2.741400	2.685200
55 H	0.464800	-1.203100	3.448600
H	-1.676500	2.295000	1.247700
H	-1.042900	2.544200	2.865300
H	1.975500	2.061100	2.685200
H	0.809500	1.004100	3.448600

49

Ni <sup>3+</sup> ^4B C_2 OPBE			
Ni	0.000000	0.000000	0.175100
N	1.473600	-1.565300	0.287100
65 N	1.415100	0.598400	-1.460100
N	1.565500	1.068200	1.239700
C	2.524300	-1.206200	1.282600
C	2.111300	0.003500	2.102800
C	2.547300	1.766700	0.367600
70 C	1.995900	1.890200	-1.033100
C	1.988800	-1.789700	-1.083000
C	2.409000	-0.477500	-1.714700
H	2.717400	-2.048100	1.957700

H	1.207100	2.648300	-1.079500
75 H	2.778600	2.215600	-1.735000
H	0.890900	0.768400	-2.315000
H	1.341500	-0.257400	2.840100
H	3.466400	-1.019800	0.759800
H	2.544700	-0.616300	-2.794600
80 H	2.774400	2.760200	0.773100
H	1.053800	-2.442800	0.586200
H	3.379200	-0.154700	-1.328400
H	2.970400	0.372500	2.685700
H	1.113900	1.757900	1.838900
85 H	2.837700	-2.487800	-1.082500
H	3.488300	1.210400	0.379900
H	1.195400	-2.273000	-1.662500
N	-1.415100	-0.598400	-1.460100
N	-1.565500	-1.068200	1.239700
90 N	-1.473600	1.565300	0.287100
C	-2.409000	0.477500	-1.714700
C	-1.995900	-1.890200	-1.033100
H	-0.890900	-0.768400	-2.315000
C	-2.111300	-0.003500	2.102800
95 C	-2.547300	-1.766700	0.367600
H	-1.113900	-1.757900	1.838900
C	-1.988800	1.789700	-1.083000
C	-2.524300	1.206200	1.282600
H	-1.053800	2.442800	0.586200
100 H	-2.544700	0.616300	-2.794600
H	-3.379200	0.154700	-1.328400
H	-2.778600	-2.215600	-1.735000
H	-1.207100	-2.648300	-1.079500
H	-1.341500	0.257400	2.840100
105 H	-2.970400	-0.372500	2.685700
H	-2.774400	-2.760200	0.773100
H	-3.488300	-1.210400	0.379900
H	-1.195400	2.273000	-1.662500
H	-2.837700	2.487800	-1.082500
110 H	-2.717400	2.048100	1.957700
H	-3.466400	1.019800	0.759800

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Ni <sup>3+</sup> ^4E D_3 SSB-D			
115 Ni	0.000000000	0.000000000	0.000000000
N	0.269737470	1.583567582	1.428537335
N	-1.506278489	-0.558184289	1.428537335
N	1.236541019	-1.025383292	1.428537335
C	1.285619166	1.208886715	2.433569427
120 C	2.109063723	0.033766508	1.953753675
C	0.404117022	-1.717822215	2.433569427
C	-1.025289208	-1.843386017	1.953753675
C	-1.083774516	1.809619508	1.953753675
C	-1.689736189	0.508935500	2.433569427
125 H	1.943730612	2.051490676	2.643296663
H	-1.103307450	-2.572242684	1.146112480
H	-1.661494752	-2.200298657	2.768401847
H	-2.392253032	-0.728139992	0.971950773
H	2.779281234	0.330629062	1.146112480
130 H	0.784372012	0.965058473	3.367033869
H	-2.748508347	0.657574750	2.643296663
H	0.804777735	-2.709065426	2.643296663
H	0.565538786	2.435821894	0.971950773
H	-1.227951160	0.196756852	3.367033869
135 H	2.736261909	-0.338747335	2.768401847
H	1.826714246	-1.707681902	0.971950773
H	-1.074767157	2.539045992	2.768401847
H	0.443579148	-1.161815325	3.367033869
H	-1.675973784	2.241613622	1.146112480
140 N	-1.506278489	0.558184289	-1.428537335
N	1.236541019	1.025383292	-1.428537335
N	0.269737470	-1.583567582	-1.428537335
C	-1.689736189	-0.508935500	-2.433569427
C	-1.025289208	1.843386017	-1.953753675
145 H	-2.392253032	0.728139992	-0.971950773
C	2.109063723	-0.033766508	-1.953753675

	C	0.404117022	1.717822215	-2.433569427
	H	1.826714246	1.707681902	-0.971950773
	C	-1.083774516	-1.809619508	-1.953753675
	C	1.285619166	-1.208886715	-2.433569427
5	H	0.565538786	-2.435821894	-0.971950773
	H	-2.748508347	-0.657574750	-2.643296663
	H	-1.227951160	-0.196756852	-3.367033869
	H	-1.661494752	2.200298657	-2.768401847
	H	-1.103307450	2.572242684	-1.146112480
10	H	2.779281234	-0.330629062	-1.146112480
	H	2.736261909	0.338747335	-2.768401847
	H	0.804777735	2.709065426	-2.643296663
	H	0.443579148	1.161815325	-3.367033869
	H	-1.675973784	-2.241613622	-1.146112480
15	H	-1.074767157	-2.539045992	-2.768401847
	H	1.943730612	-2.051490676	-2.643296663
	H	0.784372012	-0.965058473	-3.367033869

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20 Ni<sup>3+</sup> ^4B C\_2 SSB-D

	Ni	0.000000000	0.000000000	0.222851726
	N	-1.424960256	1.576942170	0.284126089
	N	-1.307937738	-0.617553329	-1.422543304
	N	-1.531359160	-1.043025358	1.271098749
25	C	-2.501796155	1.215147231	1.232753627
	C	-2.087870981	0.038167924	2.093476624
	C	-2.490367025	-1.735229701	0.386902470
	C	-1.894210955	-1.893774991	-0.988833272
	C	-1.869645197	1.770974943	-1.104352507
30	C	-2.281796866	0.450826925	-1.720099479
	H	-2.747030161	2.057752668	1.877630723
	H	-1.096117003	-2.635322449	-0.981849746
	H	-2.648755011	-2.238442107	-1.700922777
	H	-0.759330408	-0.803625005	-2.250070947
35	H	-1.318506996	0.329184947	2.811751427
	H	-3.405483322	0.979168913	0.676039174
	H	-2.392299682	0.572206383	-2.797811041
	H	-2.750896213	-2.710593497	0.796634292
	H	-1.021779219	2.452645021	0.588269301
40	H	-3.255017557	0.149049168	-1.341897053
	H	-2.943685179	-0.313997428	2.677782054
	H	-1.107709673	-1.723961942	1.889203913
	H	-2.702927109	2.473852632	-1.166653458
	H	-3.409261774	-1.155945468	0.345404327
45	H	-1.037857388	2.215030360	-1.649959272
	N	1.307937738	0.617553329	-1.422543304
	N	1.531359160	1.043025358	1.271098749
	N	1.424960256	-1.576942170	0.284126089
	C	2.281796866	-0.450826925	-1.720099479
50	C	1.894210955	1.893774991	-0.988833272
	H	0.759330408	0.803625005	-2.250070947
	C	2.087870981	-0.038167924	2.093476624
	C	2.490367025	1.735229701	0.386902470
	H	1.107709673	1.723961942	1.889203913
55	C	1.869645197	-1.770974943	-1.104352507
	C	2.501796155	-1.215147231	1.232753627
	H	1.021779219	-2.452645021	0.588269301
	H	2.392299682	-0.572206383	-2.797811041
	H	3.255017557	-0.149049168	-1.341897053
60	H	2.648755011	2.238442107	-1.700922777
	H	1.096117003	2.635322449	-0.981849746
	H	1.318506996	-0.329184947	2.811751427
	H	2.943685179	0.313997428	2.677782054
	H	2.750896213	2.710593497	0.796634292
65	H	3.409261774	1.155945468	0.345404327
	H	1.037857388	-2.215030360	-1.649959272
	H	2.702927109	-2.473852632	-1.166653458
	H	2.747030161	-2.057752668	1.877630723
	H	3.405483322	-0.979168913	0.676039174

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