Supplementary Information

Comparison of the reactivity and structures for the neutral and cationic bis(imino)pyridyl iron and cobalt species by DFT calculations

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22. Coordinates of all optimized structures:

Optimized Structures:

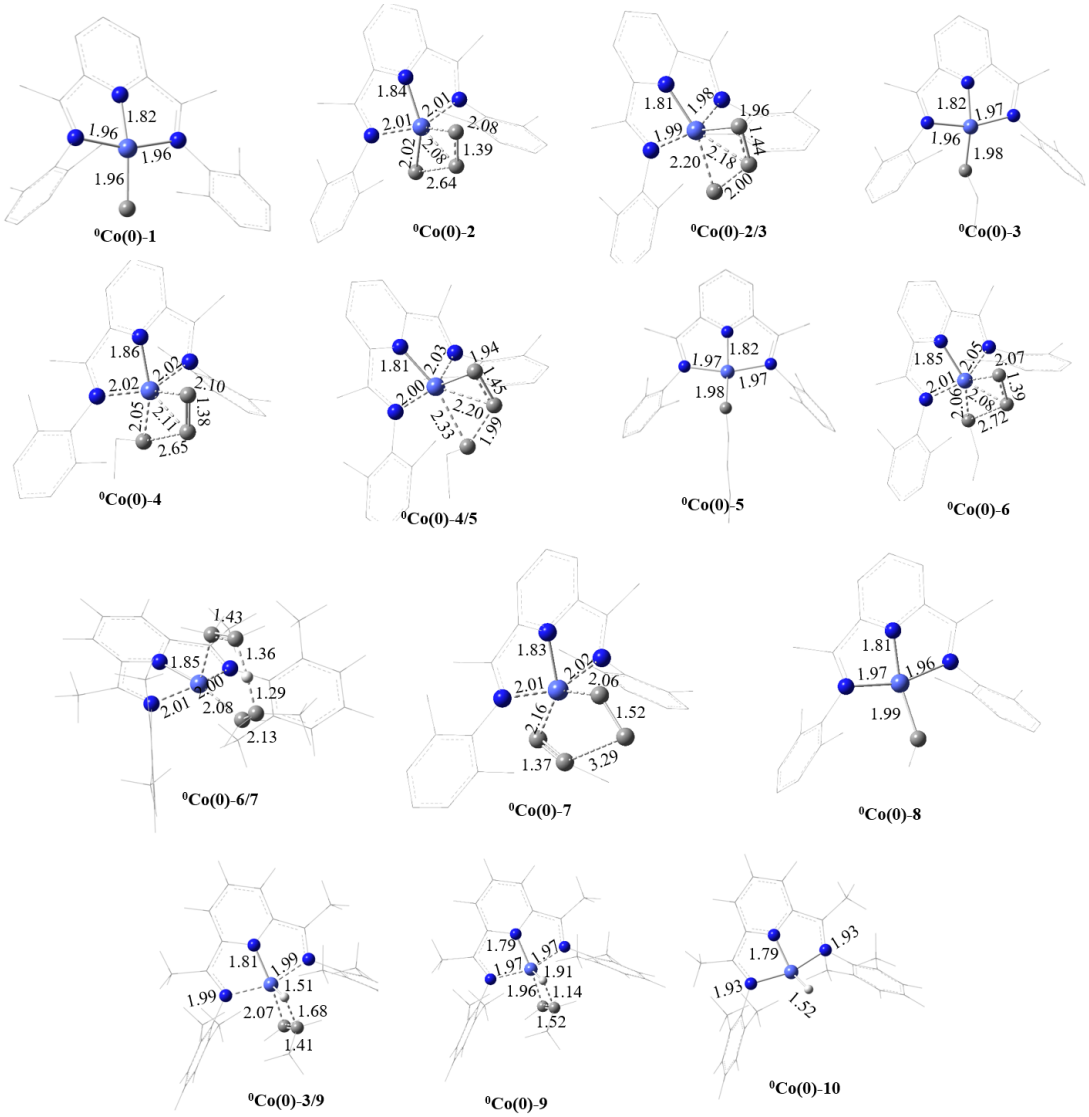

Figure S1 The DFT optimized structures of the neutral cobalt system **^{0}Co(0)** in Figure 1. The bond distance is listed for the active center in Å.

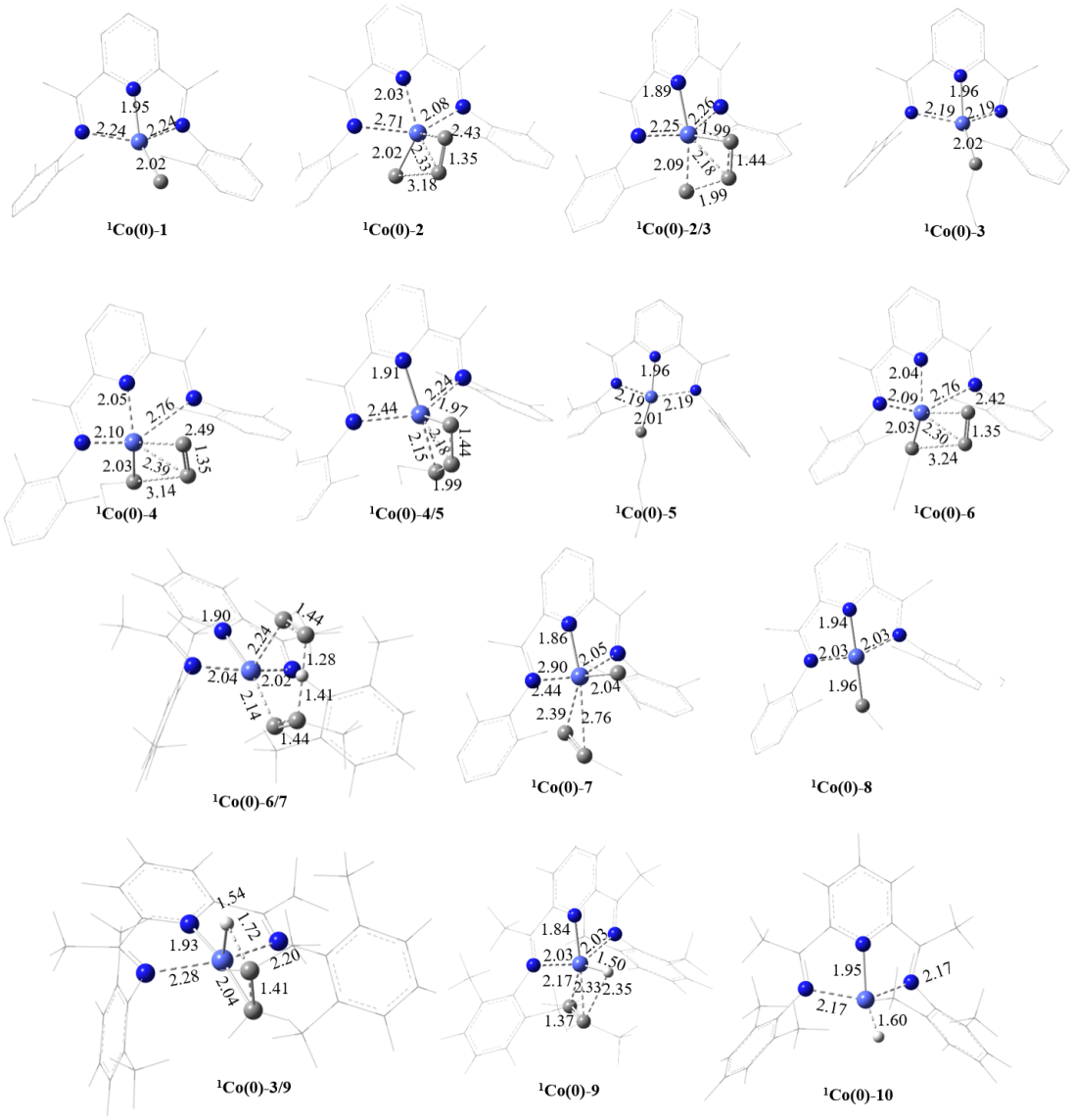

Figure S2 The DFT optimized structures of the neutral cobalt system **¹Co(0)** in Figure 1. The bond distance is listed for the active center in Å.

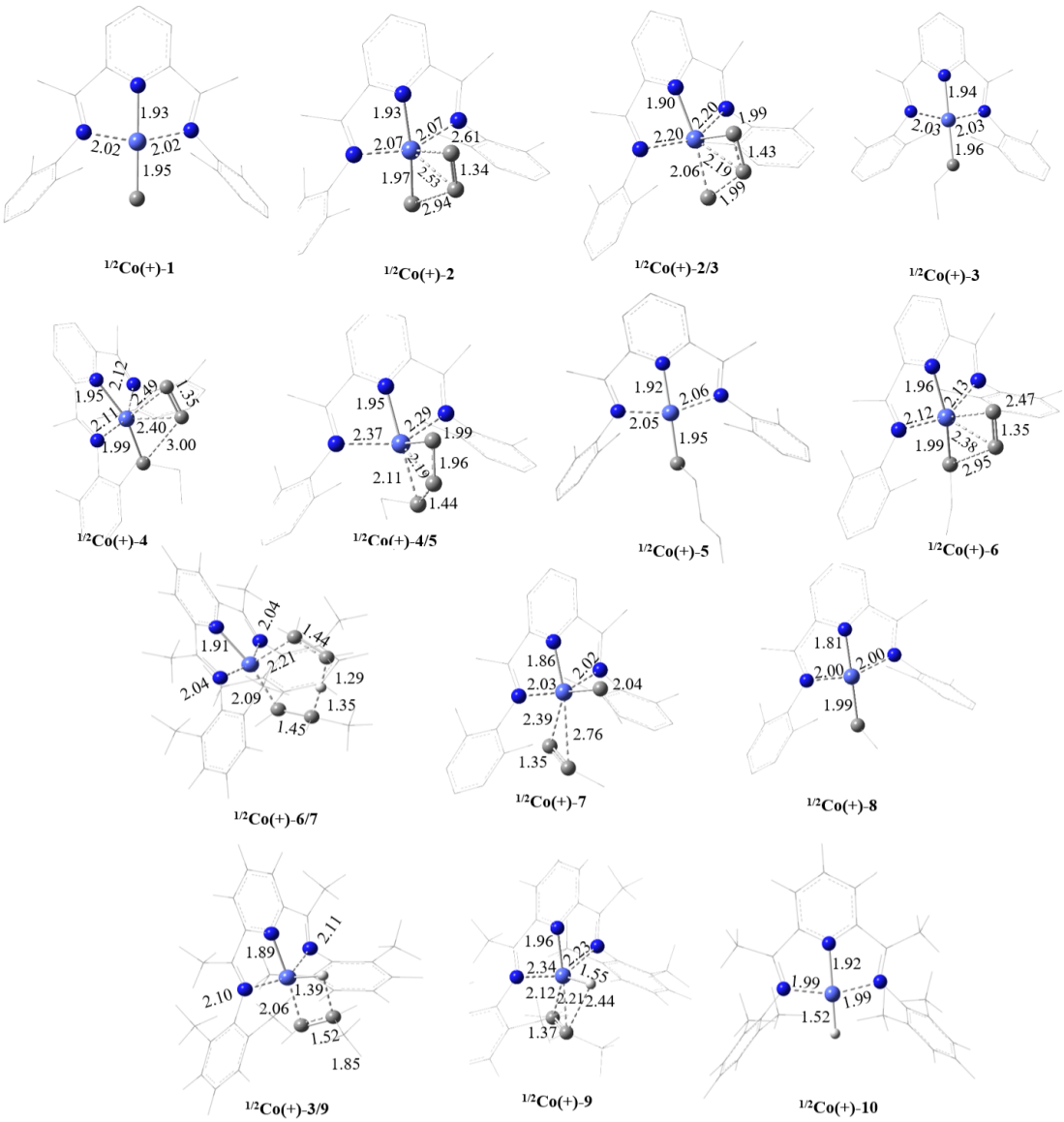

Figure S3 The DFT optimized structures of the cation cobalt system **$^{1/2}$Co(+)** in Figure 3. The bond distance is listed for the active center in Å.

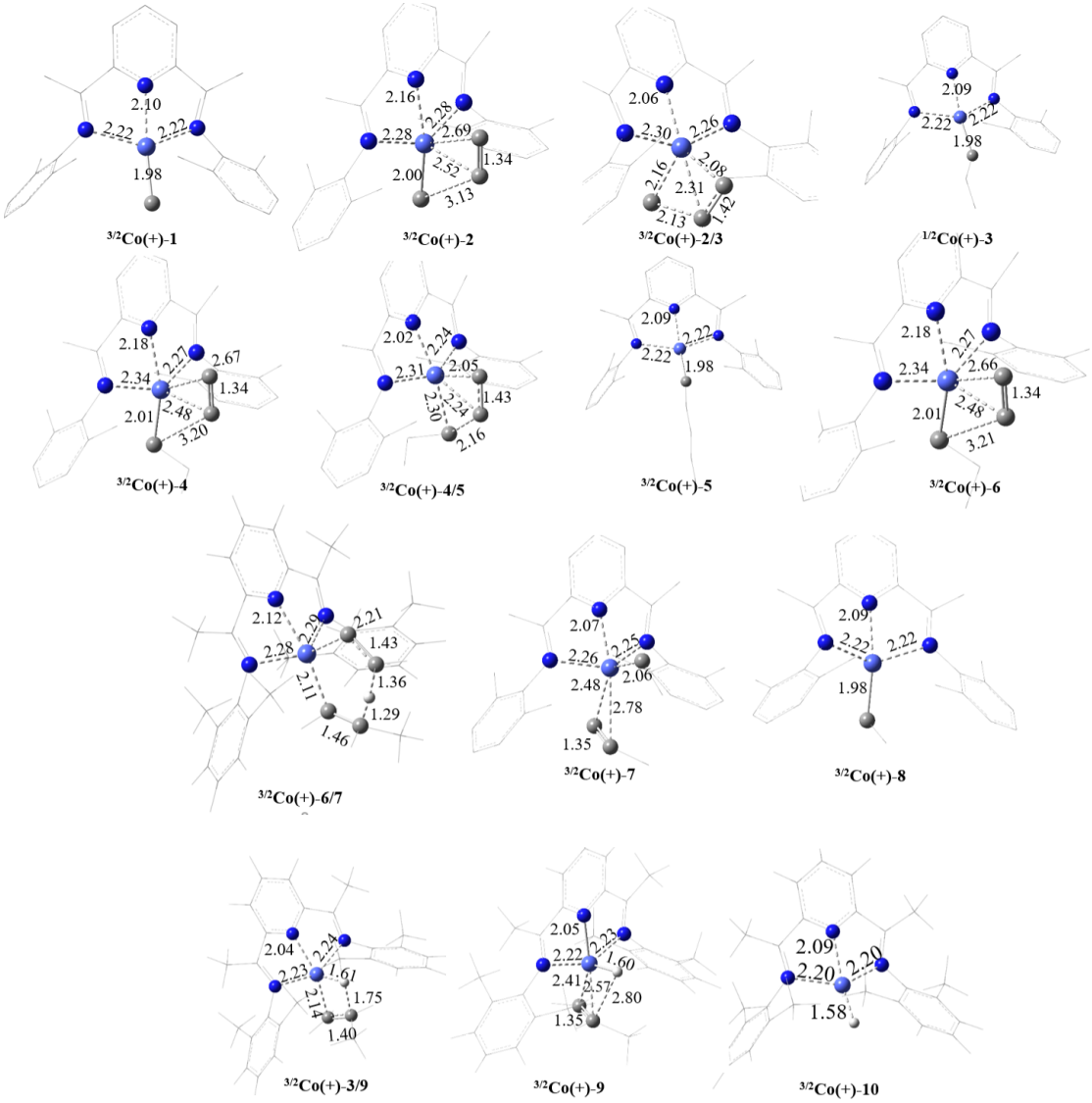

Figure S4 The DFT optimized structures of the cation cobalt system **$^{3/2}$Co(+)** in Figure 3. The bond distance is listed for the active center in Å.

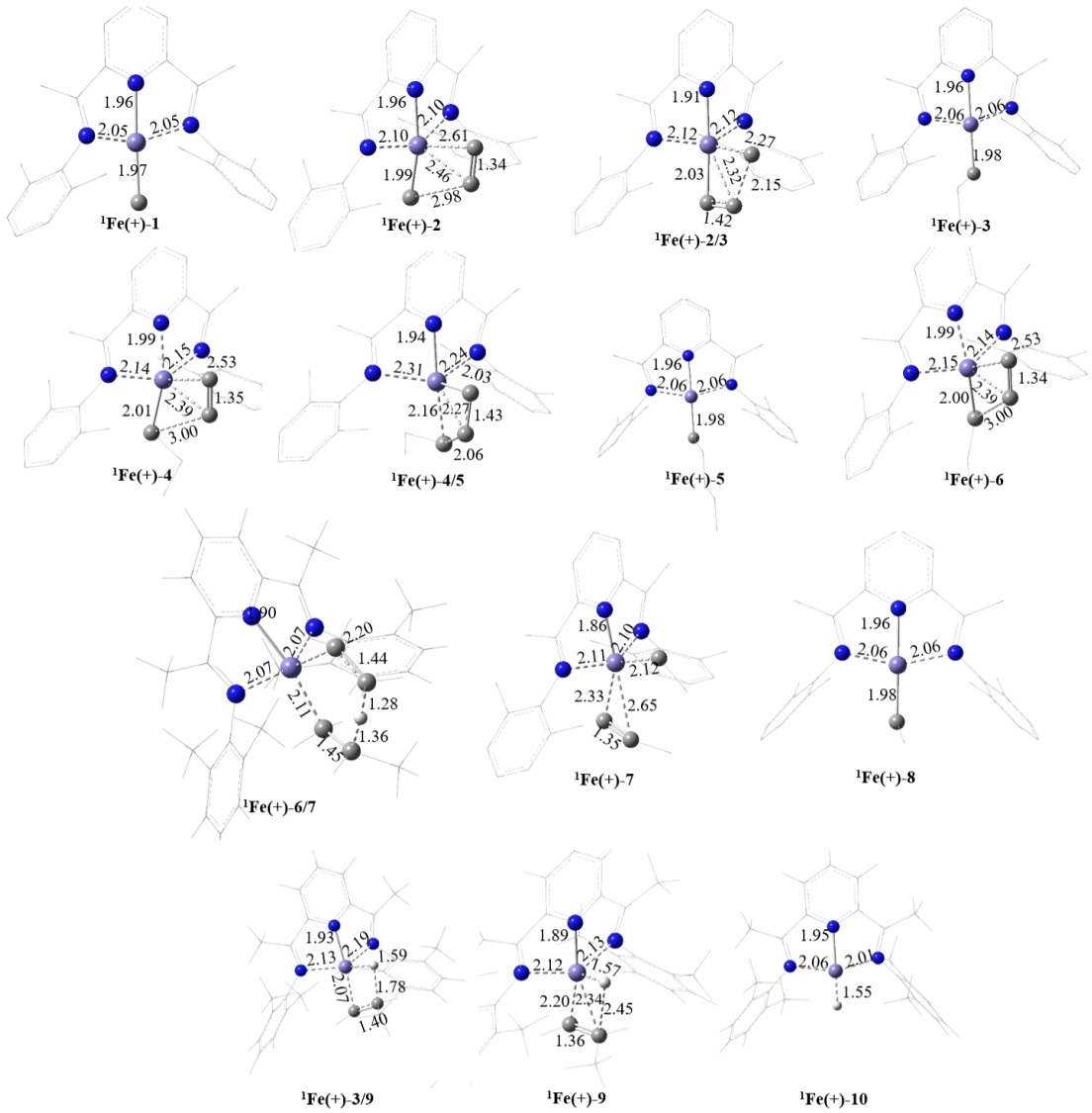

Figure S5 The DFT optimized structures of the cation iron system **¹Fe(+)** in Figure 5. The bond distance is listed for the active center in Å.

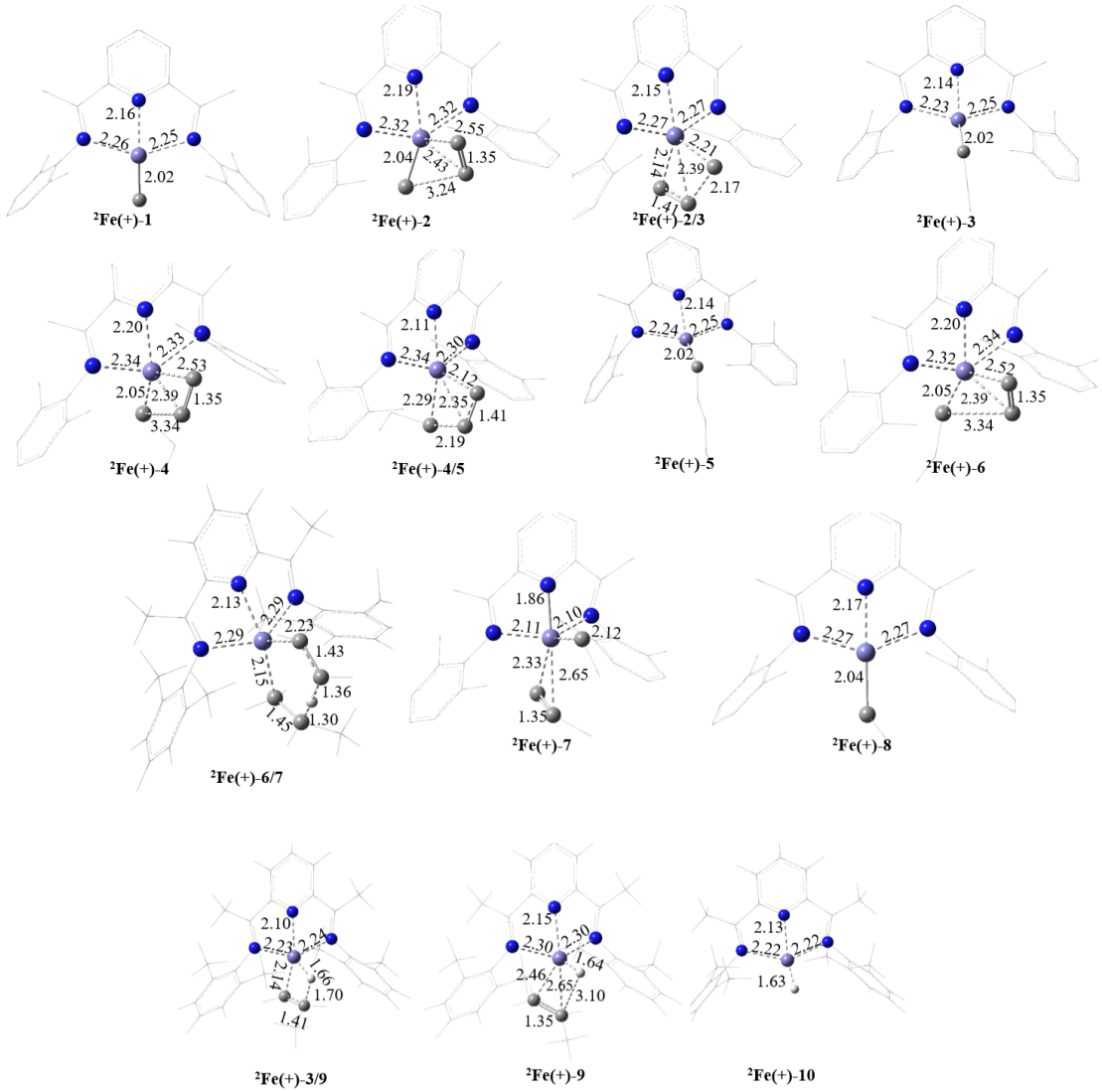

Figure S6 The DFT optimized structures of the cation iron system **²Fe(+)** in Figure 5. The bond distance is listed for the active center in Å.

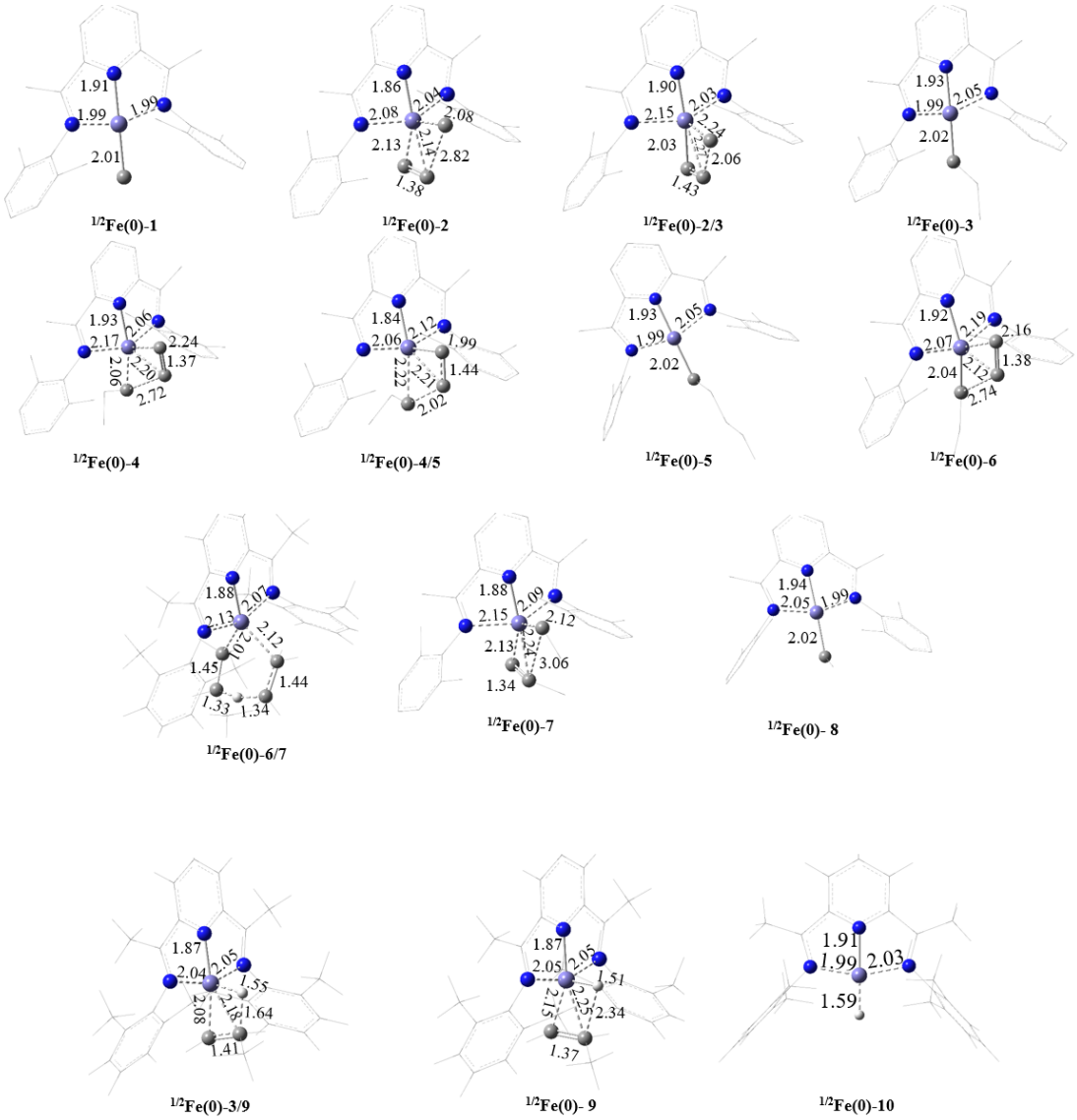

Figure S7 The DFT optimized structures of the neutral iron system **$^{1/2}$Fe(0)** in Figure 6. The bond distance is listed for the active center in Å.

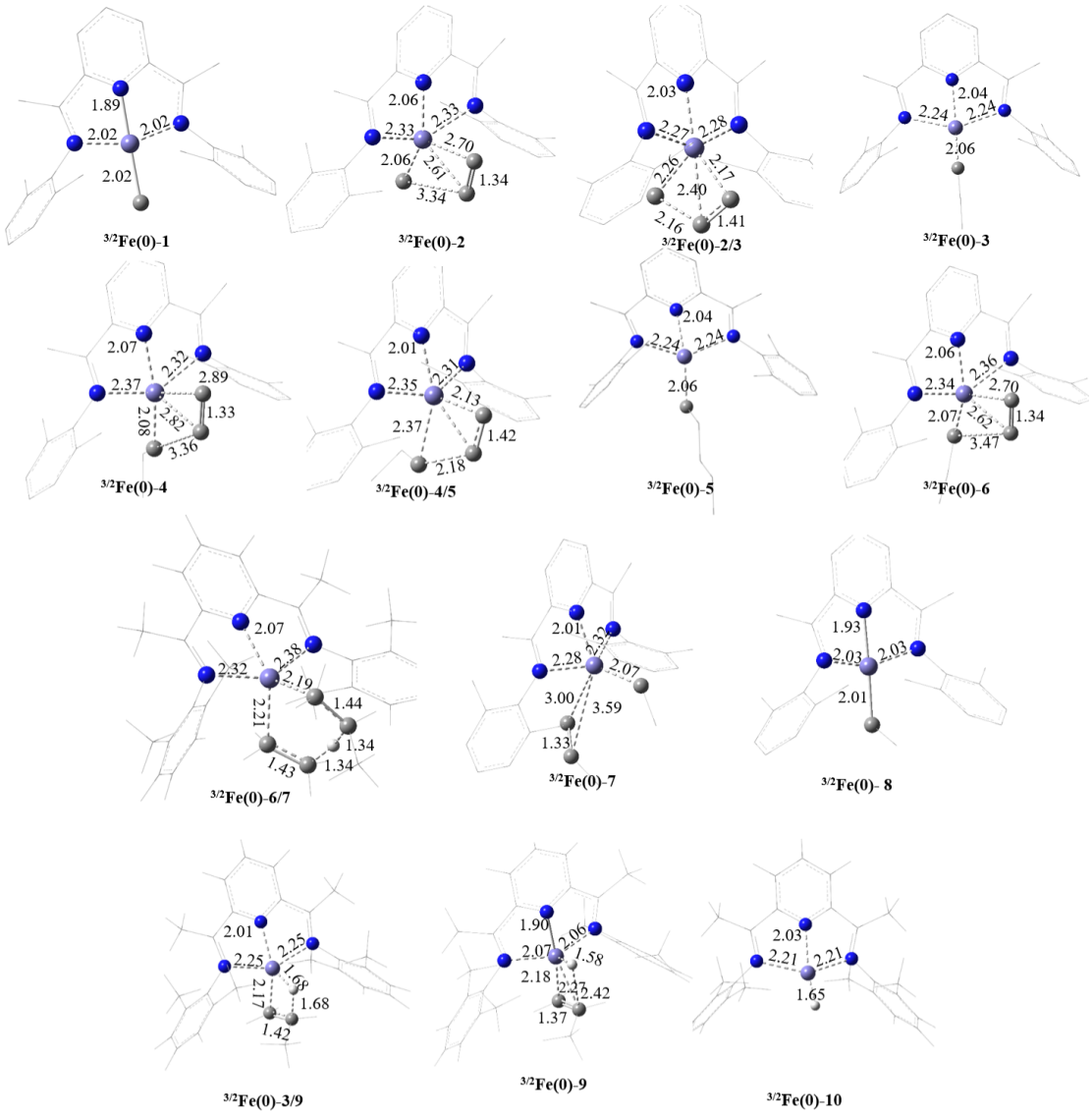

Figure S8 The DFT optimized structures of the neutral cobalt system **$^{3/2}$Fe(0)** in Figure 6. The bond distance is listed for the active center in Å.

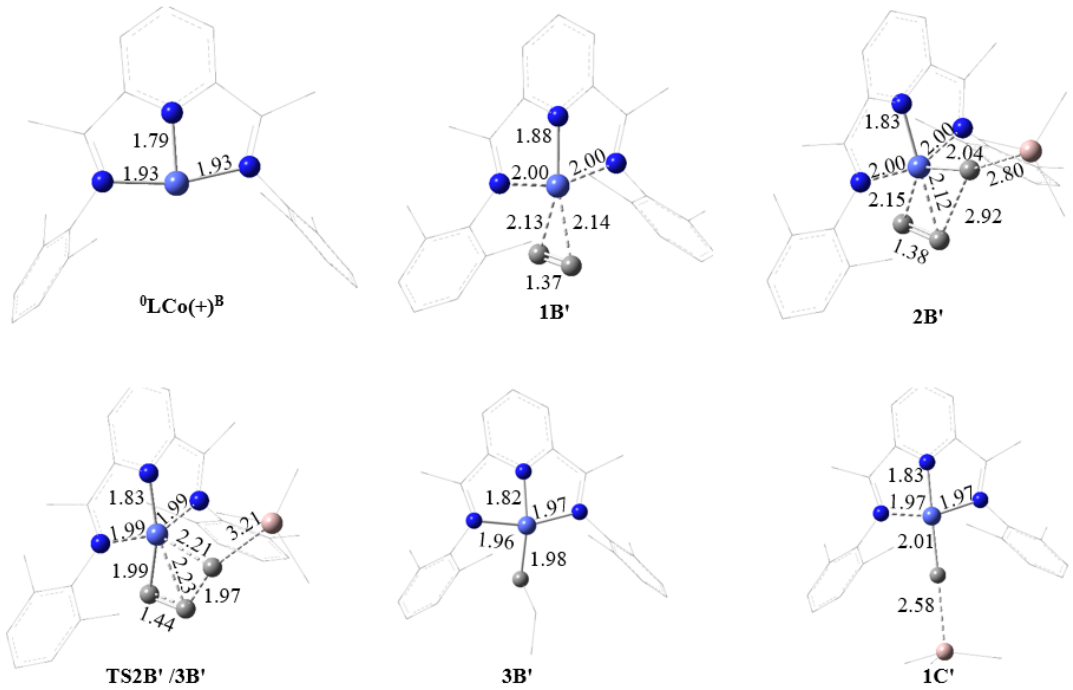

Figure S9 The DFT optimized structures of the cobalt system ^{0}**LCo(+)^{B}** in Figure 9. The bond distance is listed for the active center in Å.

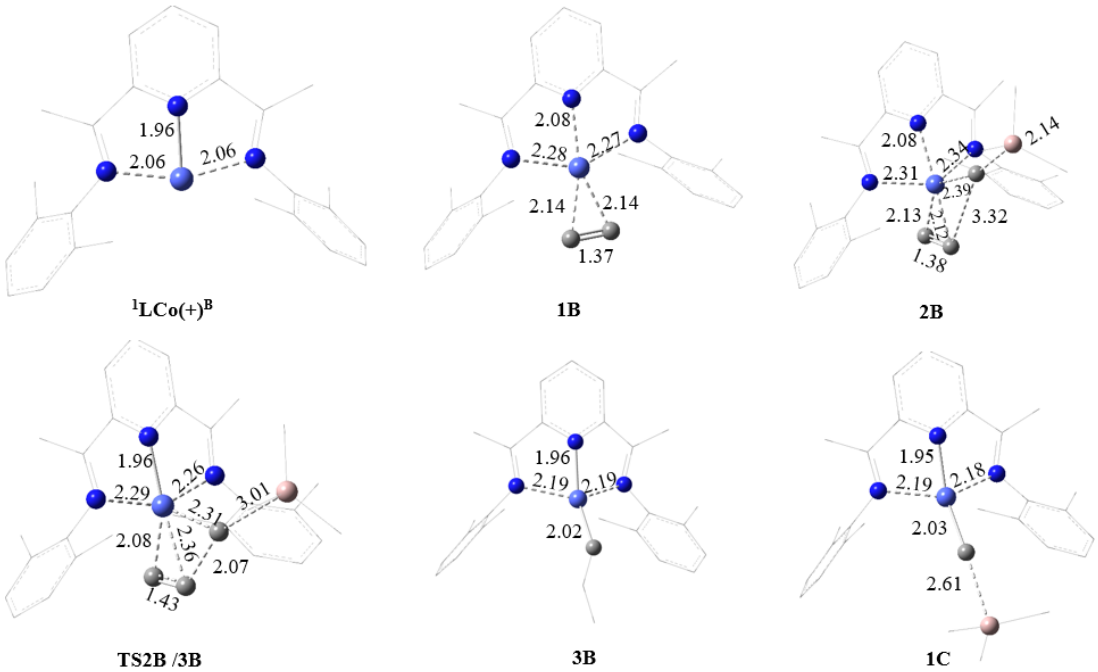

Figure S10 The DFT optimized structures of the cobalt system ^{1}**LCo(+)^{B}** in Figure 9. The bond distance is listed for the active center in Å.

Table S1 The factors for calculating the structure parameter Δ in **^{0}Co(0)**.

^{0}Co(0)	d_1	d_1'	d_2	d_2'	d_3	d_3'	Δ
1	1.372	1.372	1.445	1.445	1.318	1.318	0.100
2	1.376	1.376	1.436	1.436	1.325	1.325	0.085
TS-2/3	1.384	1.385	1.424	1.423	1.340	1.341	0.061
3	1.374	1.374	1.442	1.442	1.320	1.320	0.096
4	1.373	1.373	1.436	1.436	1.328	1.328	0.086
TS-4/5	1.385	1.384	1.420	1.422	1.342	1.341	0.058
5	1.375	1.375	1.442	1.442	1.320	1.320	0.095

Table S2 The factors for calculating the structure parameter Δ in **^{1}Co(0)**.

^{1}Co(0)	d_1	d_1'	d_2	d_2'	d_3	d_3'	Δ
1	1.372	1.372	1.461	1.461	1.304	1.304	0.123
2	1.368	1.383	1.484	1.441	1.285	1.323	0.123
TS-2/3	1.377	1.377	1.454	1.455	1.308	1.307	0.112
3	1.369	1.370	1.455	1.455	1.313	1.313	0.114
4	1.386	1.369	1.438	1.485	1.325	1.284	0.120
TS-4/5	1.376	1.385	1.463	1.443	1.299	1.315	0.109
5	1.370	1.370	1.455	1.455	1.312	1.312	0.114

Table S3 The factors for calculating the structure parameter Δ in **$^{1/2}$Co(+)**.

$^{1/2}$Co(+)	d_1	d_1'	d_2	d_2'	d_3	d_3'	Δ
1	1.337	1.337	1.491	1.491	1.297	1.297	0.174
2	1.341	1.341	1.486	1.486	1.296	1.296	0.167
TS-2/3	1.349	1.350	1.485	1.486	1.290	1.290	0.166
3	1.337	1.337	1.490	1.490	1.297	1.297	0.173
4	1.343	1.342	1.484	1.483	1.295	1.296	0.165
TS-4/5	1.350	1.350	1.492	1.489	1.283	1.285	0.174
5	1.340	1.340	1.485	1.485	1.297	1.297	0.167

Table S4 The factors for calculating the structure parameter Δ in **$^{3/2}$Co(+)**.

$^{3/2}$Co(+)	d_1	d_1'	d_2	d_2'	d_3	d_3'	Δ
1	1.338	1.338	1.497	1.497	1.286	1.286	0.185
2	1.338	1.338	1.496	1.496	1.283	1.283	0.185
TS-2/3	1.345	1.344	1.494	1.494	1.285	1.284	0.180
3	1.338	1.338	1.496	1.496	1.288	1.288	0.183
4	1.339	1.339	1.496	1.495	1.282	1.284	0.185
TS-4/5	1.345	1.345	1.487	1.485	1.290	1.292	0.168
5	1.338	1.338	1.495	1.495	1.288	1.288	0.183

Table S5 The factors for calculating the structure parameter Δ in **^{1}Fe(+)**.

^{1}Fe(+)	d_1	d_1'	d_2	d_2'	d_3	d_3'	Δ
1	1.344	1.344	1.481	1.481	1.300	1.300	0.159
2	1.352	1.352	1.473	1.473	1.302	1.302	0.146
TS-2/3	1.357	1.357	1.467	1.467	1.305	1.305	0.136
3	1.347	1.347	1.476	1.476	1.302	1.302	0.150
4	1.352	1.352	1.471	1.472	1.300	1.301	0.145
TS-4/5	1.360	1.360	1.474	1.470	1.294	1.298	0.144
5	1.348	1.348	1.475	1.474	1.303	1.303	0.149

Table S6 The factors for calculating the structure parameter Δ in **^{2}Fe(+)**.

^{2}Fe(+)	d_1	d_1'	d_2	d_2'	d_3	d_3'	Δ
1	1.337	1.337	1.498	1.498	1.285	1.285	0.187
2	1.342	1.342	1.492	1.497	1.284	1.283	0.182
TS-2/3	1.343	1.344	1.491	1.491	1.285	1.285	0.177
3	1.339	1.339	1.495	1.496	1.289	1.288	0.182
4	1.343	1.342	1.496	1.491	1.283	1.286	0.180
TS-4/5	1.347	1.347	1.488	1.487	1.288	1.289	0.170
5	1.339	1.339	1.496	1.495	1.288	1.288	0.182

Table S7 The factors for calculating the structure parameter Δ in **$^{1/2}$Fe(0)**.

$^{1/2}$Fe(0)	d_1	d_1'	d_2	d_2'	d_3	d_3'	Δ
1	1.369	1.369	1.447	1.447	1.332	1.332	0.097
2	1.371	1.375	1.441	1.432	1.323	1.334	0.086
TS-2/3	1.365	1.381	1.458	1.431	1.31	1.341	0.095
3	1.375	1.356	1.432	1.461	1.346	1.313	0.099
4	1.362	1.376	1.462	1.431	1.306	1.337	0.101
TS-4/5	1.388	1.381	1.425	1.435	1.336	1.324	0.073
5	1.373	1.355	1.43	1.461	1.346	1.314	0.098

Table S8 The factors for calculating the structure parameter Δ in **$^{3/2}$Fe(0)**.

$^{3/2}$Fe(0)	d_1	d_1'	d_2	d_2'	d_3	d_3'	Δ
1	1.371	1.365	1.448	1.443	1.332	1.331	0.095
2	1.379	1.379	1.457	1.456	1.305	1.305	0.115
TS-2/3	1.377	1.378	1.452	1.451	1.308	1.309	0.109
3	1.373	1.373	1.454	1.454	1.311	1.311	0.112
4	1.378	1.380	1.459	1.453	1.302	1.307	0.114
TS-4/5	1.375	1.379	1.456	1.447	1.306	1.315	0.107
5	1.371	1.371	1.454	1.454	1.311	1.311	0.112

Table S9 The NBO charge distribution for sM(q)-1 and sM(q)-2, M includes iron and cobalt, s means the spin states and the q refers to the charge number.

^{s}M(*q*)-1	$^{1/2}$Co(+)	$^{3/2}$Co(+)	^{1}Fe(+)	^{2}Fe(+)	^{0}Co(0)	^{1}Co(0)	$^{1/2}$Fe(0)	$^{3/2}$Fe(0)
PBI	0.060	-0.089	-0.030	-0.095	-0.449	-0.705	-0.540	-0.760
M	0.746	1.060	0.837	1.090	0.428	0.911	0.617	0.818
CH_3	-0.321	-0.466	-0.320	-0.484	-0.365	-0.529	-0.451	-0.426
2Ar	0.515	0.496	0.514	0.492	0.385	0.327	0.374	0.369
^{s}M(*q*)-2	$^{1/2}$Co(+)	$^{3/2}$Co(+)	^{1}Fe(+)	^{2}Fe(+)	^{0}Co(0)	^{1}Co(0)	$^{1/2}$Fe(0)	$^{3/2}$Fe(0)
PBI	0.049	-0.073	-0.065	-0.072	-0.402	-0.677	-0.393	-0.774
M	0.648	1.010	0.968	1.020	0.192	0.831	0.283	0.968
CH_3	-0.294	-0.488	-0.272	-0.469	-0.201	-0.485	-0.248	-0.549
C_2H_4	0.098	0.078	0.103	0.072	0.038	0.036	0.010	0.054
2Ar	0.498	0.472	0.490	0.449	0.373	0.295	0.347	0.301

Table S10 The factors for calculating the structure parameter Δ in ^{0}Co(+)^{B}.

^{0}Co(+)^{B}	d_1	d_1'	d_2	d_2'	d_3	d_3'	Δ
LCo(+)^{B}	1.350	1.350	1.477	1.477	1.302	1.302	0.150
1B	1.343	1.343	1.479	1.479	1.299	1.299	0.158
2B	1.375	1.375	1.435	1.435	1.327	1.327	0.084
TS2B/3B	1.381	1.381	1.433	1.433	1.330	1.330	0.077
3B	1.374	1.374	1.442	1.442	1.320	1.320	0.095
1C	1.364	1.364	1.452	1.452	1.312	1.312	0.114

Table S11 The factors for calculating the structure parameter Δ in ^{1}Co(+)^{B}.

^{1}Co(+)^{B}	d_1	d_1'	d_2	d_2'	d_3	d_3'	Δ
LCo(+)^{B}	1.334	1.334	1.497	1.497	1.298	1.298	0.181
1B	1.342	1.342	1.492	1.492	1.283	1.283	0.180
2B	1.346	1.345	1.484	1.485	1.288	1.288	0.168
TS2B/3B	1.376	1.375	1.457	1.456	1.306	1.306	0.116
3B	1.369	1.370	1.455	1.455	1.313	1.313	0.114
1C	1.368	1.368	1.458	1.458	1.310	1.310	0.119

Coordinate of all optimized structures:

B3LYP/6-311G*[SDD]

^{0}Co(0)

^{0}Co(0)-1

Atom	x	y	z
C	-1.18944000	2.46497300	0.13456600
C	-1.20792100	3.85634600	0.11032400
C	0.00003800	4.55956200	0.10668100
C	1.20798300	3.85632100	0.11037800
C	1.18947800	2.46494900	0.13462600
N	0.00000900	1.78253800	0.17006300
H	0.00004900	5.64323200	0.08689200
H	-2.15189700	4.38958900	0.08895000
H	2.15197100	4.38954600	0.08902600
C	-2.30239900	1.54378200	0.10287700
C	2.30242100	1.54375000	0.10289100
N	1.93606400	0.27914700	0.03822500
N	-1.93607200	0.27917200	0.03815400
C	3.72112400	2.03708100	0.14205400
H	3.95869500	2.61631600	-0.75651500
H	3.87604200	2.69942900	0.99884700
H	4.43216300	1.21623500	0.21152000
C	-3.72109400	2.03713400	0.14209300
H	-3.87599600	2.69938000	0.99897000
H	-3.95865800	2.61648500	-0.75640000
H	-4.43214700	1.21629100	0.21146500
C	2.92510800	-0.75630600	0.00804500
C	3.24299700	-1.42675600	1.20172600
C	3.51234400	-1.12009400	-1.21626400
C	4.18181300	-2.45947500	1.15213300
C	4.44457000	-2.16065300	-1.21968600
C	4.78300300	-2.82629600	-0.04703600
H	4.43771500	-2.98377200	2.06829400
H	4.90220800	-2.45448100	-2.15985100
H	5.50647400	-3.63509200	-0.06884200
C	-2.92513100	-0.75626500	0.00792900
C	-3.51213500	-1.12021500	-1.21644100
C	-3.24324900	-1.42656100	1.20164000
C	-4.44435400	-2.16078400	-1.21990400
C	-4.18204600	-2.45929400	1.15200300
C	-4.78300400	-2.82627800	-0.04723400
H	-4.90181100	-2.45473700	-2.16011800

H	-4.43811500	-2.98347300	2.06818400
H	-5.50645800	-3.63508800	-0.06907500
C	-3.13696600	-0.41694300	-2.49668000
H	-3.52347300	0.60740700	-2.53207600
H	-2.05168000	-0.35234100	-2.60547700
H	-3.53908600	-0.94664800	-3.36246700
C	-2.58813800	-1.04118300	2.50418000
H	-1.49840300	-1.10532000	2.43424500
H	-2.82083400	-0.01106200	2.79215700
H	-2.91690000	-1.69537000	3.31403000
C	3.13739800	-0.41665600	-2.49647600
H	2.05212700	-0.35210400	-2.60547600
H	3.52384200	0.60772400	-2.53164100
H	3.53972500	-0.94620800	-3.36226000
C	2.58763000	-1.04156200	2.50419100
H	2.82022000	-0.01146500	2.79233800
H	1.49791200	-1.10574700	2.43404100
H	2.91627000	-1.69583400	3.31402200
Co	-0.00004800	-0.02519700	-0.02513500
C	0.00012500	-1.83613300	-0.76790400
H	0.00001300	-2.45919200	0.14722100
H	-0.88856200	-2.12704100	-1.33545600
H	0.88895400	-2.12699900	-1.33524900

^{0}Co(0)-2

Atom	x	y	z
C	1.19341500	2.46349400	-0.09732300
C	1.20648500	3.84999700	-0.21801300
C	-0.00022100	4.55164400	-0.27494800
C	-1.20687000	3.84982400	-0.21779800
C	-1.19343800	2.46340300	-0.09711400
N	-0.00000300	1.78225400	-0.02749900
H	-0.00027600	5.63105800	-0.37311700
H	2.14836600	4.38343600	-0.27895300
H	-2.14895100	4.38297400	-0.27850800
C	2.31277500	1.56474300	-0.07977700
C	-2.31290100	1.56474000	-0.07950000
N	-1.97207500	0.28847000	0.02848200
N	1.97176300	0.28846100	0.02837100
C	-3.72397000	2.06280400	-0.24501800
H	-3.88447100	2.98391600	0.31941100
H	-3.94204600	2.28479000	-1.29563700
H	-4.45396000	1.32808900	0.09008100
C	3.72406300	2.06180100	-0.24618100

H	3.94616900	2.27044400	-1.29871700
H	3.88194800	2.98996800	0.30713900
H	4.45336100	1.33183100	0.10075300
C	-2.99663400	-0.71140800	-0.09203100
C	-3.30103900	-1.20160800	-1.37852700
C	-3.68110100	-1.19361400	1.04067000
C	-4.23940200	-2.22803400	-1.50082400
C	-4.61787500	-2.21793000	0.86835100
C	-4.88747300	-2.74758900	-0.38674800
H	-4.46363600	-2.62001300	-2.48872700
H	-5.14768900	-2.59501400	1.73849700
H	-5.61112200	-3.54883500	-0.49820300
C	2.99654800	-0.71121200	-0.09200100
C	3.68117700	-1.19294900	1.04083600
C	3.30109400	-1.20170600	-1.37835100
C	4.61842200	-2.21686300	0.86877200
C	4.23993100	-2.22774500	-1.50037600
C	4.88830100	-2.74668200	-0.38620200
H	5.14835700	-2.59353400	1.73902400
H	4.46425800	-2.61994100	-2.48817600
H	5.61232500	-3.54761500	-0.49746200
C	3.47689400	-0.61546700	2.42238900
H	3.29398900	0.46018700	2.39749600
H	2.63061600	-1.07173900	2.94202200
H	4.36234900	-0.78697600	3.03844000
C	2.67318100	-0.61090200	-2.61669800
H	1.64291800	-0.30582900	-2.44332900
H	3.22408700	0.27665700	-2.95014000
H	2.68841300	-1.32733500	-3.44060600
C	-3.47717900	-0.61616200	2.42227800
H	-2.63030500	-1.07159500	2.94167000
H	-3.29545100	0.45970100	2.39748500
H	-4.36233300	-0.78870100	3.03847000
C	-2.67357800	-0.60977500	-2.61659800
H	-3.22375600	0.27892300	-2.94823100
H	-1.64282800	-0.30605200	-2.44366100
H	-2.69035600	-1.32500300	-3.44151700
C	-0.00005200	-1.81277400	-0.69901300
H	-0.00005300	-1.60239200	-1.77373400
H	0.88416400	-2.41303800	-0.47665400
H	-0.88430900	-2.41298500	-0.47667200
C	0.00002700	-1.33712400	1.89877000
H	0.91011300	-1.92250600	1.87697000

H	-0.90993100	-1.92270400	1.87685200
C	-0.00014300	-0.02482800	2.34924900
H	-0.91220500	0.46531900	2.66500400
H	0.91178200	0.46553700	2.66506000
Co	0.00000200	-0.03606600	0.27046500

^{0}Co(0)-2/3

Atom	x	y	z
C	1.20267100	2.51469200	-0.11794800
C	1.19911600	3.90078100	-0.24317400
C	-0.01311700	4.59487600	-0.28465900
C	-1.22027700	3.89262000	-0.21275600
C	-1.21133800	2.50702200	-0.08870000
N	-0.00203400	1.83709900	-0.02247200
H	-0.01800500	5.67388500	-0.38872600
H	2.13387100	4.44438400	-0.31717200
H	-2.15950900	4.43086400	-0.26442200
C	2.30882400	1.62009000	-0.11194000
C	-2.31224700	1.60430100	-0.06306800
N	-1.94002400	0.32040400	0.03261500
N	1.94116800	0.33534800	-0.00238500
C	-3.74643300	2.03976700	-0.17693800
H	-4.33349300	1.73932800	0.69631900
H	-3.82792200	3.12194100	-0.27349100
H	-4.23558300	1.59138800	-1.04721100
C	3.73954800	2.05891200	-0.24793100
H	3.81197400	3.13163000	-0.42525500
H	4.32390400	1.83202600	0.64973200
H	4.23774400	1.55120900	-1.07900600
C	-2.94785500	-0.68832700	-0.10795000
C	-3.19626500	-1.19004800	-1.40541900
C	-3.66611000	-1.18370400	0.99661100
C	-4.13289900	-2.21130500	-1.56773500
C	-4.59686800	-2.20794700	0.78696900
C	-4.82675400	-2.72887500	-0.47874500
H	-4.32041200	-2.60254200	-2.56351700
H	-5.15440300	-2.59125900	1.63715600
H	-5.55130400	-3.52469200	-0.61967600
C	2.93663300	-0.68542500	-0.13031400
C	3.67150400	-1.14874900	0.97823400
C	3.15539200	-1.23734300	-1.41294700
C	4.57167600	-2.20442400	0.79319400
C	4.06023700	-2.29055000	-1.55002500
C	4.75863900	-2.78522400	-0.45337600

H	5.13921100	-2.56496100	1.64694400
H	4.22164700	-2.72332500	-2.53322200
H	5.45680800	-3.60741200	-0.57491000
C	3.55389900	-0.53222900	2.35370800
H	4.53779400	-0.46844600	2.82601000
H	3.13002500	0.47027500	2.32536300
H	2.92227000	-1.13023800	3.01781200
C	2.46848300	-0.67373300	-2.63292700
H	1.41999600	-0.43814100	-2.44563300
H	2.93788600	0.26345100	-2.95311400
H	2.52680300	-1.37049800	-3.47162100
C	-3.48703200	-0.64074900	2.39516100
H	-2.74129100	-1.20909400	2.95898800
H	-3.16438000	0.40009900	2.39860800
H	-4.42503600	-0.70540700	2.95202900
C	-2.47613600	-0.62643700	-2.60519300
H	-2.73563100	0.42281400	-2.77900100
H	-1.39230100	-0.65376200	-2.47662700
H	-2.73043200	-1.18481800	-3.50829600
C	-0.01984700	-2.09202300	-0.11817500
H	0.24016700	-1.66638400	-1.08894900
H	0.68717500	-2.89640300	0.06172700
H	-1.03004100	-2.48515800	-0.16483000
C	0.11415100	-1.53704200	1.79362100
H	1.07016000	-2.02291400	1.94453000
H	-0.71645000	-2.19561100	2.02684000
C	0.02451900	-0.17463500	2.25275100
H	-0.90279400	0.17516900	2.68837900
H	0.91037500	0.28805700	2.67067200
Co	0.00980500	0.06255000	0.31027000

^{0}Co(0)-3

Atom	x	y	z
C	-1.19022100	2.69903200	0.09065500
C	-1.20735300	4.08769000	0.00535300
C	0.00000000	4.79119800	-0.02662900
C	1.20735400	4.08769000	0.00535100
C	1.19022200	2.69903200	0.09065400
N	0.00000000	2.01600700	0.16461300
H	0.00000000	5.87291900	-0.09399800
H	-2.15153800	4.61892900	-0.04276000
H	2.15153900	4.61892800	-0.04276300
C	-2.30446000	1.78299600	0.08871100

C	2.30446000	1.78299600	0.08871000
N	1.94226600	0.51438700	0.05862700
N	-1.94226700	0.51438800	0.05862800
C	3.72183800	2.28156300	0.12352900
H	3.96964000	2.82413600	-0.79484800
H	3.86562700	2.97785800	0.95474200
H	4.43392700	1.46611300	0.23464300
C	-3.72183800	2.28156400	0.12353100
H	-3.86562600	2.97785800	0.95474500
H	-3.96963900	2.82413900	-0.79484500
H	-4.43392700	1.46611500	0.23464300
C	2.93470200	-0.51700000	0.06980300
C	3.20928900	-1.17556200	1.28220100
C	3.57632800	-0.88764200	-1.12540900
C	4.14833000	-2.20879500	1.27967500
C	4.50493000	-1.93131000	-1.08214900
C	4.79362400	-2.58913000	0.10766500
H	4.36988500	-2.72251000	2.21060900
H	5.00217300	-2.23128900	-2.00003600
H	5.51507200	-3.39987800	0.12111200
C	-2.93470300	-0.51699900	0.06980300
C	-3.57632800	-0.88764100	-1.12540900
C	-3.20928900	-1.17556300	1.28220100
C	-4.50492900	-1.93131000	-1.08215000
C	-4.14833000	-2.20879700	1.27967400
C	-4.79362300	-2.58913100	0.10766300
H	-5.00217200	-2.23128800	-2.00003700
H	-4.36988400	-2.72251200	2.21060800
H	-5.51507100	-3.39987900	0.12111000
C	-3.28783500	-0.17559600	-2.42416800
H	-3.78451900	0.80004800	-2.47138300
H	-2.21902700	0.00185900	-2.55616400
H	-3.64496800	-0.76086800	-3.27382200
C	-2.51468600	-0.76865000	2.55763000
H	-1.42689000	-0.81983900	2.45470800
H	-2.75036600	0.26212600	2.84046600
H	-2.80881900	-1.41710400	3.38517900
C	3.28783400	-0.17559800	-2.42416800
H	2.21902600	0.00185800	-2.55616400
H	3.78451900	0.80004600	-2.47138500
H	3.64496600	-0.76087100	-3.27382300
C	2.51468600	-0.76864800	2.55763000
H	2.75036500	0.26212800	2.84046400

H	1.42689000	-0.81983800	2.45470800
H	2.80882000	-1.41710100	3.38518000
C	-0.00000100	-1.52365300	-0.97712000
H	-0.87897400	-1.60105400	-1.62855400
H	0.87897200	-1.60105400	-1.62855500
C	0.00000000	-2.72839400	-0.01594600
H	-0.87712800	-2.69397500	0.64142400
H	0.87712800	-2.69397500	0.64142400
C	0.00000000	-4.08374500	-0.74323900
H	-0.88312800	-4.18430000	-1.38210000
H	0.88312900	-4.18429900	-1.38210000
H	0.00000100	-4.92387500	-0.03852200
Co	0.00000000	0.20716300	-0.01227000

^{0}Co(0)-4

Atom	x	y	z
C	1.19275100	2.61014300	-0.33263400
C	1.20730800	3.96768400	-0.64207700
C	-0.00007800	4.65222500	-0.80238800
C	-1.20744000	3.96764600	-0.64211300
C	-1.19283400	2.61010800	-0.33265900
N	-0.00003400	1.94587300	-0.18603900
H	-0.00009000	5.70686900	-1.05273300
H	2.14941800	4.48881100	-0.76902000
H	-2.14957700	4.48872400	-0.76908100
C	2.31243600	1.72431600	-0.17844500
C	-2.31249200	1.72429200	-0.17840000
N	-1.97159000	0.47042400	0.09400400
N	1.97157000	0.47044400	0.09393000
C	-3.72523100	2.20455800	-0.37895600
H	-3.87081700	3.18817300	0.07327800
H	-3.96906800	2.29982500	-1.44267900
H	-4.44804300	1.51985600	0.06160000
C	3.72517800	2.20450600	-0.37914100
H	3.96947100	2.29813700	-1.44290500
H	3.87043300	3.18883000	0.07162900
H	4.44791500	1.52058200	0.06276300
C	-2.99409200	-0.53673100	0.02925500
C	-3.32213400	-1.06059400	-1.24174900
C	-3.65831100	-0.99536000	1.18095300
C	-4.24858200	-2.10052500	-1.32086400
C	-4.58263100	-2.03806800	1.05282800
C	-4.86738200	-2.60359500	-0.18137800
H	-4.48799500	-2.51787800	-2.29471700

H	-5.09137000	-2.39827500	1.94312200
H	-5.57944500	-3.41898900	-0.25965100
C	2.99410300	-0.53667500	0.02904300
C	3.65871900	-0.99501400	1.18064100
C	3.32172800	-1.06085400	-1.24193200
C	4.58301700	-2.03773000	1.05248300
C	4.24816000	-2.10080000	-1.32107600
C	4.86735300	-2.60356900	-0.18167400
H	5.09204900	-2.39771100	1.94270200
H	4.48725500	-2.51840600	-2.29490000
H	5.57939800	-3.41897600	-0.25998800
C	3.48162500	-0.35886300	2.53985600
H	4.44112600	0.01779600	2.90899300
H	2.78743200	0.47737200	2.52126500
H	3.12264600	-1.07932100	3.28044700
C	2.73941800	-0.48801100	-2.51275900
H	1.72090500	-0.12736600	-2.37455800
H	3.33826200	0.35756500	-2.87106700
H	2.73501400	-1.23457600	-3.30960900
C	-3.48080400	-0.35954100	2.54026200
H	-2.78689400	0.47693200	2.52157600
H	-4.44025700	0.01670100	2.90993800
H	-3.12123900	-1.08008500	3.28048400
C	-2.74014700	-0.48742000	-2.51257500
H	-3.33847600	0.35888600	-2.87000400
H	-1.72124700	-0.12770700	-2.37474100
H	-2.73683000	-1.23350600	-3.30987900
C	0.00008800	-1.83897800	0.26567200
H	0.87775900	-2.23092700	0.79361700
H	-0.87649700	-2.23164800	0.79489000
C	-0.00071000	-2.42723000	-1.14796100
H	0.87219300	-2.08721400	-1.70964100
H	-0.87520000	-2.08858500	-1.70798300
C	0.00045300	-3.96580600	-1.14534300
H	0.88399000	-4.35765600	-0.63106300
H	-0.88156400	-4.35896900	-0.62945200
H	-0.00018500	-4.37424300	-2.16312700
Co	-0.00008600	0.20227700	0.46109500
C	0.00044700	-0.39268200	2.48610800
H	0.91095600	-0.94173900	2.67441100
H	-0.90972500	-0.94202200	2.67521600
C	0.00020600	0.98432100	2.40666100
H	-0.91235900	1.56059600	2.51044600

H	0.91261800	1.56095000	2.50977300

^{0}Co(0)-4/5

Atom	x	y	z
C	1.22933400	2.61767600	-0.26830000
C	1.25028100	3.98570500	-0.52148400
C	0.05165800	4.69127000	-0.65674600
C	-1.16445300	4.01638800	-0.52959700
C	-1.17942600	2.64810800	-0.27525200
N	0.01674300	1.96083100	-0.14904000
H	0.06590600	5.75507800	-0.86436400
H	2.19488800	4.50686900	-0.62086600
H	-2.09557200	4.56035300	-0.63515900
C	2.33234600	1.72976800	-0.14138300
C	-2.30157000	1.78617900	-0.15321400
N	-1.96636800	0.50619400	0.06923800
N	1.97313500	0.45417500	0.06147000
C	-3.72356300	2.25078200	-0.30188400
H	-3.78156800	3.33433800	-0.39889400
H	-4.20438500	1.81429900	-1.18306700
H	-4.33415200	1.96164200	0.55838200
C	3.76545000	2.17466900	-0.24027400
H	4.29570800	1.67053000	-1.05346300
H	3.84101500	3.24760600	-0.41217100
H	4.31747500	1.94753100	0.67709500
C	-3.01717700	-0.46665600	0.00311500
C	-3.34439800	-1.01208300	-1.25818300
C	-3.71243500	-0.88160200	1.15747900
C	-4.31785300	-2.01172200	-1.33022900
C	-4.68576100	-1.87757100	1.03655200
C	-4.98190600	-2.45359800	-0.19253100
H	-4.56004800	-2.44103500	-2.29843300
H	-5.22255200	-2.19767600	1.92524400
H	-5.73560800	-3.23128500	-0.26513000
C	3.01350200	-0.53221000	-0.01317100
C	3.71905900	-0.97606600	1.12130500
C	3.33718500	-1.04602100	-1.29300500
C	4.66630400	-1.99672800	0.97115600
C	4.29420900	-2.05509200	-1.39668900
C	4.94606300	-2.54764200	-0.27003800
H	5.20207700	-2.34585600	1.85011300
H	4.53003000	-2.45915000	-2.37705900
H	5.68067900	-3.34105300	-0.36520200
C	3.56969600	-0.34045100	2.48423900

H	4.52380300	0.09128700	2.80433700
H	2.82996000	0.45503600	2.49211500
H	3.28691700	-1.07123800	3.24766300
C	2.69474100	-0.49382200	-2.54270200
H	1.63204900	-0.29658200	-2.40355000
H	3.15216300	0.45769900	-2.83633200
H	2.81645200	-1.18346500	-3.38066700
C	-3.45703200	-0.27035500	2.51435000
H	-2.64374100	-0.77466600	3.04377400
H	-3.18656600	0.78376300	2.44732200
H	-4.34685200	-0.35173400	3.14289900
C	-2.70759200	-0.50850200	-2.53176000
H	-3.29359500	0.31051000	-2.96538700
H	-1.70294400	-0.12230700	-2.36545300
H	-2.65899100	-1.29867800	-3.28455200
C	-0.26394400	-2.08033900	0.56326300
H	0.15476000	-2.90690900	1.13782600
H	-1.34505000	-2.14813200	0.65722900
C	0.15486500	-2.33636800	-0.89142100
H	1.23801200	-2.28354900	-0.98806100
H	-0.26457800	-1.58970200	-1.56665300
C	-0.31267400	-3.73218900	-1.34051300
H	0.12817800	-4.51804700	-0.71880900
H	-1.40027700	-3.82877000	-1.27780000
H	-0.01802000	-3.92725000	-2.37695000
Co	-0.01036400	0.23501600	0.40592800
C	0.17555700	-1.03086500	2.20052200
H	1.16910800	-1.43156900	2.35658400
H	-0.58191400	-1.63404700	2.69114000
C	0.03897300	0.40172600	2.33356100
H	-0.89140400	0.79509600	2.72711100
H	0.90725100	0.98290500	2.62445400

^{0}Co(0)-5

Atom	x	y	z
C	1.19080900	-3.06892500	0.04151500
C	1.20743800	-4.45501400	-0.07766500
C	0.00000500	-5.15755700	-0.12643500
C	-1.20742900	-4.45501700	-0.07766200
C	-1.19080300	-3.06892700	0.04151700
N	0.00000300	-2.38788700	0.13356400
H	0.00000600	-6.23729200	-0.22034200
H	2.15155800	-4.98499400	-0.13936100
H	-2.15154800	-4.98499900	-0.13935600

C	2.30475700	-2.15342900	0.06080000
C	-2.30475300	-2.15343400	0.06080100
N	-1.94201300	-0.88422900	0.05837800
N	1.94201500	-0.88422500	0.05837800
C	-3.72241100	-2.65181300	0.08702100
H	-3.97238900	-3.17361100	-0.84270800
H	-3.86542400	-3.36612900	0.90291600
H	-4.43371500	-1.83848700	0.21742400
C	3.72241600	-2.65180500	0.08701700
H	3.86542700	-3.36613500	0.90290100
H	3.97239900	-3.17358800	-0.84272000
H	4.43371800	-1.83848100	0.21743600
C	-2.93201500	0.14850800	0.09642900
C	-3.19294400	0.78662600	1.32294600
C	-3.58378700	0.54278900	-1.08575300
C	-4.12780400	1.82329600	1.34770000
C	-4.50777800	1.58919900	-1.01513000
C	-4.78246200	2.22710400	0.18867800
H	-4.33902100	2.32078200	2.28977700
H	-5.01263300	1.90717700	-1.92275600
H	-5.50082600	3.03996500	0.22341400
C	2.93201500	0.14851300	0.09643000
C	3.58378900	0.54279500	-1.08575000
C	3.19293900	0.78663300	1.32294800
C	4.50777800	1.58920700	-1.01512400
C	4.12779700	1.82330500	1.34770400
C	4.78245800	2.22711400	0.18868300
H	5.01263500	1.90718600	-1.92274900
H	4.33900900	2.32079300	2.28978200
H	5.50082000	3.03997600	0.22342100
C	3.31267500	-0.14731900	-2.40009000
H	3.83003300	-1.11109200	-2.46629400
H	2.24829200	-0.34397900	-2.53926300
H	3.65987200	0.46303300	-3.23611700
C	2.48785100	0.35521800	2.58449400
H	1.40091600	0.41025500	2.47423400
H	2.71954900	-0.68144800	2.84816300
H	2.77635900	0.98649700	3.42716700
C	-3.31266600	-0.14732500	-2.40009200
H	-2.24828000	-0.34396400	-2.53927100
H	-3.83000400	-1.11110800	-2.46629000
H	-3.65988100	0.46301700	-3.23612000
C	-2.48785800	0.35521100	2.58449400

H	-2.71955700	-0.68145500	2.84816200
H	-1.40092300	0.41024800	2.47423700
H	-2.77636900	0.98649000	3.42716600
C	0.00000100	1.15303200	-0.97333600
H	0.87909900	1.23026900	-1.62398300
H	-0.87909700	1.23026900	-1.62398200
C	-0.00000100	2.35299600	-0.00662200
H	0.87769100	2.31591900	0.65116800
H	-0.87769300	2.31591400	0.65116800
C	-0.00000400	3.71685900	-0.72255600
H	0.87690100	3.77327500	-1.38069100
H	-0.87690900	3.77327100	-1.38069100
Co	0.00000000	-0.57766200	-0.01012800
C	-0.00000700	4.91800300	0.22953300
H	-0.87599200	4.85769300	0.88791400
H	0.87597800	4.85769600	0.88791500
C	-0.00000900	6.26771400	-0.49338600
H	-0.00001400	7.10515100	0.21132900
H	0.88187700	6.37591500	-1.13320300
H	-0.88189200	6.37590800	-1.13320900

^{0}Co(0)-6

Atom	x	y	z
C	1.05483200	2.70133200	0.24281300
C	1.01042000	4.07671600	0.46290800
C	-0.22051900	4.72060100	0.58758400
C	-1.39729700	3.97294300	0.48938000
C	-1.32673800	2.60202600	0.26746900
N	-0.11004200	1.97282600	0.14337600
H	-0.26392400	5.78886400	0.76548700
H	1.92897800	4.64539000	0.54787600
H	-2.36025400	4.45909100	0.59590600
C	2.20854600	1.85958900	0.13999200
C	-2.41907600	1.67394000	0.18450100
N	-2.04715000	0.42015200	-0.01899100
N	1.92057800	0.57745500	-0.05500800
C	-3.84224100	2.12619000	0.38486800
H	-4.05834800	2.28355200	1.44729800
H	-4.02955200	3.07343200	-0.12532200
H	-4.55642800	1.39411000	0.01295500
C	3.60596600	2.38976000	0.31959100
H	3.66189300	3.45078200	0.07465700
H	3.94437000	2.27436100	1.35501300
H	4.32293000	1.86072600	-0.30829100

C	-3.05736300	-0.59969900	0.03143300
C	-3.75682700	-0.99748800	-1.12441500
C	-3.33597400	-1.19156000	1.28102400
C	-4.68679800	-2.03679200	-1.01568300
C	-4.26925300	-2.22836600	1.33988500
C	-4.93443900	-2.66227200	0.19943500
H	-5.22981800	-2.34881700	-1.90320000
H	-4.47488600	-2.69723900	2.29773100
H	-5.65407800	-3.47247400	0.26023300
C	3.00612900	-0.36061000	-0.00114500
C	3.36887400	-0.89253800	1.25296200
C	3.70297400	-0.73363700	-1.16800600
C	4.37542200	-1.85984300	1.30511300
C	4.70941500	-1.69799800	-1.06527500
C	5.03593800	-2.27480100	0.15590400
H	4.64379200	-2.28716800	2.26712200
H	5.24774700	-1.99216000	-1.96177800
H	5.81309900	-3.03025100	0.21323900
C	2.73900600	-0.41158800	2.53873700
H	3.32770400	0.40130800	2.98061500
H	1.72927700	-0.03506200	2.38739100
H	2.69997700	-1.21418800	3.27855000
C	3.43260100	-0.09685600	-2.51127100
H	2.58816100	-0.55783100	-3.02907900
H	3.20873300	0.96803400	-2.42549300
H	4.30371200	-0.20135400	-3.16170200
C	-2.67272100	-0.70022200	2.54437100
H	-1.61272800	-0.49787300	2.39293400
H	-3.13080700	0.23123900	2.89675500
H	-2.77375800	-1.43417100	3.34630300
C	-3.58091100	-0.30832900	-2.45757200
H	-3.48643000	0.77444800	-2.35167000
H	-2.69350700	-0.65381500	-2.99259600
H	-4.44151700	-0.50334000	-3.10086000
C	0.01746400	-1.71164600	0.49164300
H	0.40739700	-1.49383700	1.49370900
H	-1.03356900	-1.97860800	0.61541800
C	0.74302300	-2.93908500	-0.06125600
H	1.78000800	-2.70767800	-0.32366600
H	0.26362800	-3.27558600	-0.98798000
C	0.74424600	-4.11921000	0.92360400
H	1.26110400	-3.85902200	1.85314600
H	-0.27631100	-4.41472000	1.18880600

H	1.24632400	-4.99723100	0.50141600
Co	-0.03243600	0.17985100	-0.31992400
C	-0.05366100	-0.88622000	-2.10189800
H	0.87072400	-1.43654700	-2.20468700
H	-0.94423300	-1.50124200	-2.12861900
C	-0.10707000	0.47465800	-2.36747400
H	-1.04282300	0.97496300	-2.58278200
H	0.78168400	1.02693600	-2.64788700

^{0}Co(0)-TS6/7

Atom	x	y	z
C	1.16009900	2.70705900	-0.02135400
C	1.17633700	4.09369400	-0.13443700
C	-0.03424900	4.78585000	-0.24347500
C	-1.24041400	4.08222200	-0.23516900
C	-1.22621100	2.69330200	-0.11457400
N	-0.03045100	2.02822100	-0.00488300
H	-0.03664100	5.86617600	-0.33371600
H	2.11583300	4.63464300	-0.14098600
H	-2.17776300	4.61927300	-0.32078100
C	2.27978500	1.81099300	0.12766500
C	-2.33525600	1.77930900	-0.03776400
N	-1.97031900	0.50380700	0.03178100
N	1.93803300	0.53172700	0.15815100
C	-3.76377800	2.24264500	0.04784500
H	-4.18458000	2.04453000	1.03916900
H	-3.84983100	3.31264100	-0.13887800
H	-4.40323800	1.72258900	-0.66921000
C	3.68578500	2.32809400	0.26748200
H	4.33325000	1.59863700	0.75287900
H	4.12565700	2.55587600	-0.71012500
H	3.70972000	3.24791400	0.85539400
C	-2.98869000	-0.46717100	0.31238600
C	-3.69885000	-1.10099600	-0.72318200
C	-3.24425600	-0.78547200	1.66142800
C	-4.66682600	-2.05163500	-0.38536700
C	-4.21761800	-1.74347000	1.95294200
C	-4.92875000	-2.37611200	0.94000600
H	-5.22157100	-2.54174600	-1.18041100
H	-4.41514500	-1.99508900	2.99095000
H	-5.68231000	-3.11880000	1.18225800
C	2.93906400	-0.45852100	0.42816000
C	3.03455200	-0.96084900	1.74436500
C	3.79111600	-0.93593800	-0.58428000

C	3.95584900	-1.97439600	2.01061000
C	4.69721100	-1.95553700	-0.27219000
C	4.77786400	-2.48197900	1.00938200
H	4.02827700	-2.36801500	3.02026200
H	5.35008300	-2.33332200	-1.05436800
H	5.48242200	-3.27725100	1.23127300
C	2.20061700	-0.38466000	2.86192600
H	2.53251900	0.62575800	3.12543300
H	1.14901400	-0.30197600	2.58353400
H	2.27567300	-1.00031700	3.76046300
C	3.80250900	-0.35172700	-1.97638600
H	2.88555700	0.18345700	-2.20984400
H	4.63338700	0.35363500	-2.09373300
H	3.94315900	-1.13261300	-2.72795700
C	-2.47762400	-0.11879900	2.77614800
H	-1.40078200	-0.25466200	2.65015200
H	-2.65023900	0.96153500	2.80867700
H	-2.76599400	-0.53015600	3.74552600
C	-3.42869500	-0.79482800	-2.17463700
H	-3.38000200	0.27808700	-2.37478900
H	-2.47216100	-1.21612900	-2.49168000
H	-4.20790100	-1.21911000	-2.81119300
C	-0.03972900	-1.88105500	0.07737800
H	0.57088100	-1.85845200	0.98559000
H	-1.07303100	-2.13026500	0.32506000
C	0.51798400	-2.79546900	-0.90852200
H	1.59244800	-2.97361900	-0.81725800
H	0.53763100	-2.10700400	-1.99947300
C	-0.25163000	-4.03927400	-1.31821100
H	-0.23153700	-4.78174100	-0.51217700
H	-1.30283800	-3.80697600	-1.51350000
H	0.16851300	-4.51277700	-2.21196100
Co	-0.01213900	0.18622700	-0.18740400
C	0.40216800	-1.16340600	-2.96598400
H	1.37940200	-1.28651500	-3.42935700
H	-0.38543900	-1.67345300	-3.52117200
C	0.09479300	0.07112300	-2.30857600
H	-0.90108400	0.46046900	-2.50161900
H	0.85662100	0.84235400	-2.40955600

^{0}Co(0)-7

Atom	x	y	z
C	-1.26036600	2.52471000	-0.11679000
C	-1.28219500	3.91904200	-0.10824300

C	-0.08748600	4.63612900	-0.15715300
C	1.12707300	3.94420800	-0.17991600
C	1.12715400	2.55454000	-0.18288600
N	-0.05733700	1.85238900	-0.20222500
H	-0.10032100	5.71994900	-0.15566900
H	-2.22616100	4.44894000	-0.06050300
H	2.06562500	4.48701600	-0.18976300
C	-2.36243400	1.61848000	-0.07755400
C	2.26147900	1.68360100	-0.20050800
N	1.94864800	0.39538400	-0.11022400
N	-1.99663300	0.33769900	-0.03108500
C	3.65736700	2.22914400	-0.35632200
H	3.72228300	2.90544200	-1.21314300
H	3.95564700	2.80126900	0.52840200
H	4.38919600	1.43695600	-0.49935800
C	-3.79735800	2.06699500	-0.13231200
H	-3.88012400	3.15074800	-0.05969600
H	-4.28104200	1.76090400	-1.06480400
H	-4.38282200	1.63120900	0.68117400
C	2.99931900	-0.56225200	-0.31067200
C	3.78613800	-1.00522400	0.76816000
C	3.23989200	-1.03171100	-1.61859500
C	4.77084600	-1.96782400	0.52933700
C	4.23017500	-1.99883700	-1.81090100
C	4.98687000	-2.47525000	-0.74639200
H	5.37406100	-2.32046900	1.36107300
H	4.41198800	-2.37395700	-2.81397200
H	5.74865800	-3.23038700	-0.91253700
C	-3.02274900	-0.64358100	-0.24419400
C	-3.33762600	-0.99089100	-1.57932700
C	-3.70153900	-1.24953800	0.82801400
C	-4.29504900	-1.97935500	-1.80930400
C	-4.65605800	-2.23438000	0.54946300
C	-4.94842900	-2.60810100	-0.75410300
H	-4.53164000	-2.25595400	-2.83279700
H	-5.17931900	-2.70464700	1.37772900
H	-5.68753600	-3.37840800	-0.95039100
C	-2.68978100	-0.29036900	-2.75052500
H	-3.18149500	0.66557300	-2.96477900
H	-1.63930500	-0.06312500	-2.56485300
H	-2.76242800	-0.89830500	-3.65484700
C	-3.47593900	-0.84032700	2.26340500
H	-2.71882100	-0.06672800	2.35636800

H	-4.40398200	-0.46180100	2.70484700
H	-3.16244300	-1.69133300	2.87516400
C	2.50193700	-0.46337200	-2.80670700
H	1.45008900	-0.27846800	-2.58739600
H	2.93297200	0.49784400	-3.10974600
H	2.56954800	-1.13375600	-3.66624700
C	3.61769400	-0.42525800	2.14861700
H	4.15946100	0.52295600	2.24470100
H	2.57441200	-0.21840500	2.37433700
H	4.01282000	-1.10127200	2.90993100
C	-0.07133800	-1.87968000	-0.72554700
H	-0.95626700	-1.80247200	-1.33963200
H	0.85342000	-2.08615100	-1.25163600
C	-0.15212600	-2.13042700	0.62345200
H	-1.13745500	-2.16512400	1.07688800
H	-0.80541400	-1.12418900	3.30255200
C	0.92163500	-2.87741800	1.37130800
H	0.62643400	-3.93274600	1.44233400
H	1.87881700	-2.84697100	0.85227800
H	1.06818800	-2.52468700	2.39085200
Co	-0.02051000	0.06810100	0.20532500
C	-0.05220000	-0.33722900	3.38427000
H	-0.27363800	0.21362300	4.31043900
H	0.90848400	-0.82990100	3.54846200
C	-0.03593600	0.61041700	2.18957900
H	0.82793400	1.28041800	2.26541500
H	-0.92263700	1.25193000	2.22388300

^{0}Co(0)-8

Atom	x	y	z
C	1.19171000	2.55097400	-0.18993400
C	1.20737200	3.94145400	-0.15270900
C	-0.00000800	4.64595300	-0.14650800
C	-1.20738400	3.94144800	-0.15270600
C	-1.19171300	2.55096800	-0.18993200
N	0.00000000	1.86462500	-0.24592500
H	-0.00001000	5.72931100	-0.11561100
H	2.15141400	4.47424600	-0.11999300
H	-2.15142800	4.47423400	-0.11998500
C	2.30473100	1.63764900	-0.14610000
C	-2.30473300	1.63763700	-0.14609900
N	-1.94131000	0.37034000	-0.06187900
N	1.94131000	0.37035000	-0.06186600
C	-3.72280400	2.13312900	-0.20101700

H	-3.97752100	2.69855300	0.70164300
H	-3.86328100	2.80715500	-1.05074200
H	-4.43332400	1.31401200	-0.29467100
C	3.72280000	2.13314500	-0.20103800
H	3.86328000	2.80711400	-1.05080800
H	3.97750600	2.69863200	0.70158500
H	4.43332500	1.31402600	-0.29463100
C	-2.92978900	-0.66328800	-0.02294900
C	-3.18077200	-1.39988800	-1.19559800
C	-3.59150600	-0.96131200	1.18188900
C	-4.11539100	-2.43552500	-1.14378600
C	-4.51334400	-2.01195000	1.18932700
C	-4.77867800	-2.74514800	0.03910100
H	-4.31933000	-3.00762400	-2.04421900
H	-5.02432900	-2.25663400	2.11608900
H	-5.49591200	-3.55935700	0.06476400
C	2.92979100	-0.66327500	-0.02293000
C	3.59146800	-0.96133000	1.18192400
C	3.18081000	-1.39985100	-1.19558700
C	4.51331300	-2.01196100	1.18936300
C	4.11543300	-2.43548400	-1.14377100
C	4.77868900	-2.74512900	0.03912800
H	5.02427000	-2.25666600	2.11613500
H	4.31939900	-3.00756300	-2.04421100
H	5.49592800	-3.55933300	0.06479300
C	3.33425200	-0.16570700	2.43818500
H	3.88915200	0.77929700	2.43853500
H	2.27759800	0.08204200	2.54934900
H	3.64958600	-0.72434800	3.32171900
C	2.46575000	-1.07246100	-2.48257400
H	1.38005300	-1.14119200	-2.36653200
H	2.67602500	-0.05276700	-2.81923700
H	2.76522500	-1.75651000	-3.27897700
C	-3.33434700	-0.16563900	2.43813000
H	-2.27770800	0.08216900	2.54930400
H	-3.88929600	0.77933700	2.43844000
H	-3.64966600	-0.72426700	3.32167700
C	-2.46568700	-1.07251100	-2.48257500
H	-2.67594400	-0.05281500	-2.81924200
H	-1.37999200	-1.14125400	-2.36651400
H	-2.76515600	-1.75655800	-3.27898100
C	0.00001900	-1.54644500	1.16670300
H	0.87925800	-1.56732200	1.81910000

H	-0.87920400	-1.56729800	1.81912300
C	-0.00000800	-2.81636700	0.29254900
H	0.88365600	-2.88065000	-0.35026600
H	-0.88369500	-2.88063500	-0.35023600
Co	0.00001100	0.07221600	0.02890300
H	-0.00000600	-3.72888000	0.90699500

^{0}Co(0)-TS3/9

Atom	x	y	z
C	-1.14806300	2.57073500	0.06427900
C	-1.14032900	3.96128900	0.08726200
C	0.07196200	4.65397900	0.11689200
C	1.27039900	3.93797000	0.11188700
C	1.25180400	2.54726100	0.08769200
N	0.04433400	1.86685500	0.07855600
H	0.08235000	5.73763100	0.13278400
H	-2.07386100	4.51137300	0.07970500
H	2.21474700	4.46934500	0.12332500
C	-2.26512300	1.69098400	0.00045500
C	2.35319800	1.64732700	0.04739600
N	1.98553300	0.36714900	-0.00668200
N	-1.92422100	0.40209300	-0.03366300
C	3.78859600	2.09511900	0.05452100
H	3.86810800	3.17976800	-0.00569900
H	4.30660800	1.77542700	0.96392900
H	4.34557400	1.67308800	-0.78598100
C	-3.68903300	2.17273900	-0.04944900
H	-3.73892300	3.25843000	-0.12061300
H	-4.22222500	1.75821800	-0.90900900
H	-4.25151400	1.87314400	0.83977100
C	3.02062900	-0.61907000	-0.08229800
C	3.57686700	-1.15311600	1.09778300
C	3.45938900	-1.05245000	-1.34957600
C	4.55614000	-2.14379600	0.98481900
C	4.44117100	-2.04487400	-1.41406200
C	4.98508500	-2.59359800	-0.25872400
H	4.98604100	-2.56503300	1.88913300
H	4.78084600	-2.38816200	-2.38709500
H	5.74215800	-3.36847100	-0.32683200
C	-2.99182000	-0.54820700	-0.12362000
C	-3.39586500	-1.00582200	-1.39366900
C	-3.62951300	-1.00338200	1.04675600
C	-4.42409700	-1.94932900	-1.46786900
C	-4.65691500	-1.94309300	0.92471800

C	-5.05112000	-2.42055400	-0.31999300
H	-4.73666800	-2.31305200	-2.44253400
H	-5.14886300	-2.30558000	1.82288800
H	-5.84608500	-3.15581200	-0.39538000
C	-2.77507800	-0.45709100	-2.65519100
H	-3.17025700	0.53763900	-2.89114500
H	-1.69402600	-0.34744200	-2.56104800
H	-2.99068700	-1.10262900	-3.50930600
C	-3.23322500	-0.48811700	2.40908000
H	-2.15574000	-0.33980500	2.48717300
H	-3.70253900	0.47828700	2.62544100
H	-3.54743000	-1.18064300	3.19290900
C	2.92564700	-0.43124400	-2.61794000
H	1.85745000	-0.22142500	-2.55199400
H	3.41889900	0.52437600	-2.83017700
H	3.10268400	-1.08313900	-3.47608000
C	3.15939800	-0.65712300	2.46154000
H	3.65481400	0.28786200	2.71162300
H	2.08626200	-0.47073600	2.51852900
H	3.43065500	-1.37720100	3.23657700
C	0.02836100	-1.82000300	-0.76003300
H	-0.92793900	-2.07047200	-1.20474400
H	0.87958500	-1.87960700	-1.42565500
C	0.21107100	-2.04196100	0.61985800
H	0.04393000	-0.60839900	1.47163700
H	1.23968800	-2.16565200	0.94058000
C	-0.75456300	-2.86417400	1.44709100
H	-1.78889900	-2.73050700	1.13700900
H	-0.50618500	-3.92301200	1.30829100
H	-0.67999600	-2.64559600	2.51541100
Co	0.02711400	0.05491400	0.11635000

^{0}Co(0)-9

Atom	x	y	z
C	1.28344900	2.58177800	-0.13753300
C	1.31540900	3.97098300	-0.10553800
C	0.12310600	4.70061200	-0.09213800
C	-1.09905100	4.02253000	-0.09741600
C	-1.12615300	2.63306600	-0.13000300
N	0.06376800	1.91609400	-0.17903200
H	0.14632200	5.78377800	-0.06448000
H	2.26671100	4.49037300	-0.08140600
H	-2.02731500	4.58172400	-0.06695200
C	2.36910700	1.66289900	-0.12378000

C	-2.24870500	1.76025500	-0.11296600
N	-1.90968700	0.46996100	-0.06041800
N	1.97749000	0.38795400	-0.06917300
C	-3.66998900	2.24728200	-0.16057600
H	-4.14493600	2.22039600	0.82578600
H	-3.72202600	3.27382100	-0.52342500
H	-4.27925200	1.62713800	-0.82164400
C	3.80903400	2.09157200	-0.17273300
H	3.90449600	3.10599500	-0.56041300
H	4.27557000	2.07110700	0.81792000
H	4.39707300	1.43110000	-0.81320200
C	-2.94733500	-0.51420400	-0.06975500
C	-3.25063700	-1.16312000	-1.28632400
C	-3.63739600	-0.84170600	1.11282300
C	-4.23313900	-2.15346300	-1.29140500
C	-4.61000000	-1.84675800	1.06160500
C	-4.90756400	-2.50273300	-0.12482700
H	-4.47205900	-2.65607600	-2.22411800
H	-5.13867300	-2.11221900	1.97306100
H	-5.66366500	-3.28125400	-0.14405100
C	2.97265500	-0.64007100	-0.06671800
C	3.64331100	-0.98840200	1.12070900
C	3.24612100	-1.31723800	-1.27525000
C	4.56387900	-2.04217800	1.08322300
C	4.17823500	-2.35490700	-1.26723200
C	4.83092000	-2.72548300	-0.09464200
H	5.07718100	-2.32302800	1.99891200
H	4.39474700	-2.87792600	-2.19421800
H	5.54725100	-3.54095700	-0.10320400
C	3.42762500	-0.25039300	2.42163800
H	4.27092200	0.41568100	2.63681300
H	2.52301000	0.35437100	2.40895000
H	3.35713000	-0.94944500	3.25915200
C	2.56464300	-0.91824700	-2.56111300
H	1.47947900	-1.02965600	-2.49735700
H	2.74869100	0.13099200	-2.80962400
H	2.92060600	-1.52831400	-3.39376600
C	-3.38389100	-0.13122900	2.42207100
H	-2.43765500	0.40668300	2.42334800
H	-4.17877100	0.59274200	2.63459400
H	-3.37315600	-0.84045700	3.25383500
C	-2.55434900	-0.77725800	-2.56850700
H	-2.74017100	0.26894300	-2.83009300

H	-1.46964500	-0.88205500	-2.49202400
H	-2.89985400	-1.39629900	-3.39889500
C	0.00965700	-1.16240500	1.50226800
H	0.85515800	-1.15260600	2.18431100
H	-0.92836900	-1.22734700	2.04881500
C	0.12742900	-2.16236300	0.36964400
H	1.15585500	-2.50941800	0.26768300
H	-0.05828000	-1.64703800	-0.63312900
C	-0.83054600	-3.35927900	0.40728400
H	-0.60504100	-3.97591400	1.28233600
H	-1.87213700	-3.04680000	0.47964100
H	-0.72594200	-3.98744300	-0.48304000
Co	0.02595600	0.14348600	0.04531000

^{0}Co(0)-10

Atom	x	y	z
C	-1.19939700	2.42431300	-0.16148500
C	-1.21006000	3.81360500	-0.11279200
C	0.00001200	4.51591100	-0.11293600
C	1.21007800	3.81360100	-0.11281700
C	1.19940900	2.42430700	-0.16151400
N	0.00000100	1.74620600	-0.25784600
H	0.00001400	5.59905000	-0.07555800
H	-2.15211100	4.34862700	-0.05928600
H	2.15213500	4.34861500	-0.05933000
C	-2.29981400	1.50062500	-0.08341000
C	2.29981700	1.50061400	-0.08347300
N	1.91054200	0.23798200	-0.00214700
N	-1.91055900	0.23799200	-0.00208400
C	3.72988600	1.96109800	-0.09089700
H	3.92303800	2.62320700	-0.93968100
H	3.96572200	2.52578700	0.81748900
H	4.42018700	1.12108000	-0.15040700
C	-3.72988100	1.96112300	-0.09081700
H	-3.92303200	2.62328000	-0.93956100
H	-4.42018300	1.12111300	-0.15039100
H	-3.96573100	2.52574600	0.81760500
C	2.85088200	-0.84014600	0.02356100
C	3.39828200	-1.26706200	1.24735000
C	3.15889300	-1.49321800	-1.18418100
C	4.27065900	-2.35815300	1.23593500
C	4.03549900	-2.57987100	-1.14747400
C	4.59021300	-3.01300700	0.05174800
H	4.69839800	-2.69924700	2.17420600

H	4.28087100	-3.09179200	-2.07346900
H	5.26674000	-3.86173500	0.06398700
C	-2.85090400	-0.84013200	0.02361100
C	-3.15896800	-1.49312200	-1.18416100
C	-3.39823100	-1.26713700	1.24739900
C	-4.03555100	-2.57979200	-1.14748700
C	-4.27059700	-2.35823900	1.23595000
C	-4.59020000	-3.01301700	0.05173600
H	-4.28095800	-3.09165800	-2.07350300
H	-4.69828300	-2.69940400	2.17421900
H	-5.26670900	-3.86175900	0.06395200
C	-2.56192400	-1.03190400	-2.49127000
H	-2.87857500	-0.01652700	-2.74943400
H	-1.46930400	-1.01294300	-2.45091700
H	-2.86048200	-1.69094800	-3.30877300
C	-3.04763000	-0.57425900	2.53865900
H	-1.96375800	-0.50380600	2.65748600
H	-3.44042900	0.44752000	2.57475800
H	-3.45923900	-1.11426600	3.39365100
C	2.56175200	-1.03214800	-2.49129900
H	1.46912800	-1.01338700	-2.45091200
H	2.87823300	-0.01673700	-2.74951800
H	2.86038600	-1.69119000	-3.30877900
C	3.04775400	-0.57409300	2.53858200
H	3.44063900	0.44765600	2.57461400
H	1.96389100	-0.50354900	2.65742800
H	3.45933800	-1.11408400	3.39359600
H	0.00002300	-0.81000700	1.41817600
Co	0.00001100	-0.00345500	0.12451000

^{1}Co(0)

^{1}Co(0)-1

Atom	x	y	z
C	-1.18657500	2.36864300	0.13461400
C	-1.20456800	3.75292600	0.26948600
C	-0.00000200	4.45991500	0.31884900
C	1.20456400	3.75293600	0.26952200
C	1.18658900	2.36864600	0.13467500
N	0.00001100	1.69254600	0.00696200
H	-0.00000500	5.53855500	0.42484800
H	-2.14655400	4.28252800	0.34971400
H	2.14654500	4.28254800	0.34975200
C	-2.37122400	1.51410400	0.14346700
C	2.37123000	1.51410500	0.14356500

N	2.14346100	0.23042300	0.10936100
N	-2.14345300	0.23042500	0.10938700
C	3.74332700	2.13870400	0.21001200
H	3.93258100	2.77734400	-0.65798700
H	3.84243800	2.76721100	1.09970000
H	4.52062200	1.37791900	0.24896800
C	-3.74332000	2.13871800	0.20981000
H	-3.84256800	2.76695000	1.09968600
H	-3.93239400	2.77762800	-0.65801900
H	-4.52064200	1.37794500	0.24842000
C	3.19230300	-0.72851100	0.10985800
C	3.44905000	-1.43118500	1.30341300
C	3.88644400	-1.03636900	-1.07669600
C	4.43018000	-2.42370900	1.29881900
C	4.85512500	-2.04256700	-1.03607300
C	5.13370900	-2.73119000	0.13906500
H	4.63806700	-2.96460900	2.21762900
H	5.39253700	-2.29039400	-1.94690700
H	5.88876100	-3.51071100	0.14889900
C	-3.19230400	-0.72850200	0.10985700
C	-3.88636800	-1.03641300	-1.07674200
C	-3.44916000	-1.43108500	1.30342900
C	-4.85508200	-2.04257200	-1.03612200
C	-4.43033000	-2.42358000	1.29882700
C	-5.13377700	-2.73111200	0.13904600
H	-5.39243600	-2.29044800	-1.94697600
H	-4.63830600	-2.96439900	2.21766400
H	-5.88885500	-3.51060800	0.14886500
C	-3.58450600	-0.31638600	-2.36738900
H	-3.91186600	0.72855700	-2.34366500
H	-2.51293100	-0.31399100	-2.57807900
H	-4.09354700	-0.79639300	-3.20538200
C	-2.67702900	-1.11539400	2.56000500
H	-1.59998000	-1.24426300	2.41086600
H	-2.82246500	-0.08066300	2.88517200
H	-2.98158000	-1.76837800	3.38023600
C	3.58473200	-0.31622100	-2.36731300
H	2.51316800	-0.31367300	-2.57805100
H	3.91221900	0.72867900	-2.34350600
H	4.09375300	-0.79623100	-3.20531700
C	2.67685000	-1.11552400	2.55995400
H	2.82255700	-0.08089200	2.88533400
H	1.59978200	-1.24403400	2.41066800

H	2.98112300	-1.76874300	3.38010000
Co	0.00003600	-0.21477200	-0.38311300
C	-0.00002800	-1.56696000	-1.87893800
H	-0.88485700	-2.21467400	-1.86271000
H	-0.00006900	-1.06149800	-2.85511600
H	0.88479300	-2.21468400	-1.86275000

^{1}Co(0)-2

Atom	x	y	z
C	1.18519200	2.34289400	-0.03836600
C	1.18085300	3.74798300	-0.05708000
C	-0.01153500	4.43916900	-0.00396200
C	-1.20983200	3.70667900	0.03881000
C	-1.17695800	2.32051400	0.04131600
N	0.00211200	1.62806800	0.01913200
H	-0.02782100	5.52318000	-0.00562800
H	2.11918500	4.28662200	-0.10789100
H	-2.15558800	4.23123800	0.05832100
C	2.40087600	1.57077500	-0.07369000
C	-2.43444700	1.53366700	0.00388200
N	-2.34735800	0.25638900	0.10906200
N	2.26518700	0.25969100	0.03914600
C	-3.73988700	2.27828400	-0.19136100
H	-3.92730100	2.96493400	0.63911400
H	-3.72582000	2.87439500	-1.10728300
H	-4.57586900	1.58395400	-0.24591000
C	3.73424800	2.26193800	-0.23323500
H	3.77077100	2.86500200	-1.14557200
H	3.93905400	2.93482700	0.60575500
H	4.54669900	1.53908100	-0.27825900
C	-3.47761100	-0.58949500	-0.04457100
C	-3.85762100	-0.99673900	-1.34179400
C	-4.16005200	-1.07550400	1.08915600
C	-4.89769000	-1.91853300	-1.47539900
C	-5.20166900	-1.98814400	0.90395400
C	-5.56736100	-2.42011600	-0.36519700
H	-5.18597600	-2.24144400	-2.47165900
H	-5.73320400	-2.36058900	1.77516600
H	-6.37330700	-3.13632100	-0.48868600
C	3.39712100	-0.60849400	-0.04512600
C	4.03709800	-1.06052500	1.12495300
C	3.83267600	-1.04884900	-1.31432100
C	5.08816200	-1.97552200	1.00724100
C	4.88071900	-1.96793200	-1.38358400

C	5.50549100	-2.43831900	-0.23346200
H	5.58560700	-2.32286000	1.90870500
H	5.21143200	-2.31508700	-2.35821700
H	6.31929700	-3.15284700	-0.30578500
C	3.62751500	-0.58418600	2.49826100
H	3.22618600	0.42978000	2.48261300
H	2.86099800	-1.23270800	2.93557400
H	4.48036100	-0.59765400	3.18097500
C	3.20161800	-0.52215400	-2.57841400
H	2.11384300	-0.58145900	-2.53736700
H	3.45993400	0.52898500	-2.74943100
H	3.54391600	-1.08728000	-3.44756700
C	-3.80189700	-0.62240300	2.48411900
H	-2.88326400	-1.09505800	2.84328600
H	-3.64867400	0.45819000	2.54315200
H	-4.59516700	-0.88245900	3.18799100
C	-3.18009900	-0.43113800	-2.56512500
H	-3.48994100	0.60350400	-2.75402100
H	-2.09514100	-0.42942300	-2.46048400
H	-3.43668000	-1.01189400	-3.45329400
C	-0.04179500	-1.80753100	-1.42003000
H	0.02316000	-1.44048900	-2.45158200
H	0.72702700	-2.58608800	-1.31686100
H	-1.01515900	-2.29774800	-1.30966000
C	-0.17780600	-1.81453700	1.75996800
H	0.67235500	-2.48415600	1.67597200
H	-1.13014500	-2.20826400	1.42602000
C	-0.07501200	-0.61863500	2.37665400
H	-0.93602800	0.01740400	2.52963900
H	0.86299900	-0.26723100	2.78561200
Co	0.28410700	-0.38511000	-0.01984000

^{1}Co(0)-TS-2/3

Atom	x	y	z
C	1.18988900	2.39933000	-0.20220800
C	1.20525700	3.78742900	-0.29688400
C	0.00455000	4.50068000	-0.31720100
C	-1.19848600	3.79228700	-0.28042800
C	-1.18694000	2.40410000	-0.18659300
N	0.00061400	1.71178000	-0.11169800
H	0.00632000	5.58268600	-0.38035300
H	2.14893300	4.31627800	-0.36491300
H	-2.14105900	4.32468200	-0.33504100
C	2.37695700	1.55927300	-0.24442500

C	-2.37585000	1.56749200	-0.21282800
N	-2.18139000	0.28740800	-0.02897600
N	2.18284100	0.28035400	-0.05638400
C	-3.72539600	2.19178800	-0.48030800
H	-3.98741500	2.91382300	0.29936000
H	-3.73407600	2.73089500	-1.43200300
H	-4.50903900	1.43669100	-0.51300600
C	3.72307200	2.17998200	-0.53670400
H	3.71483000	2.71879100	-1.48853200
H	4.00220100	2.90137000	0.23756500
H	4.50354400	1.42230200	-0.58460100
C	-3.23820500	-0.65304400	-0.15271400
C	-3.43632000	-1.29074900	-1.39556100
C	-4.01945100	-1.00782100	0.96603700
C	-4.41238500	-2.28428600	-1.49532200
C	-4.98748200	-2.00454400	0.81938300
C	-5.18604700	-2.64609900	-0.39808500
H	-4.56651600	-2.77694200	-2.45124900
H	-5.59362400	-2.27836600	1.67839900
H	-5.93984500	-3.42133500	-0.49131900
C	3.23418600	-0.66588400	-0.17527900
C	4.04703500	-0.97999800	0.93359800
C	3.39718400	-1.34931600	-1.39892200
C	5.00166200	-1.99145400	0.80051100
C	4.36392900	-2.35289300	-1.48637300
C	5.16172100	-2.68150200	-0.39584200
H	5.62932900	-2.23675300	1.65267300
H	4.49148300	-2.88053500	-2.42744700
H	5.90576000	-3.46725800	-0.47883900
C	3.91211800	-0.23089100	2.23636100
H	4.16043900	0.82969300	2.12587200
H	2.89388300	-0.27137800	2.62806700
H	4.58077800	-0.64564700	2.99337700
C	2.56442800	-0.98414800	-2.60295800
H	1.49434300	-1.00663400	-2.38159200
H	2.78287700	0.02949600	-2.95509100
H	2.75440700	-1.66941900	-3.43148400
C	-3.82530200	-0.33004400	2.29977700
H	-2.83537200	-0.53369100	2.71510300
H	-3.91414700	0.75765400	2.22731500
H	-4.56761300	-0.67578200	3.02204200
C	-2.62180500	-0.89490500	-2.60208700
H	-2.83837200	0.13014500	-2.92076100

H	-1.54904800	-0.93230400	-2.39621200
H	-2.83014500	-1.55399500	-3.44727800
C	-0.11927300	-2.19313400	0.40293000
H	0.15327700	-1.91482900	-0.63371800
H	0.54687500	-3.01357100	0.66037100
H	-1.15096700	-2.53843500	0.41173800
C	0.13138600	-1.34796300	2.18412400
H	1.10411500	-1.78714700	2.37938400
H	-0.67338800	-1.96842800	2.56978900
C	0.02236400	0.07527200	2.37336800
H	-0.90815700	0.48457700	2.75424400
H	0.90411400	0.62489700	2.68898600
Co	-0.00259100	-0.11118800	0.38949500

^{1}Co(0)-3

Atom	x	y	z
C	1.18583200	2.67571500	0.10616600
C	1.20677500	4.06507000	0.03196000
C	0.00009800	4.77249000	0.03276400
C	-1.20661600	4.06512200	0.03195700
C	-1.18572700	2.67577300	0.10617000
N	0.00002700	2.00769300	0.25831300
H	0.00011800	5.85468700	-0.02788900
H	2.14657300	4.59810200	-0.05356500
H	-2.14638800	4.59819900	-0.05356500
C	2.33869100	1.79857900	-0.03424000
C	-2.33863600	1.79868500	-0.03424700
N	-2.05967300	0.52199100	-0.15754700
N	2.05967500	0.52188100	-0.15758000
C	-3.73055200	2.37676500	-0.05949200
H	-3.99218600	2.82686700	0.90323900
H	-3.80972000	3.16383000	-0.81412600
H	-4.47265300	1.61497600	-0.29141600
C	3.73064800	2.37654900	-0.05941500
H	3.80990700	3.16361100	-0.81404500
H	3.99229200	2.82661600	0.90332500
H	4.47268900	1.61470000	-0.29133600
C	-3.07620400	-0.46536400	-0.29120600
C	-3.21970600	-1.09301600	-1.54538200
C	-3.84885400	-0.87263800	0.81430800
C	-4.16372200	-2.11081300	-1.68210500
C	-4.77505500	-1.90403300	0.63291200
C	-4.94028100	-2.51858300	-0.60207400
H	-4.28437700	-2.59294100	-2.64792300

H	-5.36918100	-2.23072500	1.48160900
H	-5.66318700	-3.31932700	-0.72086900
C	3.07621000	-0.46549600	-0.29117000
C	3.84876300	-0.87277300	0.81441300
C	3.21984800	-1.09310100	-1.54534300
C	4.77497400	-1.90417000	0.63309100
C	4.16387300	-2.11091000	-1.68199300
C	4.94030600	-2.51871300	-0.60188900
H	5.36900600	-2.23089500	1.48184100
H	4.28462400	-2.59301500	-2.64781000
H	5.66321100	-3.31946800	-0.72062100
C	3.69351600	-0.23103100	2.17159700
H	4.24269300	0.71447700	2.24066500
H	2.64878200	-0.01641300	2.40142300
H	4.08234800	-0.88584500	2.95384600
C	2.37357200	-0.66452000	-2.71722000
H	1.30655000	-0.74220500	-2.48831900
H	2.55477500	0.37878400	-2.99361100
H	2.57777100	-1.28294500	-3.59348300
C	-3.69364100	-0.23092400	2.17150900
H	-2.64886800	-0.01661600	2.40146900
H	-4.24253300	0.71474800	2.24053400
H	-4.08276300	-0.88562700	2.95370300
C	-2.37327200	-0.66448400	-2.71716200
H	-2.55424100	0.37887400	-2.99347000
H	-1.30628000	-0.74241400	-2.48817900
H	-2.57751000	-1.28280800	-3.59348800
C	-0.00008100	-1.59217100	1.58988000
H	0.87493800	-1.59032100	2.25564500
H	-0.87489800	-1.59010100	2.25590000
C	-0.00039300	-2.89071600	0.76399600
H	0.87524500	-2.91651000	0.10201300
H	-0.87623800	-2.91625300	0.10227700
C	-0.00041100	-4.17018800	1.61519300
H	0.88218500	-4.20890700	2.26221300
H	-0.88284900	-4.20870900	2.26244000
H	-0.00058800	-5.07527900	0.99641500
Co	0.00003100	0.05375100	0.42648100

^{1}Co(0)-4

Atom	x	y	z
C	1.19426900	2.41273000	-0.52134700
C	1.23531200	3.75138500	-0.87879700
C	0.04223800	4.48102800	-1.02022600

C	-1.15321900	3.82786500	-0.81350700
C	-1.16682200	2.46960300	-0.44873700
N	0.01292100	1.75989400	-0.29237700
H	0.06543400	5.52973300	-1.29405800
H	2.18346200	4.24027700	-1.05604100
H	-2.08907500	4.36016000	-0.92905900
C	2.45206900	1.63141600	-0.41403200
C	-2.39011400	1.74659400	-0.22958500
N	-2.27302100	0.49429100	0.18827200
N	2.38795000	0.44965500	0.08328900
C	-3.71871300	2.42783400	-0.46047300
H	-3.83353100	3.29534300	0.19728000
H	-3.82297400	2.78836600	-1.48821800
H	-4.54753400	1.75270300	-0.25739800
C	3.73298400	2.26450100	-0.92101900
H	3.63519200	2.58095400	-1.96235200
H	3.99276200	3.15152900	-0.33606100
H	4.56365800	1.56531400	-0.85032000
C	-3.41593400	-0.35722100	0.26777500
C	-3.97169000	-0.89119200	-0.91591900
C	-3.95069700	-0.70520000	1.52436500
C	-5.02851400	-1.79893000	-0.81229900
C	-5.01509600	-1.60794100	1.57946800
C	-5.54850800	-2.16457800	0.42326900
H	-5.44803500	-2.22173600	-1.72081500
H	-5.43121700	-1.87229800	2.54758300
H	-6.36956000	-2.87175000	0.48434000
C	3.52141700	-0.40294700	0.14633700
C	4.28479000	-0.47526400	1.32981500
C	3.82570200	-1.22692000	-0.95741200
C	5.32523000	-1.40463900	1.39914000
C	4.87069800	-2.14555100	-0.83836100
C	5.61568600	-2.24536500	0.33088800
H	5.91712500	-1.46256300	2.30820400
H	5.10155300	-2.78849400	-1.68288100
H	6.42211900	-2.96760000	0.40659200
C	4.01556300	0.44418700	2.49623000
H	4.00002000	1.49600900	2.19540900
H	3.05328900	0.23702600	2.97104100
H	4.78715500	0.33305400	3.26059700
C	3.06552900	-1.09845800	-2.25329700
H	1.98972400	-1.04333200	-2.08651500
H	3.35287300	-0.19168500	-2.79870600

H	3.26752700	-1.94735700	-2.90920700
C	-3.41354600	-0.10912100	2.80205100
H	-2.48163500	-0.59034400	3.11244400
H	-3.20634400	0.95826300	2.69972100
H	-4.12806700	-0.23628500	3.61809600
C	-3.47263200	-0.48209000	-2.28052900
H	-3.92647900	0.46132000	-2.60462800
H	-2.39174300	-0.34321100	-2.29893000
H	-3.72977900	-1.23482200	-3.02843600
C	0.00299600	-2.07678200	-0.38498500
H	1.07227600	-2.30430500	-0.27322900
H	-0.50076900	-2.69393600	0.37879600
C	-0.48201700	-2.54668200	-1.76119600
H	-0.09558900	-1.89322300	-2.55531100
H	-1.57205400	-2.45923200	-1.81497200
C	-0.09571300	-3.99612500	-2.09515800
H	0.99178900	-4.12527400	-2.08998300
H	-0.50733700	-4.69056700	-1.35513900
H	-0.46334100	-4.30408900	-3.08133200
Co	-0.29214800	-0.18158000	0.28542300
C	0.39315400	-0.84084600	2.47383700
H	1.34917700	-1.27050900	2.20080900
H	-0.39487500	-1.54798500	2.70983800
C	0.22405100	0.48493300	2.63177700
H	-0.71467300	0.90468000	2.97158000
H	1.03169900	1.18430200	2.46212200

^{1}Co(0)-TS-4/5

Atom	x	y	z
C	1.14936700	2.52116500	-0.30167000
C	1.13233900	3.90704500	-0.47066900
C	-0.07430100	4.59199400	-0.54061500
C	-1.26417500	3.85598600	-0.46315100
C	-1.22501400	2.47898100	-0.29224900
N	-0.02985200	1.80414400	-0.18907600
H	-0.09658100	5.66852700	-0.66414900
H	2.06692100	4.45002800	-0.54911600
H	-2.21602000	4.36576500	-0.54633200
C	2.36047800	1.73722100	-0.25466600
C	-2.43445000	1.65648900	-0.26051600
N	-2.28529200	0.38833100	-0.02043500
N	2.21996700	0.45855500	0.02014700
C	-3.77339100	2.30833900	-0.53301300
H	-4.00123800	3.06900300	0.21939100

H	-3.78446800	2.80556200	-1.50658400
H	-4.57637300	1.57358000	-0.51914300
C	3.69356400	2.39822600	-0.52416400
H	3.71384800	2.88319400	-1.50448400
H	3.90881800	3.17137800	0.22020200
H	4.50586700	1.67422300	-0.49076500
C	-3.38002000	-0.51344600	-0.08631300
C	-3.66862200	-1.14880500	-1.31367800
C	-4.12291700	-0.82799100	1.07098700
C	-4.66459600	-2.12740800	-1.34894500
C	-5.11248000	-1.81054100	0.98778100
C	-5.38004900	-2.46923800	-0.20713700
H	-4.88246400	-2.62197400	-2.29146700
H	-5.68428600	-2.05580700	1.87838300
H	-6.14763900	-3.23524300	-0.25013900
C	3.32681900	-0.42878300	-0.04737100
C	4.02785700	-0.77931200	1.12517100
C	3.67197700	-1.01420900	-1.28481900
C	5.04700000	-1.73127100	1.04304400
C	4.69386600	-1.96617900	-1.32023900
C	5.37838000	-2.33166900	-0.16652200
H	5.58914000	-2.00038400	1.94527500
H	4.95684200	-2.42105300	-2.27125600
H	6.16899500	-3.07390800	-0.21081900
C	3.70584500	-0.12265500	2.44414500
H	3.78420300	0.96692100	2.38533900
H	2.68639900	-0.34127500	2.76886300
H	4.38791700	-0.46436200	3.22545400
C	2.97323200	-0.60432500	-2.55811100
H	1.88699600	-0.60602700	-2.44789000
H	3.25077200	0.41055700	-2.86258100
H	3.23517900	-1.27392300	-3.37989500
C	-3.89555300	-0.09233900	2.36821800
H	-2.86437200	-0.17204400	2.71509900
H	-4.10695300	0.97740300	2.26890500
H	-4.54538300	-0.48240000	3.15420000
C	-2.94793800	-0.75293500	-2.57920900
H	-3.28262400	0.22570800	-2.94151300
H	-1.86990200	-0.67518100	-2.43055000
H	-3.13451600	-1.47486100	-3.37702700
C	0.36928000	-2.08607200	0.81737400
H	1.45796300	-2.13762000	0.85705200
H	-0.01825100	-2.93160800	1.38452100

C	-0.14898300	-2.23352400	-0.62015500
H	0.06256400	-1.34151100	-1.23677400
H	-1.23473700	-2.34487100	-0.61154000
C	0.48907000	-3.44059900	-1.32817900
H	1.57556100	-3.34023400	-1.38509400
H	0.26744000	-4.36667700	-0.78936500
H	0.10365400	-3.54833400	-2.34682700
Co	0.07692600	0.02024500	0.48393800
C	-0.14341700	-0.99243600	2.40412300
H	0.63603400	-1.51248200	2.95545500
H	-1.11511600	-1.44801700	2.56923600
C	-0.09510400	0.44923200	2.39939400
H	-1.01411900	0.99931300	2.57782700
H	0.79078600	0.93913400	2.79427400

^{1}Co(0)-5

Atom	x	y	z
C	1.18576600	-3.04409300	-0.25373900
C	1.20659900	-4.43518600	-0.27448500
C	0.00006400	-5.14119000	-0.32194000
C	-1.20648900	-4.43521400	-0.27446000
C	-1.18568800	-3.04412300	-0.25371800
N	0.00002900	-2.36618900	-0.35668800
H	0.00007700	-6.22499900	-0.33442200
H	2.14664500	-4.97261800	-0.22694400
H	-2.14652100	-4.97267000	-0.22690000
C	2.34070900	-2.18024000	-0.05985600
C	-2.34065100	-2.18029600	-0.05982600
N	-2.06526200	-0.91458100	0.15079300
N	2.06529100	-0.91453100	0.15077000
C	-3.73098000	-2.76261200	-0.07746200
H	-3.97986200	-3.17059100	-1.06190000
H	-3.81561300	-3.58297000	0.64048700
H	-4.47832600	-2.01457800	0.18054100
C	3.73105200	-2.76252300	-0.07749900
H	3.81571200	-3.58287200	0.64045800
H	3.97993500	-3.17050700	-1.06193500
H	4.47838200	-2.01446900	0.18049000
C	-3.08477000	0.06058100	0.34028700
C	-3.24115500	0.60395400	1.63129800
C	-3.84669700	0.53957800	-0.74407900
C	-4.18825500	1.60958200	1.82561200
C	-4.77694600	1.55501800	-0.50405900
C	-4.95531000	2.08641800	0.76737600

H	-4.31873900	2.02719400	2.81978400
H	-5.36344500	1.93635800	-1.33503800
H	-5.68140200	2.87612300	0.93184500
C	3.08477600	0.06065400	0.34027600
C	3.84668000	0.53969300	-0.74408700
C	3.24116000	0.60400300	1.63129700
C	4.77690200	1.55515500	-0.50405600
C	4.18823400	1.60965300	1.82562300
C	4.95526400	2.08653300	0.76738900
H	5.36338200	1.93652900	-1.33503200
H	4.31871700	2.02724700	2.81980200
H	5.68133500	2.87625500	0.93186700
C	3.67100800	-0.00831100	-2.13926800
H	4.17847300	-0.97049500	-2.26854300
H	2.61849800	-0.16279500	-2.38335800
H	4.09020000	0.67758300	-2.87792800
C	2.40183400	0.10238400	2.77887300
H	1.33371600	0.21645900	2.57019400
H	2.56684500	-0.96180000	2.97312100
H	2.62738200	0.64941700	3.69637900
C	-3.67102100	-0.00844500	-2.13925200
H	-2.61851000	-0.16293000	-2.38333900
H	-4.17848400	-0.97063200	-2.26851700
H	-4.09021300	0.67743700	-2.87792300
C	-2.40180700	0.10237900	2.77887600
H	-2.56682200	-0.96179700	2.97317200
H	-1.33369300	0.21643500	2.57016700
H	-2.62733000	0.64945000	3.69636400
C	-0.00003800	1.34364800	-1.38580000
H	0.87525100	1.40674200	-2.04771000
H	-0.87538100	1.40670400	-2.04764400
C	-0.00003100	2.55119400	-0.43171300
H	0.87634900	2.50939100	0.23001400
H	-0.87636900	2.50935600	0.23006700
C	-0.00007800	3.91734600	-1.13962200
H	0.87640800	3.97667500	-1.79884100
H	-0.87661100	3.97664600	-1.79878300
Co	0.00001500	-0.40405100	-0.38344600
C	-0.00006700	5.11529800	-0.18366100
H	-0.87572900	5.05212700	0.47494000
H	0.87564400	5.05215800	0.47487700
C	-0.00011800	6.46832100	-0.90011700
H	-0.00010800	7.30227600	-0.19134200

H	0.88173800	6.57986000	-1.53944400
H	-0.88202400	6.57982700	-1.53938000

^{1}Co(0)-6

Atom	x	y	z
C	1.09882700	2.53896500	0.38145700
C	1.06808700	3.91790900	0.65294000
C	-0.13615300	4.58482400	0.72464000
C	-1.31915000	3.84744100	0.55289300
C	-1.26162400	2.48447700	0.30306600
N	-0.06939500	1.81996700	0.19685300
H	-0.17341400	5.65062900	0.91956800
H	1.99642200	4.45619200	0.79787500
H	-2.27427800	4.34873800	0.62898100
C	2.33334700	1.80555600	0.27202000
C	-2.51158000	1.68919400	0.20850300
N	-2.41814700	0.45314300	-0.12618400
N	2.23574100	0.53615300	-0.08957600
C	-3.82198400	2.37373800	0.54470200
H	-3.80889600	2.79146300	1.55450100
H	-4.02107000	3.19905700	-0.14477900
H	-4.65112000	1.67277300	0.47431900
C	3.64788500	2.49454500	0.55451400
H	3.82172900	3.32001700	-0.14327500
H	3.67796000	2.91563400	1.56401400
H	4.48227000	1.80307900	0.45639000
C	-3.53770800	-0.41910300	-0.10582000
C	-4.21867500	-0.72534700	-1.30198200
C	-3.90568700	-1.03732900	1.10883500
C	-5.24326600	-1.67391800	-1.26600100
C	-4.92840500	-1.98816100	1.09216000
C	-5.59422100	-2.31453200	-0.08336600
H	-5.77308900	-1.90860200	-2.18491600
H	-5.20592200	-2.47446800	2.02300100
H	-6.38579000	-3.05686400	-0.07680500
C	3.39740800	-0.29414600	-0.14628500
C	3.87430400	-0.89444500	1.03921100
C	4.02966100	-0.54723000	-1.37871600
C	4.96549600	-1.76182500	0.96175700
C	5.12284100	-1.41818800	-1.40828500
C	5.58844200	-2.03058600	-0.25197300
H	5.32915600	-2.23158000	1.87109400
H	5.61519000	-1.61121000	-2.35735100
H	6.43554900	-2.70776600	-0.29423900

C	3.23320000	-0.60146000	2.37268500
H	3.46294800	0.41250500	2.71863700
H	2.14630800	-0.68139900	2.32165800
H	3.59294800	-1.29423000	3.13589900
C	3.56650000	0.10178000	-2.66076000
H	2.74068100	-0.45322400	-3.11751000
H	3.22117600	1.12520100	-2.50501700
H	4.37598300	0.12775900	-3.39364900
C	-3.23735400	-0.66565700	2.40958200
H	-2.15522100	-0.58957300	2.30414000
H	-3.59596800	0.30070300	2.78356200
H	-3.45133700	-1.40866500	3.18029400
C	-3.87880900	-0.03481500	-2.60042600
H	-3.83228100	1.05234700	-2.49007000
H	-2.91106500	-0.35550700	-2.99505600
H	-4.62931200	-0.25629600	-3.36183600
C	-0.08535800	-1.81799100	0.95029100
H	0.05168200	-1.55439100	2.01106800
H	-1.14834900	-2.06972300	0.84178100
C	0.75143700	-3.06681900	0.63596300
H	1.82240500	-2.84103900	0.69768900
H	0.57995700	-3.38163600	-0.40229500
C	0.45050000	-4.26310400	1.55289500
H	0.65216000	-4.01490100	2.60044200
H	-0.60270300	-4.55505600	1.48540900
H	1.05742700	-5.13949900	1.29639300
Co	0.27022500	-0.16027600	-0.17141000
C	-0.19550400	-1.12908100	-2.20979700
H	0.67145000	-1.77599400	-2.30028700
H	-1.13319800	-1.61799700	-1.97401900
C	-0.13376500	0.18082200	-2.53400500
H	-1.01423300	0.80854400	-2.52954500
H	0.78820800	0.64449500	-2.85982900

^{1}Co(0)-TS-6/7

Atom	x	y	z
C	1.26571800	2.67836600	-0.10140100
C	1.32593600	4.06618500	-0.12518800
C	0.12770200	4.79658000	-0.14517800
C	-1.09691000	4.12963800	-0.12191200
C	-1.12092000	2.73244100	-0.10020500
N	0.06156600	2.04306900	-0.12106600
H	0.15390400	5.88025700	-0.16075800
H	2.27901600	4.58226000	-0.12731600

H	-2.01802800	4.70036900	-0.11571700
C	2.37198300	1.74624500	0.00680500
C	-2.25406600	1.85112400	-0.00338600
N	-1.94922700	0.55429500	0.05192500
N	2.02019900	0.47494800	0.07019000
C	-3.66473900	2.36369500	0.10343800
H	-3.70846700	3.44817000	0.01237900
H	-4.30816300	1.93721800	-0.67038100
H	-4.11386800	2.08943300	1.06314000
C	3.79078200	2.24366100	0.07911200
H	3.87364400	3.09881400	0.75372700
H	4.47123100	1.46885100	0.42790700
H	4.13829600	2.57479400	-0.90556800
C	-3.00335800	-0.37763100	0.31835400
C	-3.76894500	-0.93746000	-0.72144400
C	-3.24198900	-0.73863000	1.66057100
C	-4.76744500	-1.86029300	-0.39373600
C	-4.24697200	-1.66615000	1.94217900
C	-5.00851200	-2.22831700	0.92419300
H	-5.36423100	-2.29292600	-1.19171400
H	-4.43092000	-1.94858400	2.97477000
H	-5.78688000	-2.94808400	1.15691600
C	3.01033000	-0.52413800	0.34888300
C	3.15950700	-0.94359900	1.68777500
C	3.79091100	-1.09146000	-0.67396200
C	4.07050100	-1.96112400	1.97478900
C	4.68706400	-2.11262700	-0.34108800
C	4.82564500	-2.55375100	0.96822500
H	4.18559800	-2.29125200	3.00302400
H	5.28597100	-2.56136800	-1.12859000
H	5.52231100	-3.35141400	1.20560300
C	2.37967500	-0.28625700	2.79946600
H	2.65234600	0.76763900	2.91681500
H	1.30363800	-0.30900800	2.61101600
H	2.56694000	-0.78452000	3.75252100
C	3.72714900	-0.59195900	-2.09566000
H	2.73376800	-0.24000200	-2.36194800
H	4.42100600	0.24291400	-2.25046900
H	4.01251800	-1.37733300	-2.79893200
C	-2.42835900	-0.13639000	2.77899000
H	-1.35954900	-0.31875900	2.63742300
H	-2.55232100	0.94927100	2.84112100
H	-2.71886600	-0.55971300	3.74251500

C	-3.53096700	-0.58339700	-2.16808900
H	-4.37497500	-0.89711000	-2.78604800
H	-3.38320800	0.48750300	-2.32052600
H	-2.63672700	-1.07889600	-2.55222700
C	-0.03197300	-1.94664200	0.31692900
H	0.76234800	-1.94112600	1.06470000
H	-1.01336100	-2.05740400	0.78023700
C	0.20304400	-2.89796900	-0.73983700
H	1.22407800	-3.27512600	-0.82428600
H	0.24225700	-2.14685100	-1.93223600
C	-0.86028800	-3.90959000	-1.11198200
H	-0.90651700	-4.71468700	-0.36790700
H	-1.85097300	-3.44690900	-1.14208400
H	-0.66971800	-4.37451200	-2.08502100
Co	0.01551000	0.14016000	-0.14588600
C	0.18560200	-1.33023300	-2.91202400
H	1.12363000	-1.57306200	-3.41399900
H	-0.66535200	-1.75587500	-3.44859500
C	0.03831800	-0.00312000	-2.38092400
H	-0.91683000	0.48596600	-2.54200500
H	0.87337800	0.67738600	-2.52807100

^{1}Co(0)-7

Atom	x	y	z
C	-1.24402500	2.43073400	0.19166000
C	-1.30840800	3.81227100	0.28834400
C	-0.12544800	4.57373400	0.28732700
C	1.08043600	3.92091900	0.16802400
C	1.11553700	2.51586800	0.07056400
N	-0.05070600	1.77256200	0.11108200
H	-0.16797000	5.65422600	0.36772400
H	-2.26391500	4.31469500	0.35075600
H	2.00597900	4.48349700	0.15248900
C	-2.49233500	1.62654400	0.09415600
C	2.33922200	1.77761300	-0.07593600
N	2.23532600	0.45303600	-0.03265100
N	-2.38568500	0.36159500	-0.08753100
C	3.65138000	2.50306200	-0.25246600
H	3.63273700	3.17911500	-1.11274800
H	3.89235900	3.10949700	0.62738400
H	4.47062500	1.80072700	-0.39807100
C	-3.82046800	2.35322200	0.17526400
H	-3.90864600	2.90518200	1.11461800
H	-3.93148100	3.07603800	-0.63753900

H	-4.64785300	1.64868900	0.11546900
C	3.33546100	-0.38401300	-0.37351500
C	4.06066500	-1.04540800	0.63893200
C	3.64627000	-0.59800500	-1.73384900
C	5.06499100	-1.94257000	0.26893000
C	4.65624200	-1.50832600	-2.05798800
C	5.35988000	-2.18491800	-1.06877600
H	5.62539400	-2.45424400	1.04621000
H	4.89050000	-1.68438000	-3.10424100
H	6.13847100	-2.89170700	-1.33770600
C	-3.50398000	-0.46725600	-0.35150000
C	-3.94206700	-0.61139200	-1.68567800
C	-4.09883900	-1.21712500	0.68376000
C	-4.96440900	-1.52138400	-1.96165700
C	-5.12170400	-2.11122200	0.36012000
C	-5.55445300	-2.27233400	-0.95144700
H	-5.30013700	-1.63834900	-2.98825800
H	-5.58365100	-2.68846900	1.15606300
H	-6.34526900	-2.97803500	-1.18438400
C	-3.33830500	0.21306400	-2.79670800
H	-3.68143800	1.25333800	-2.76346300
H	-2.24802300	0.24612300	-2.73919300
H	-3.61569500	-0.18749500	-3.77373100
C	-3.65595800	-1.04346600	2.11362700
H	-2.57868500	-1.17651900	2.22188200
H	-3.88156300	-0.03998100	2.49044500
H	-4.15734200	-1.75960300	2.76764200
C	2.93358000	0.15680200	-2.83042700
H	1.87414900	0.29688900	-2.61122200
H	3.35951700	1.15718400	-2.96709900
H	3.02474900	-0.36429200	-3.78606900
C	3.79189800	-0.75907000	2.09450300
H	4.03576900	0.27816400	2.34766500
H	2.74118300	-0.89758800	2.35111400
H	4.39258900	-1.40622800	2.73696100
C	0.04871000	-1.66013500	-1.28047700
H	-0.70795800	-1.04767300	-1.75184500
H	1.00985700	-1.73818300	-1.77623800
C	-0.22560000	-2.39190100	-0.18121600
H	-1.23288200	-2.36265700	0.22588300
H	-0.62613100	-2.27421300	3.13893300
C	0.70968900	-3.41287600	0.40432000
H	0.34404500	-4.41933900	0.16755600

H	1.71919700	-3.31939600	-0.00104800
H	0.76246800	-3.34581800	1.49174700
Co	0.37956400	-0.15028800	0.61144000
C	0.10968300	-1.52753700	3.45939100
H	-0.08215800	-1.34459300	4.52661400
H	1.09063300	-2.01302700	3.40504000
C	0.04094700	-0.24677600	2.62023100
H	0.76010800	0.48428700	3.02079500
H	-0.94184100	0.22283300	2.75959600

^{1}Co(0)-8

Atom	x	y	z
C	1.19666600	2.55800900	-0.01270700
C	1.21441600	3.95017900	-0.04884700
C	-0.00001300	4.64639800	-0.07164100
C	-1.21445400	3.95015800	-0.04874000
C	-1.19664100	2.55801100	-0.01261300
N	0.00000300	1.90104300	-0.00563000
H	-0.00001700	5.73007400	-0.10243800
H	2.15000100	4.49667900	-0.06349400
H	-2.15006500	4.49661800	-0.06331500
C	2.31049300	1.63571000	0.02025400
C	-2.31050500	1.63571700	0.02040600
N	-1.96662900	0.35255400	0.04697400
N	1.96658600	0.35252500	0.04685200
C	-3.73781400	2.10825100	0.01167600
H	-3.81391800	3.15510000	0.30514100
H	-4.18580700	2.01065300	-0.98316000
H	-4.35504000	1.51893500	0.69205400
C	3.73785800	2.10806700	0.01161900
H	4.18676600	2.00794500	-0.98253600
H	3.81388900	3.15559200	0.30265000
H	4.35441000	1.52030000	0.69398200
C	-2.99364000	-0.64262600	0.05295700
C	-3.52081500	-1.10415600	-1.16623000
C	-3.42529200	-1.17496100	1.28178300
C	-4.49853700	-2.10182400	-1.13269000
C	-4.40838500	-2.16663000	1.26936700
C	-4.94546900	-2.62967200	0.07298900
H	-4.90820000	-2.47039400	-2.06878500
H	-4.74906000	-2.58413800	2.21244300
H	-5.70366700	-3.40628100	0.08034600
C	2.99364500	-0.64260200	0.05289400
C	3.42537700	-1.17480200	1.28175400

C	3.52078700	-1.10424500	-1.16626800
C	4.40853500	-2.16640800	1.26939600
C	4.49858400	-2.10184000	-1.13266900
C	4.94560900	-2.62952800	0.07304500
H	4.74926200	-2.58381400	2.21249900
H	4.90822100	-2.47048800	-2.06874400
H	5.70386100	-3.40608400	0.08045000
C	2.83836900	-0.68716900	2.58229500
H	3.02546400	0.37892100	2.74627300
H	1.75306200	-0.82098100	2.59934700
H	3.26016900	-1.23216200	3.42901200
C	3.04668600	-0.54400700	-2.48508600
H	1.95795900	-0.46526600	-2.52056700
H	3.44231100	0.46030900	-2.67230500
H	3.36803700	-1.17792500	-3.31382000
C	-2.83833200	-0.68733200	2.58234600
H	-1.75299000	-0.82086000	2.59932400
H	-3.02570500	0.37869400	2.74643900
H	-3.25994900	-1.23252200	3.42902500
C	-3.04684300	-0.54371400	-2.48500700
H	-3.44255700	0.46059900	-2.67205600
H	-1.95812300	-0.46490200	-2.52056400
H	-3.36821200	-1.17754200	-3.31380200
C	0.00000500	-1.98624900	0.21918700
H	0.87775700	-2.30340500	0.79866500
H	-0.87760200	-2.30339000	0.79889500
C	-0.00017700	-2.74940300	-1.11396600
H	0.88207500	-2.51833800	-1.72085600
H	-0.88257100	-2.51830600	-1.72063600
Co	0.00000000	-0.00357600	0.06901600
H	-0.00017900	-3.83989400	-0.97331200

^{1}Co(0)-TS-3/9

Atom	x	y	z
C	-1.22413900	2.49189100	-0.01006300
C	-1.25398500	3.88030200	0.02525200
C	-0.05406900	4.60104100	0.03968200
C	1.14928300	3.90283100	-0.02514200
C	1.14298400	2.50890900	-0.06057100
N	-0.03712000	1.80909800	-0.01241100
H	-0.06259900	5.68422900	0.07930400
H	-2.20114600	4.40640600	0.02904300
H	2.08865300	4.44268700	-0.05312600
C	-2.41785000	1.64952000	-0.09422900

C	2.33077100	1.68239700	-0.18402900
N	2.13357600	0.38984600	-0.11559300
N	-2.20833900	0.36783700	-0.09204300
C	3.67465400	2.33121900	-0.41082400
H	3.65154700	2.99521500	-1.27965200
H	3.97227800	2.93892600	0.44971400
H	4.44994400	1.58509000	-0.57584500
C	-3.77868600	2.29440800	-0.20496100
H	-4.00171200	2.89922700	0.67919100
H	-3.82928200	2.96048300	-1.07095300
H	-4.56169700	1.54516500	-0.30775900
C	3.21041900	-0.52878500	-0.21121700
C	4.01103200	-0.79537100	0.91889500
C	3.41344000	-1.22738000	-1.41930500
C	5.00553400	-1.77161300	0.81848200
C	4.42223100	-2.19098600	-1.47476200
C	5.21505400	-2.46902800	-0.36592800
H	5.62146800	-1.98573100	1.68751900
H	4.58517200	-2.72979400	-2.40391400
H	5.99060400	-3.22600900	-0.42456900
C	-3.26499900	-0.57377700	-0.15712800
C	-3.53682700	-1.21176300	-1.38498000
C	-3.96062600	-0.93529200	1.01489400
C	-4.51380600	-2.20812100	-1.41953000
C	-4.92692300	-1.94107600	0.93295900
C	-5.20665500	-2.57749900	-0.27109900
H	-4.73034500	-2.70077400	-2.36320200
H	-5.46386500	-2.22812700	1.83276900
H	-5.95772100	-3.35973300	-0.31388900
C	-2.80253200	-0.80639800	-2.63850600
H	-3.04399400	0.21931300	-2.93696100
H	-1.71880800	-0.84076000	-2.49839100
H	-3.06069000	-1.46224800	-3.47240300
C	-3.68082100	-0.24908600	2.33017800
H	-2.61131100	-0.09743600	2.48894400
H	-4.15026900	0.74009300	2.37915900
H	-4.07436000	-0.83304000	3.16483400
C	2.57143400	-0.92413600	-2.63302000
H	1.50618800	-1.05357600	-2.42238900
H	2.69889400	0.11017400	-2.96828100
H	2.83651000	-1.57865200	-3.46588900
C	3.80799900	-0.04213700	2.21096200
H	4.25380200	0.95819100	2.17111100

H	2.74853400	0.09208100	2.43726200
H	4.27472400	-0.56905600	3.04590700
C	-0.01102700	-2.13157100	-0.07492800
H	-0.86063000	-2.38228900	-0.70456700
H	0.95023700	-2.51151500	-0.41196000
C	-0.21684800	-1.93147500	1.30284500
H	-1.24506600	-1.98301200	1.65047600
H	-0.13741500	-0.25416500	1.68754300
C	0.79978700	-2.37776700	2.33098200
H	0.65497100	-3.44474900	2.53841500
H	1.82009200	-2.25089400	1.96703300
H	0.70029300	-1.83750500	3.27561400
Co	0.00967500	-0.10782300	0.16077000

^{1}Co(0)-9

Atom	x	y	z
C	1.20182400	2.48713400	-0.05973400
C	1.23280800	3.87416600	-0.17084900
C	0.03857700	4.59514300	-0.20394600
C	-1.16248800	3.89874800	-0.11215200
C	-1.15146700	2.50833100	-0.00520400
N	0.02040600	1.80394700	0.00456000
H	0.04726600	5.67546800	-0.29283900
H	2.18039100	4.39570100	-0.22520600
H	-2.10341100	4.43536400	-0.12425100
C	2.41671300	1.66239700	0.00342100
C	-2.36389100	1.69694900	0.08287800
N	-2.18118500	0.41149600	0.09252400
N	2.23792200	0.38460400	0.07720600
C	-3.71214600	2.37424200	0.13689800
H	-3.76671800	3.08276200	0.96839500
H	-3.90757300	2.93863200	-0.78047200
H	-4.51245000	1.64650700	0.25833500
C	3.76819400	2.33711700	-0.02676200
H	3.91135200	2.88930300	-0.96057200
H	3.87027200	3.05551800	0.79156900
H	4.57129900	1.60747200	0.05980700
C	-3.27511800	-0.49272700	0.14811700
C	-3.87536300	-0.93489700	-1.04770500
C	-3.68440600	-1.00066000	1.39702500
C	-4.88497500	-1.89712500	-0.96739300
C	-4.69894900	-1.96015900	1.42833500
C	-5.29763800	-2.41182500	0.25718400
H	-5.35098100	-2.24659400	-1.88440000

H	-5.01911900	-2.35714400	2.38755800
H	-6.08018100	-3.16274900	0.29818800
C	3.32202200	-0.52732900	0.13639900
C	3.75030700	-1.00321100	1.39171100
C	3.88170200	-1.02417000	-1.05813100
C	4.74881400	-1.97817000	1.43116900
C	4.87679300	-2.00073500	-0.96920300
C	5.31160500	-2.47933300	0.26201800
H	5.08493800	-2.34920400	2.39530100
H	5.31203100	-2.39136900	-1.88471400
H	6.08178000	-3.24245800	0.31019900
C	3.15669800	-0.45394300	2.66542600
H	3.46330100	0.58300600	2.84234200
H	2.06421600	-0.45161400	2.63415100
H	3.47360500	-1.04074100	3.52989800
C	3.42145600	-0.50970000	-2.39973700
H	2.33226100	-0.44262200	-2.45071400
H	3.80969000	0.49558300	-2.60118900
H	3.77039500	-1.15848500	-3.20585300
C	-3.05264700	-0.50348800	2.67337100
H	-1.96150700	-0.53473800	2.61940500
H	-3.32426100	0.53721900	2.88195700
H	-3.37245400	-1.10322300	3.52790900
C	-3.44596500	-0.37706400	-2.38196600
H	-3.81416900	0.64504700	-2.52849000
H	-2.35796800	-0.33603500	-2.46681000
H	-3.83859200	-0.98277800	-3.20143700
C	-0.19822500	-2.10255400	0.67390300
H	0.45997600	-2.01511200	1.53537600
H	-1.23604200	-2.34024600	0.88583500
C	0.32168000	-2.28262100	-0.58541500
H	1.40177500	-2.28848800	-0.70019300
H	-0.01761300	-0.13388300	-1.69058800
C	-0.45254200	-2.88905500	-1.72546200
H	-0.25970900	-3.96945300	-1.76940500
H	-1.52826400	-2.75081800	-1.60245400
H	-0.16046600	-2.46355700	-2.68714500
Co	-0.03419700	-0.15034700	-0.14573100

^{1}Co(0)-10

Atom	x	y	z
C	1.18677900	2.37112400	0.07071000
C	1.20880300	3.73077700	0.36482600
C	0.00000000	4.42652800	0.48011500

C	-1.20880300	3.73077600	0.36482900
C	-1.18677900	2.37112300	0.07071200
N	0.00000000	1.74031800	-0.17481500
H	0.00000000	5.48488500	0.71402900
H	2.14867600	4.24457700	0.53113100
H	-2.14867600	4.24457600	0.53113700
C	2.33188700	1.46921600	0.06896900
C	-2.33188700	1.46921500	0.06897100
N	-2.03739000	0.19220200	0.00715900
N	2.03739000	0.19220200	0.00715600
C	-3.73175400	2.02061100	0.15180000
H	-4.47074100	1.22271400	0.19424700
H	-3.85518900	2.64177000	1.04357700
H	-3.95761500	2.65176900	-0.71322900
C	3.73175400	2.02061300	0.15179600
H	3.85519100	2.64176700	1.04357600
H	4.47074200	1.22271600	0.19423900
H	3.95761400	2.65177400	-0.71323000
C	-3.04823500	-0.81404000	0.03358500
C	-3.70490000	-1.19936400	-1.15054300
C	-3.30618600	-1.46373400	1.25528900
C	-4.63874200	-2.23622900	-1.08056700
C	-4.24971500	-2.49254900	1.27822500
C	-4.91601800	-2.87931200	0.12064400
H	-5.14929600	-2.54481600	-1.98817400
H	-4.45736000	-2.99767300	2.21718700
H	-5.64273000	-3.68482800	0.15270700
C	3.04823500	-0.81403900	0.03358500
C	3.30618600	-1.46373100	1.25528900
C	3.70489800	-1.19936800	-1.15054400
C	4.24971400	-2.49254800	1.27822700
C	4.63873800	-2.23623400	-1.08056600
C	4.91601400	-2.87931500	0.12064600
H	4.45735900	-2.99767000	2.21719000
H	5.14929000	-2.54482400	-1.98817300
H	5.64272500	-3.68483200	0.15271100
C	2.57759300	-1.05651800	2.51177200
H	2.81441900	-0.03004600	2.81009900
H	1.49282300	-1.09665500	2.37566000
H	2.83965100	-1.71198300	3.34457400
C	3.39695900	-0.53010000	-2.46620200
H	2.32685100	-0.57345900	-2.68528700
H	3.68523800	0.52654200	-2.46985400

H	3.93298500	-1.01759200	-3.28281900
C	-2.57759100	-1.05652500	2.51177100
H	-1.49282100	-1.09666200	2.37565700
H	-2.81441500	-0.03005300	2.81010100
H	-2.83964700	-1.71199100	3.34457300
C	-3.39696100	-0.53009300	-2.46620000
H	-3.68524000	0.52654900	-2.46985100
H	-2.32685300	-0.57345300	-2.68528500
H	-3.93298700	-1.01758400	-3.28281900
H	0.00000300	-1.17469800	-1.87940400
Co	0.00000200	-0.14968800	-0.65013400

$^{1/2}$Co(+)

$^{1/2}$Co(+)-1

Atom	x	y	z
C	1.17635900	2.47981300	0.00491500
C	1.21366000	3.87448200	0.00737000
C	0.00066100	4.56623300	0.00829200
C	-1.21245800	3.87470400	0.00627200
C	-1.17550400	2.47996400	0.00386600
N	0.00040500	1.84466000	0.00340600
H	0.00076700	5.65005400	0.01031400
H	2.15325200	4.41271800	0.00833700
H	-2.15190800	4.41312300	0.00641300
C	2.32105000	1.52458800	0.00089400
C	-2.32053800	1.52488300	-0.00128700
N	-1.98553000	0.27198100	0.00770700
N	1.98546900	0.27201900	0.00989200
C	-3.71797400	2.05996600	-0.01711600
H	-3.89007600	2.69797200	0.85541500
H	-3.87662700	2.68254300	-0.90328000
H	-4.45735400	1.26337200	-0.01579400
C	3.71882200	2.05887200	-0.01347400
H	3.87931100	2.68024900	-0.90015100
H	3.88986600	2.69787300	0.85856900
H	4.45774900	1.26187300	-0.00998100
C	-3.00054600	-0.75404100	-0.00306800
C	-3.44185600	-1.25060000	-1.23891900
C	-3.46289000	-1.25932700	1.22185100
C	-4.39747400	-2.26905200	-1.22434300
C	-4.41863000	-2.27729300	1.18382500
C	-4.88646200	-2.77743500	-0.02624000
H	-4.75541300	-2.66924200	-2.16739600
H	-4.79303000	-2.68372400	2.11772300

H	-5.62636900	-3.57016800	-0.03548100
C	3.00020700	-0.75439100	-0.00086900
C	3.45607000	-1.26383600	1.22465300
C	3.44776300	-1.24693800	-1.23621000
C	4.41164800	-2.28198600	1.18833300
C	4.40282900	-2.26596100	-1.21992200
C	4.88540000	-2.77845900	-0.02097100
H	4.78122600	-2.69144500	2.12286000
H	4.76544400	-2.66331100	-2.16241900
H	5.62501300	-3.57146800	-0.02902800
C	2.92663100	-0.74386800	2.53772200
H	3.16090500	0.31443300	2.69342400
H	1.83788300	-0.84541400	2.59810500
H	3.35481200	-1.29569700	3.37487300
C	2.91464500	-0.70737300	-2.54032100
H	1.82343200	-0.77875900	-2.58910100
H	3.17622100	0.34480100	-2.69502500
H	3.31822700	-1.26642900	-3.38486600
C	-2.94053200	-0.73578900	2.53634700
H	-1.85162200	-0.83198100	2.60108800
H	-3.18064500	0.32142800	2.69044300
H	-3.36921400	-1.28906400	3.37228900
C	-2.90143400	-0.71515400	-2.54167100
H	-3.16102800	0.33686800	-2.70056000
H	-1.81004000	-0.78775800	-2.58434400
H	-3.30096800	-1.27607000	-3.38689400
Co	0.00018300	-0.08428900	0.02603200
C	-0.00003600	-2.03166400	0.04887500
H	-0.01450600	-2.39141400	-0.99070500
H	0.89528500	-2.44766700	0.51966300
H	-0.88441900	-2.44455200	0.54277900

$^{1/2}$Co(+)-2

Atom	x	y	z
C	1.17038600	2.43915600	-0.33753900
C	1.20319800	3.81132600	-0.59074400
C	-0.00598300	4.50047300	-0.68225600
C	-1.21431300	3.81485400	-0.55842100
C	-1.17841900	2.44284800	-0.30562300
N	-0.00284600	1.81330600	-0.16275000
H	-0.00696600	5.56726400	-0.87320200
H	2.14282600	4.33300900	-0.72116900
H	-2.15570700	4.33889300	-0.66464000
C	2.32526800	1.50528700	-0.29840100

C	-2.33359500	1.51090400	-0.24435800
N	-2.02548200	0.26669100	-0.05037300
N	2.01785200	0.26087600	-0.10564500
C	-3.71443500	2.04868100	-0.47152300
H	-3.97262600	2.78063600	0.30003100
H	-3.76855700	2.56668500	-1.43374800
H	-4.46219000	1.25980700	-0.46399800
C	3.70494300	2.04260400	-0.53253600
H	3.74054600	2.61211000	-1.46567500
H	3.99102300	2.72730700	0.27221600
H	4.44414400	1.24746300	-0.58610600
C	-3.04939900	-0.75111900	-0.08873000
C	-3.21737100	-1.46063000	-1.29108600
C	-3.81587300	-1.03376600	1.05474500
C	-4.15860200	-2.49144700	-1.31822900
C	-4.74122000	-2.07849700	0.97756400
C	-4.91010200	-2.80785600	-0.19292000
H	-4.30023400	-3.05039300	-2.23754400
H	-5.33818000	-2.31664500	1.85198700
H	-5.63033700	-3.61772200	-0.22945500
C	3.03925300	-0.75814300	-0.12757400
C	3.84638500	-0.99228000	0.99803400
C	3.15858100	-1.52954800	-1.30025500
C	4.75453900	-2.05557800	0.94075900
C	4.08882800	-2.56798600	-1.31140000
C	4.87460800	-2.84156400	-0.19624600
H	5.37830800	-2.25855600	1.80574000
H	4.19546900	-3.16980500	-2.20801900
H	5.58344600	-3.66196800	-0.21819700
C	3.81708200	-0.12367700	2.23364000
H	4.61458300	0.62706300	2.20319700
H	2.87704700	0.41091800	2.35998500
H	3.98354100	-0.71922800	3.13327300
C	2.34983200	-1.21675600	-2.53418100
H	1.27953200	-1.16887500	-2.32160800
H	2.63456900	-0.25354700	-2.97151900
H	2.50216100	-1.97730900	-3.30059400
C	-3.69718600	-0.23003600	2.32685100
H	-2.66549600	-0.13356300	2.66660100
H	-4.09296200	0.78457300	2.20832100
H	-4.26398100	-0.69835900	3.13200500
C	-2.44949300	-1.09768600	-2.53778700
H	-2.78393500	-0.14122800	-2.95497800

H	-1.37714900	-1.00759900	-2.35009400
H	-2.58869400	-1.85226700	-3.31261900
C	-0.02769200	-2.05367400	0.14838300
H	-0.11498100	-2.36554700	-0.90028700
H	0.88908300	-2.49584300	0.54607200
H	-0.88530100	-2.47567600	0.67875800
C	0.13449900	-0.54722300	2.66847300
H	1.08896300	-1.05764600	2.68946300
H	-0.73675800	-1.18057300	2.77365900
C	0.04289200	0.78977100	2.64220000
H	-0.90992200	1.30136400	2.71879000
H	0.92189900	1.42437900	2.63585100
Co	-0.00442600	-0.08799400	0.18680800

$^{1/2}$Co(+)-TS-2/3

Atom	x	y	z
C	1.17516800	2.43931000	-0.24115900
C	1.20121900	3.81606100	-0.46642000
C	-0.00202400	4.51097700	-0.55049600
C	-1.20353900	3.81551900	-0.44810700
C	-1.17312800	2.43908100	-0.22160200
N	0.00193800	1.79416100	-0.07368200
H	-0.00354100	5.58122000	-0.72052200
H	2.14252800	4.33746900	-0.58210100
H	-2.14674500	4.33634700	-0.55009400
C	2.36857100	1.55408300	-0.23914300
C	-2.36567700	1.55375100	-0.19830600
N	-2.11132500	0.29377000	-0.08753400
N	2.11187300	0.29416500	-0.13602500
C	-3.72772900	2.16350700	-0.37228500
H	-3.94357600	2.87427500	0.43084500
H	-3.78425500	2.71687100	-1.31434500
H	-4.50574500	1.40384600	-0.37889900
C	3.73033000	2.16039800	-0.42302200
H	3.76250700	2.76941100	-1.33079300
H	3.98206600	2.81730900	0.41507100
H	4.49754600	1.39365600	-0.50235500
C	-3.15131700	-0.69275800	-0.15270000
C	-3.30654200	-1.38652700	-1.36805600
C	-3.92925900	-1.00276600	0.97871900
C	-4.26388800	-2.40077500	-1.43297300
C	-4.87103100	-2.02926700	0.86354700
C	-5.04065900	-2.72577900	-0.32716400
H	-4.39967700	-2.93828800	-2.36599100

H	-5.48051600	-2.28081600	1.72558200
H	-5.77772600	-3.51847800	-0.39303600
C	3.13559700	-0.70672200	-0.19507600
C	3.95832800	-0.97665300	0.91461300
C	3.22452900	-1.46465600	-1.38078300
C	4.85938600	-2.04224400	0.81808700
C	4.14864300	-2.50827400	-1.43098100
C	4.95653100	-2.80499000	-0.33821700
H	5.49573900	-2.26900700	1.66780200
H	4.23425600	-3.09367900	-2.34085000
H	5.66229100	-3.62672400	-0.39019600
C	3.92740200	-0.14510600	2.17512000
H	4.58873000	0.72484100	2.09635200
H	2.93190900	0.23049000	2.41181600
H	4.27538000	-0.72587500	3.03079200
C	2.39216800	-1.12367000	-2.59232900
H	1.33189000	-1.00487400	-2.35160100
H	2.71342700	-0.18158100	-3.04935500
H	2.47617400	-1.89944100	-3.35424000
C	-3.77003800	-0.27443500	2.29153800
H	-2.79205800	-0.45695300	2.74427700
H	-3.87628900	0.80896000	2.18824700
H	-4.52397900	-0.60455100	3.00679900
C	-2.49093100	-1.02508100	-2.58480900
H	-2.75615100	-0.03677600	-2.97495400
H	-1.41887400	-0.99892100	-2.36835600
H	-2.65102600	-1.74446200	-3.38863500
C	-0.08586400	-2.10384000	0.53782200
H	0.20695600	-1.91082500	-0.51173400
H	0.57009600	-2.90260700	0.87113300
H	-1.12109100	-2.43304800	0.57012700
C	0.18817400	-1.14433800	2.26011100
H	1.17847300	-1.53639800	2.45952700
H	-0.59554900	-1.76098500	2.68790800
C	0.03344600	0.27734200	2.33542300
H	-0.90823600	0.68594400	2.68840100
H	0.89553100	0.87682100	2.61203700
Co	0.00796100	-0.04965700	0.37310800

$^{1/2}$Co(+)-3

Atom	x	y	z
C	1.17470800	2.69827300	-0.08589800
C	1.21225500	4.09101800	-0.16459400
C	0.00017100	4.78233000	-0.20567600

C	-1.21196800	4.09110100	-0.16462600
C	-1.17451500	2.69836000	-0.08593200
N	0.00007400	2.06124200	-0.05462000
H	0.00020500	5.86439500	-0.26767600
H	2.15199000	4.62815500	-0.19336300
H	-2.15166200	4.62830900	-0.19341300
C	2.32346600	1.75177800	-0.02165100
C	-2.32330500	1.75191900	-0.02173500
N	-1.99775000	0.49924800	0.06103600
N	1.99785900	0.49910800	0.06097800
C	-3.71737800	2.29689500	-0.04765500
H	-3.86216700	3.00650400	0.77273000
H	-3.89534600	2.84493500	-0.97824300
H	-4.46234900	1.51033900	0.03885900
C	3.71755600	2.29671000	-0.04742800
H	3.89560100	2.84479100	-0.97797800
H	3.86231300	3.00627500	0.77300000
H	4.46249400	1.51012600	0.03908700
C	-3.02372100	-0.51346300	0.11431200
C	-3.56707200	-0.99711600	-1.08654100
C	-3.40441800	-1.01570700	1.36931300
C	-4.52298900	-2.01278900	-1.00314400
C	-4.36848400	-2.02546700	1.39986900
C	-4.92385300	-2.52313900	0.22612600
H	-4.95417400	-2.40629900	-1.91800300
H	-4.68089400	-2.42692400	2.35840800
H	-5.66645000	-3.31224600	0.26951200
C	3.02377700	-0.51368400	0.11427900
C	3.40440900	-1.01599200	1.36927400
C	3.56714700	-0.99729300	-1.08657400
C	4.36841600	-2.02580500	1.39980500
C	4.52302500	-2.01301000	-1.00320300
C	4.92380200	-2.52344800	0.22605400
H	4.68076400	-2.42735400	2.35832600
H	4.95422000	-2.40648900	-1.91806900
H	5.66635500	-3.31259700	0.26944600
C	2.80555200	-0.47858600	2.64479900
H	3.05847800	0.57417300	2.80922900
H	1.71321700	-0.54987900	2.63903700
H	3.16699500	-1.03663600	3.50892200
C	3.15619700	-0.43968900	-2.42792600
H	2.07191500	-0.33243400	-2.51645900
H	3.59491500	0.54715000	-2.61336900

H	3.48926700	-1.09208000	-3.23569000
C	-2.80558600	-0.47825600	2.64483200
H	-1.71326500	-0.54978000	2.63918700
H	-3.05829900	0.57457800	2.80909400
H	-3.16722700	-1.03612300	3.50899000
C	-3.15602500	-0.43966200	-2.42792500
H	-3.59480200	0.54711200	-2.61356400
H	-2.07174400	-0.33232800	-2.51637100
H	-3.48895600	-1.09219700	-3.23563000
C	-0.00014300	-1.82476600	0.27520700
H	0.88300200	-2.12098300	0.85503300
H	-0.88371300	-2.12041900	0.85468900
C	-0.00015000	-2.57186300	-1.06433800
H	0.87760900	-2.28894300	-1.65822400
H	-0.87728900	-2.28810900	-1.65874800
C	-0.00085800	-4.09984400	-0.90012400
H	0.88156300	-4.43565000	-0.34804500
H	-0.88388400	-4.43494500	-0.34859300
H	-0.00075000	-4.60673400	-1.86995900
Co	0.00002600	0.12638100	0.09084100

$^{1/2}$Co(+)-4

Atom	x	y	z
N	-0.12730100	2.01706300	-0.08560000
C	-1.32453400	2.60543900	-0.23882700
C	-2.45225400	1.64121200	-0.23377500
N	-2.11654500	0.39819800	-0.09654700
C	-3.12321100	-0.63223400	-0.16987300
C	-3.25937300	-1.31581600	-1.39536200
C	-2.47422800	-0.90447100	-2.61574900
H	-2.62515500	-1.61354200	-3.43031600
C	-4.17693600	-2.36312500	-1.46640500
C	-4.93580800	-2.73008300	-0.35915600
C	-4.79956500	-2.03095800	0.83118900
C	-3.90233700	-0.96311900	0.95060300
C	-3.85900800	-0.19407400	2.25038800
H	-2.97749900	0.43678200	2.34712600
H	-5.40322400	-2.30595700	1.69083800
H	-4.29509000	-2.89710000	-2.40360500
C	-3.84722100	2.15637500	-0.43473100
H	-4.14092500	2.80190800	0.39900800
H	-3.90644900	2.76036400	-1.34448700
H	-4.56889200	1.34746800	-0.51263700
C	-1.41541500	3.98313800	-0.44440900

C	-0.23950500	4.72794100	-0.51570700
C	0.99430900	4.08716200	-0.42099300
C	1.01699800	2.70691000	-0.21493100
C	2.22068900	1.84046200	-0.19486000
N	1.99175100	0.57403600	-0.04529900
C	3.08738200	-0.36112200	-0.13844700
C	3.33384800	-0.96174600	-1.38561700
C	4.34596700	-1.92166200	-1.46232600
C	5.09855500	-2.26364200	-0.34568700
C	4.85907800	-1.63095000	0.86851500
C	3.85544200	-0.66777300	0.99867600
H	5.45945700	-1.88455500	1.73619700
H	4.54653300	-2.39908900	-2.41608500
C	3.56634500	2.46906000	-0.40945700
H	3.77913800	3.19815600	0.37826500
H	4.36232500	1.72920600	-0.41903000
H	3.58808800	3.01042500	-1.35990000
H	1.91377700	4.65170800	-0.51344700
H	-0.28444600	5.79975900	-0.66892500
H	-2.37729300	4.46713600	-0.55410500
H	5.87738300	-3.01394600	-0.42321000
C	3.64496500	0.02586000	2.32229500
H	3.84084000	1.10159200	2.25988700
H	-5.63615300	-3.55515200	-0.42895800
C	2.58631500	-0.54882200	-2.63033100
H	2.73222100	-1.27595300	-3.43003500
C	-0.00111000	-1.87416500	-0.10055400
H	-1.04850500	-2.18872100	-0.14103300
H	0.36857700	-1.85821300	-1.13947700
H	-1.40189800	-0.85212600	-2.41448000
H	-2.78163100	0.08107000	-2.98247700
H	-3.87898500	-0.87098700	3.10731200
H	-4.73484600	0.45665300	2.34515800
H	4.31875700	-0.37735900	3.07891500
H	2.62637800	-0.09318100	2.69641000
H	2.94105500	0.41736900	-3.00707400
H	1.51235600	-0.44976400	-2.46209900
C	0.86639200	-4.26796900	-0.00107000
C	0.80350500	-2.89926800	0.69551000
H	1.41885900	-4.99424000	0.60239000
H	1.36560700	-4.19666000	-0.97178000
H	-0.13536900	-4.67277800	-0.17312800
H	1.82652000	-2.55074700	0.87101900

H	0.35082700	-3.04126600	1.68323900
C	-0.18300300	-0.46838600	2.54580700
C	-0.13620900	0.87569200	2.57537300
H	-1.11991500	-1.01126000	2.55256000
H	0.70831700	-1.06888200	2.66191200
H	-1.03462500	1.48132200	2.59450200
H	0.79876700	1.41033900	2.69741400
Co	-0.04150600	0.08799900	0.21947100

$^{1/2}$Co(+)-TS-4/5

Atom	x	y	z
C	1.12289400	2.51015400	-0.22669300
C	1.13500100	3.89238700	-0.42432800
C	-0.06981000	4.57544600	-0.53037800
C	-1.25766800	3.85803100	-0.46228100
C	-1.21483300	2.47641700	-0.26367500
N	-0.03838200	1.82819000	-0.12668000
H	-0.08298400	5.64914800	-0.67678500
H	2.07193800	4.42794700	-0.49640300
H	-2.20594600	4.36812900	-0.56417900
C	2.36793100	1.69493400	-0.16588100
C	-2.44400700	1.63110600	-0.23937800
N	-2.27275100	0.37857100	-0.02258500
N	2.21532900	0.43421000	0.03021900
C	-3.77002500	2.29327500	-0.50633300
H	-3.98687800	3.04961200	0.25364000
H	-3.76954600	2.80000100	-1.47536100
H	-4.57870800	1.56616000	-0.50196200
C	3.68760500	2.38966200	-0.37210100
H	3.72312700	2.88889000	-1.34450500
H	3.84286400	3.15836300	0.39056200
H	4.51564700	1.68694200	-0.31901800
C	-3.37018800	-0.54344800	-0.09368500
C	-3.64958200	-1.15253200	-1.33389500
C	-4.09809800	-0.87355500	1.06429300
C	-4.63967900	-2.13676900	-1.37935100
C	-5.07923900	-1.86437600	0.96660600
C	-5.34465300	-2.50251500	-0.23860600
H	-4.86189100	-2.61536000	-2.32797200
H	-5.64640000	-2.12944800	1.85341500
H	-6.10608500	-3.27284400	-0.29160100
C	3.33825400	-0.45773300	-0.03737100
C	4.00093000	-0.85143000	1.13943800
C	3.71316100	-0.96493400	-1.29688800

C	5.03213500	-1.78866200	1.03296400
C	4.74675100	-1.90350700	-1.35026000
C	5.40068500	-2.32060900	-0.19694400
H	5.55562600	-2.09716900	1.93228800
H	5.04383500	-2.30416500	-2.31434100
H	6.20124000	-3.04958500	-0.25743200
C	3.65059700	-0.26219900	2.48355100
H	3.71163500	0.83026300	2.48278000
H	2.63673900	-0.52244600	2.79593400
H	4.33246000	-0.62484100	3.25343900
C	3.05226900	-0.49271500	-2.56990600
H	1.96239600	-0.48019700	-2.49477900
H	3.36293500	0.52389900	-2.83441300
H	3.32206500	-1.13580300	-3.40843200
C	-3.90239700	-0.14035700	2.36915700
H	-4.31724100	-0.70956500	3.20234900
H	-2.85449200	0.06035200	2.58963300
H	-4.41476900	0.82845900	2.36028900
C	-2.95078700	-0.72524400	-2.60279700
H	-3.33626000	0.23337400	-2.96798400
H	-1.87445200	-0.60041400	-2.46964500
H	-3.10929200	-1.45465000	-3.39831400
C	0.26822300	-2.09504200	0.83350300
H	1.34164000	-2.23512200	0.95144600
H	-0.25077500	-2.90629700	1.33580400
C	-0.14642700	-2.08426700	-0.63612300
H	0.04498600	-1.09893800	-1.14749000
H	-1.21861800	-2.25633200	-0.72459800
C	0.62659300	-3.12988600	-1.45786000
H	1.70429800	-2.96955400	-1.40380200
H	0.41690000	-4.13304500	-1.07965000
H	0.32523300	-3.10062700	-2.50778900
Co	0.00841600	-0.03679400	0.44712800
C	-0.19328200	-0.97698200	2.40995600
H	0.56814300	-1.51863200	2.96184100
H	-1.18541100	-1.37207200	2.59656000
C	-0.06908000	0.45471400	2.34574900
H	-0.95161600	1.05599200	2.54443700
H	0.85141100	0.91002700	2.70001300

$^{1/2}$Co(+)-5

Atom	x	y	z
C	1.31877400	-2.97021300	0.34469500
C	1.41400700	-4.33911400	0.59394100

C	0.23494500	-5.07633200	0.71525500
C	-1.00354500	-4.44597100	0.58587700
C	-1.02745400	-3.07369000	0.33681500
N	0.11798800	-2.38655200	0.22697100
H	0.28138400	-6.14124400	0.91011800
H	2.37637600	-4.82546000	0.69355800
H	-1.92021900	-5.01478300	0.67921900
C	2.43148200	-2.00002300	0.17972400
C	-2.22028800	-2.20542200	0.16475100
N	-1.96569000	-0.95390400	-0.06294500
N	2.06870000	-0.77546800	-0.04816400
C	-3.58659500	-2.81063000	0.26084200
H	-3.69178100	-3.62580100	-0.46121300
H	-3.74273700	-3.24200400	1.25443200
H	-4.36792800	-2.07825300	0.07515500
C	3.84533500	-2.48281200	0.28063400
H	4.03508400	-2.90030100	1.27429900
H	4.02491800	-3.28443800	-0.44188800
H	4.55951700	-1.68399100	0.09871200
C	-3.03774600	-0.00296200	-0.21947200
C	-3.56974100	0.61258500	0.92534600
C	-3.47299800	0.31445300	-1.51668900
C	-4.56900300	1.57133900	0.74102000
C	-4.47593900	1.27762600	-1.64740800
C	-5.02010700	1.90356300	-0.53140100
H	-4.99385200	2.06276300	1.61032900
H	-4.83004100	1.53807400	-2.63955600
H	-5.79509800	2.65225000	-0.65365000
C	3.05336100	0.26574200	-0.20540700
C	3.46600300	0.61122100	-1.50288600
C	3.51963000	0.93602900	0.93700900
C	4.37968700	1.65906100	-1.63619900
C	4.42961600	1.97942600	0.75016100
C	4.85764400	2.34049600	-0.52235100
H	4.71489100	1.94272200	-2.62853300
H	4.80267500	2.51431900	1.61758100
H	5.56239300	3.15535800	-0.64639000
C	2.95488800	-0.12915400	-2.71332000
H	3.27325900	-1.17702400	-2.71984400
H	1.86133900	-0.12720900	-2.75889400
H	3.32494200	0.32673100	-3.63200600
C	3.07334700	0.54362800	2.32435500
H	1.98780300	0.43272100	2.39183300

H	3.51420500	-0.40747300	2.64307600
H	3.37550700	1.29487000	3.05464200
C	-2.89711300	-0.37218900	-2.72982500
H	-1.80669100	-0.28794100	-2.76687600
H	-3.13605500	-1.44088300	-2.74886100
H	-3.29381100	0.06375700	-3.64709800
C	-3.09819800	0.25071500	2.31269600
H	-3.45637800	-0.73713400	2.62330600
H	-2.00742700	0.23456800	2.38576500
H	-3.46810500	0.96811900	3.04581800
C	-0.04350600	1.37658900	-0.68072000
H	0.85345500	1.60165500	-1.27059700
H	-0.91359100	1.50101700	-1.33749400
C	-0.14479400	2.34284700	0.50236200
H	0.71817700	2.22318400	1.16946500
H	-1.03310100	2.11562200	1.10429000
C	-0.22017700	3.81891400	0.06881200
H	0.67005000	4.06365000	-0.52386100
H	-1.07729000	3.94968200	-0.60357400
Co	0.03743900	-0.50842600	-0.17500500
C	-0.33855600	4.79795700	1.24203400
H	0.51648700	4.66287000	1.91642500
H	-1.22968100	4.55013000	1.83242900
C	-0.41187700	6.26135400	0.79995600
H	-1.27577400	6.43931500	0.15217600
H	-0.49940100	6.93463100	1.65680600
H	0.48219100	6.55473200	0.24135300

$^{1/2}$Co(+)-6

Atom	x	y	z
C	1.02223300	2.70052400	0.23778600
C	1.00001500	4.08038300	0.44714900
C	-0.23329700	4.72425000	0.52565700
C	-1.40927100	3.98225900	0.43437000
C	-1.31861100	2.60531800	0.22382900
N	-0.12132000	2.01338700	0.08724800
H	-0.27783600	5.79569400	0.68207000
H	1.91922800	4.64187800	0.55444900
H	-2.37164700	4.46796600	0.53296700
C	2.22584600	1.83357900	0.23197200
C	-2.45024300	1.64598000	0.20439500
N	-2.12244500	0.40304400	0.05018300
N	1.99696800	0.56768200	0.08354600
C	-3.84056200	2.16767400	0.42371000

H	-3.90238500	2.70183300	1.37656900
H	-4.11134200	2.88133700	-0.36034000
H	-4.57638300	1.36797700	0.43225400
C	3.57084700	2.46126600	0.45218200
H	3.81029300	3.14924400	-0.36472400
H	3.57449100	3.04690800	1.37592200
H	4.35905200	1.71578100	0.51563900
C	-3.13879300	-0.61785900	0.13710800
C	-3.89024700	-0.97344900	-0.99641400
C	-3.32017300	-1.25507200	1.37792800
C	-4.81469800	-2.01364700	-0.86707500
C	-4.25871600	-2.28615500	1.45598400
C	-4.99619100	-2.67191200	0.34325600
H	-5.40228100	-2.30422100	-1.73192800
H	-4.41004400	-2.78889100	2.40570900
H	-5.71632600	-3.47902900	0.42037700
C	3.08949400	-0.37002900	0.17277300
C	3.28412700	-1.02391400	1.40525200
C	3.89573600	-0.64182500	-0.94460500
C	4.28377900	-1.99340400	1.48361600
C	4.88072400	-1.62717400	-0.81606300
C	5.07127800	-2.30514000	0.37979600
H	4.44628000	-2.50744700	2.42544800
H	5.50599600	-1.85802500	-1.67295900
H	5.83708400	-3.06916100	0.45619500
C	2.48550000	-0.65475000	2.63135600
H	2.79006100	0.31970800	3.02979500
H	1.41443200	-0.59457800	2.42851300
H	2.63360700	-1.38674700	3.42603800
C	3.77770400	0.11127900	-2.24856500
H	2.80103700	0.57169200	-2.38960400
H	4.52348300	0.91183300	-2.30696600
H	3.96038800	-0.54857100	-3.09894900
C	-2.56128100	-0.82060800	2.60727700
H	-1.48356200	-0.78205300	2.43320100
H	-2.86831200	0.17598900	2.94336400
H	-2.73903800	-1.50784800	3.43500900
C	-3.75134400	-0.25252500	-2.31524000
H	-4.01852000	0.80642700	-2.23760900
H	-2.73490900	-0.29848200	-2.70980500
H	-4.41005100	-0.69246000	-3.06443500
C	-0.06442800	-1.88239800	0.02462800
H	0.12598200	-1.89048700	1.11178100

H	-1.11038200	-2.17509900	-0.11192300
C	0.84282800	-2.90969200	-0.64757500
H	1.88874700	-2.59192300	-0.62336100
H	0.57649900	-3.00939200	-1.70586800
C	0.73767300	-4.29831700	0.00384400
H	1.05266600	-4.27010100	1.05124200
H	-0.28979500	-4.67325100	-0.02136400
H	1.37022800	-5.02651800	-0.51223600
Co	-0.03826900	0.08540400	-0.24097600
C	0.07458500	-0.45407500	-2.55791900
H	1.05618700	-0.90571800	-2.60796200
H	-0.76019700	-1.13738000	-2.64621600
C	-0.09168300	0.88149500	-2.57914700
H	-1.07127000	1.33640900	-2.66724100
H	0.75240500	1.55963600	-2.63113200

$^{1/2}$Co(+)-TS-6/7

Atom	x	y	z
C	1.20486300	2.68357000	0.02198200
C	1.25277100	4.07272400	-0.09680200
C	0.05092400	4.77803100	-0.16611100
C	-1.16624100	4.09762300	-0.11290200
C	-1.14869900	2.70791300	0.00606800
N	0.02083500	2.04973100	0.06774500
H	0.06267700	5.85752000	-0.26013900
H	2.19961800	4.59700800	-0.13552100
H	-2.10139600	4.64141100	-0.16327500
C	2.33776300	1.74310900	0.13482300
C	-2.30261600	1.79088900	0.10459600
N	-1.99352100	0.52718800	0.10768500
N	2.00128200	0.48633100	0.13375000
C	-3.68419200	2.35980300	0.22924500
H	-3.73943400	3.04404000	1.08100100
H	-3.94086200	2.94002600	-0.66273800
H	-4.43418900	1.58415200	0.36000900
C	3.73129400	2.27818100	0.27095000
H	4.03690700	2.78378100	-0.65082900
H	3.78124400	3.01851700	1.07402600
H	4.44993200	1.48966600	0.48023800
C	-3.02423700	-0.46035200	0.33009600
C	-3.80028700	-0.94315300	-0.73732300
C	-3.19438300	-0.93342900	1.64428100
C	-4.75167800	-1.92930100	-0.45872800
C	-4.15752500	-1.91892900	1.87066000

C	-4.92981100	-2.41936000	0.82931400
H	-5.36316200	-2.31177400	-1.26962200
H	-4.30169800	-2.29290600	2.87913700
H	-5.67319200	-3.18511700	1.02193700
C	3.00338600	-0.53015900	0.35396900
C	3.12833500	-1.04666700	1.65947400
C	3.79967900	-0.99822600	-0.70413100
C	4.04459700	-2.07663300	1.87506600
C	4.69940500	-2.03631100	-0.43750100
C	4.81886800	-2.57939100	0.83438100
H	4.15293700	-2.48467900	2.87476900
H	5.31796400	-2.41348900	-1.24595000
H	5.52056900	-3.38546000	1.01875700
C	2.34239900	-0.47542400	2.81428800
H	2.65252400	0.54890400	3.04661500
H	1.26881300	-0.44102600	2.61138100
H	2.49069000	-1.07072100	3.71578800
C	3.76511300	-0.38870200	-2.08462000
H	2.80457100	0.06371300	-2.32162900
H	4.52799300	0.39134000	-2.18677600
H	3.98284500	-1.13889400	-2.84722500
C	-2.38007500	-0.38650800	2.79031800
H	-1.30556600	-0.47488300	2.60494600
H	-2.58561900	0.67341000	2.97199100
H	-2.60176500	-0.92267500	3.71355100
C	-3.64232900	-0.43272200	-2.14838900
H	-3.72292100	0.65600800	-2.21310700
H	-2.67382900	-0.70712500	-2.57099700
H	-4.41322200	-0.85151700	-2.79598800
C	-0.02744000	-1.92058400	0.16935100
H	0.70941300	-1.98693300	0.97290000
H	-1.03009000	-2.14377900	0.53405800
C	0.34620500	-2.74170300	-0.96521800
H	1.40709700	-2.98758100	-1.03681700
H	0.33233100	-1.90969100	-2.02761200
C	-0.57339200	-3.83764400	-1.45574300
H	-0.53483100	-4.68359600	-0.76034800
H	-1.61248400	-3.50087200	-1.49533300
H	-0.28605500	-4.21236700	-2.44153300
Co	0.00330000	0.14877100	-0.08520300
C	0.21501600	-1.00623300	-2.93755700
H	1.15246900	-1.18444400	-3.46281900
H	-0.63292300	-1.44096000	-3.46767400

C	0.02800200	0.26328300	-2.29230700
H	-0.94344000	0.72589500	-2.44020900
H	0.84254600	0.97337100	-2.41790400

$^{1/2}$Co(+)-7

Atom	x	y	z
C	1.25675700	2.61087800	0.09216200
C	1.30335100	4.00122100	0.02239600
C	0.10857700	4.72290900	0.02568300
C	-1.11107400	4.04561200	0.07668600
C	-1.11203800	2.65460200	0.14430500
N	0.06142400	1.97234400	0.18636900
H	0.12731600	5.80466200	-0.02774500
H	2.25410900	4.51677600	-0.03740400
H	-2.04423500	4.59533700	0.05855900
C	2.37363000	1.67538700	0.08852100
C	-2.26175900	1.76021200	0.17803800
N	-1.95961000	0.48844500	0.07553700
N	2.02171800	0.41430600	0.01386500
C	-3.64706300	2.31478400	0.33374200
H	-3.70587300	2.97633100	1.20198200
H	-3.91823800	2.91049800	-0.54375200
H	-4.38935800	1.52887000	0.44781500
C	3.78302200	2.17913600	0.18887000
H	4.01164700	2.83506200	-0.65664300
H	3.92131400	2.76945600	1.09913500
H	4.50626400	1.36753800	0.19208800
C	-2.99532500	-0.50191200	0.26189700
C	-3.73654600	-0.98937900	-0.82643400
C	-3.23028300	-0.96134400	1.57643700
C	-4.67044200	-2.00481300	-0.58505500
C	-4.17102400	-1.97415200	1.76522600
C	-4.87885700	-2.50656600	0.69144500
H	-5.24748800	-2.39305000	-1.41884200
H	-4.35706900	-2.34121000	2.76950300
H	-5.60372300	-3.29641300	0.85563800
C	3.02204200	-0.61187000	0.20396900
C	3.31337500	-1.00792600	1.52746900
C	3.66830900	-1.20415100	-0.89505800
C	4.21224900	-2.05830400	1.72088900
C	4.56290900	-2.25153600	-0.64815300
C	4.82533900	-2.68782500	0.64306300
H	4.43796400	-2.37915300	2.73285200
H	5.06657600	-2.71844200	-1.48900400

H	5.51726800	-3.50562500	0.81226200
C	2.73655000	-0.29363500	2.72851600
H	3.31110300	0.60976500	2.96166700
H	1.70164300	0.02368700	2.58626200
H	2.77532700	-0.93001400	3.61379300
C	3.50625700	-0.70026900	-2.30857000
H	2.62017700	-0.08568900	-2.43931700
H	4.37117000	-0.09221100	-2.59542900
H	3.45581100	-1.52681000	-3.02084300
C	-2.54279900	-0.34306100	2.77122000
H	-1.47632400	-0.17425100	2.60869800
H	-2.97996100	0.63049100	3.01872400
H	-2.65344600	-0.97552700	3.65303900
C	-3.63278500	-0.41561800	-2.21878700
H	-4.53078500	0.16467700	-2.45550000
H	-2.77630900	0.24131900	-2.34447800
H	-3.56595200	-1.20635500	-2.96964900
C	-0.00394500	-2.02400900	0.84550300
H	0.82394600	-1.67945500	1.45213300
H	-0.96943800	-2.11742800	1.32715100
C	0.21814000	-2.60362100	-0.35107500
H	1.22881100	-2.58713300	-0.75244100
H	0.73842600	-1.30465700	-3.00175900
C	-0.78891500	-3.41560200	-1.10042800
H	-0.55183400	-4.47616800	-0.95019200
H	-1.80622200	-3.24866400	-0.74486100
H	-0.74765500	-3.24277100	-2.17612200
Co	0.01978500	0.14505600	-0.15219600
C	-0.08896200	-0.60043700	-3.11206000
H	-0.05618000	-0.24171900	-4.15041400
H	-1.01848700	-1.15968200	-3.00476400
C	-0.00470300	0.56872900	-2.14787400
H	-0.85463200	1.24408300	-2.27583900
H	0.90149900	1.15706600	-2.31266400

$^{1/2}$Co(+)-8

Atom	x	y	z
C	1.17463100	2.55914400	0.00898100
C	1.21214300	3.95406400	-0.00041500
C	-0.00000400	4.64649200	-0.00732300
C	-1.21215100	3.95406300	-0.00041100
C	-1.17463800	2.55914300	0.00898400
N	-0.00000300	1.92143100	0.00831800
H	-0.00000400	5.73029100	-0.01550700

H	2.15183800	4.49203600	-0.00196600
H	-2.15184600	4.49203500	-0.00196000
C	2.32348200	1.61060100	0.02786800
C	-2.32348800	1.61059900	0.02787200
N	-1.99788400	0.35537500	0.04955600
N	1.99787900	0.35537700	0.04953800
C	-3.71749700	2.15628600	0.03154900
H	-3.86055000	2.82337900	0.88721500
H	-3.89694900	2.75107000	-0.86958300
H	-4.46263500	1.36653000	0.07949200
C	3.71749100	2.15629000	0.03156400
H	3.89695300	2.75107500	-0.86956400
H	3.86053300	2.82338100	0.88723400
H	4.46262900	1.36653400	0.07951500
C	-3.02311900	-0.65927600	0.05427400
C	-3.57136400	-1.08145800	-1.16738400
C	-3.39696200	-1.22650300	1.28340000
C	-4.52492700	-2.10210300	-1.13184000
C	-4.35900600	-2.23838700	1.26645200
C	-4.91887700	-2.67615900	0.07119000
H	-4.95961400	-2.44893700	-2.06376000
H	-4.66604300	-2.68943200	2.20443700
H	-5.65938400	-3.46836300	0.07715500
C	3.02311700	-0.65927400	0.05427100
C	3.39694100	-1.22649600	1.28340500
C	3.57138200	-1.08145500	-1.16737700
C	4.35898700	-2.23837900	1.26647400
C	4.52494800	-2.10209800	-1.13181500
C	4.91887800	-2.67615200	0.07122200
H	4.66601100	-2.68942200	2.20446500
H	4.95965100	-2.44893200	-2.06372700
H	5.65938700	-3.46835500	0.07720100
C	2.79332100	-0.75355700	2.58199900
H	3.05222600	0.28724700	2.80329200
H	1.70055600	-0.81634800	2.56568200
H	3.14535300	-1.35908300	3.41757800
C	3.16792300	-0.45567000	-2.48069300
H	2.08438900	-0.34185400	-2.56975600
H	3.60878600	0.53859900	-2.61411300
H	3.50426100	-1.06678300	-3.31883200
C	-2.79335900	-0.75356700	2.58200400
H	-1.70059500	-0.81636700	2.56570300
H	-3.05225900	0.28723900	2.80329200

H	-3.14541100	-1.35908900	3.41757700
C	-3.16788200	-0.45567200	-2.48069400
H	-3.60873700	0.53860000	-2.61411800
H	-2.08434600	-0.34186400	-2.56974200
H	-3.50421200	-1.06678100	-3.31883900
C	-0.00000200	-1.97595500	0.14097800
H	0.88313600	-2.30470100	0.70050300
H	-0.88316600	-2.30470600	0.70046000
C	0.00003400	-2.63083000	-1.24470300
H	0.88428000	-2.36505000	-1.83235200
H	-0.88418400	-2.36505700	-1.83239700
Co	-0.00000200	-0.01885300	0.06009900
H	0.00003600	-3.72529100	-1.16814500

$^{1/2}$Co(+)-TS-3/9

Atom	x	y	z
C	-1.13248200	2.56200100	-0.08462200
C	-1.15020700	3.95339300	-0.17765000
C	0.05892100	4.64495000	-0.17813000
C	1.25769200	3.93728100	-0.12887200
C	1.21823000	2.54623500	-0.03860100
N	0.03612700	1.90012200	0.04024100
H	0.06746900	5.72645700	-0.24496900
H	-2.08744400	4.48906800	-0.25608400
H	2.20447000	4.46035600	-0.16940700
C	-2.30389900	1.66883100	-0.16481500
C	2.38024900	1.63769800	-0.07646200
N	2.07402900	0.37916800	-0.13944400
N	-2.01868800	0.40246500	-0.17945700
C	3.76762500	2.20821200	-0.09046300
H	3.87149000	2.94053600	-0.89596600
H	3.98500200	2.72820900	0.84749800
H	4.51738700	1.43436000	-0.23685400
C	-3.67586900	2.26418600	-0.28229800
H	-3.94714900	2.80565500	0.62892700
H	-3.70748900	2.98378000	-1.10512400
H	-4.42972600	1.50293500	-0.46728500
C	3.09078200	-0.63031300	-0.17856800
C	3.81140800	-0.96950400	0.98215100
C	3.28540600	-1.30950700	-1.39839100
C	4.73467100	-2.01670300	0.89340700
C	4.22795900	-2.33700300	-1.43714400
C	4.94606600	-2.69443900	-0.30014700
H	5.29475400	-2.29867100	1.77949700

H	4.39871400	-2.86203800	-2.37142100
H	5.66852100	-3.50196100	-0.34551400
C	-3.05624400	-0.58485200	-0.24453800
C	-3.17431500	-1.32625600	-1.43752500
C	-3.87859400	-0.83841800	0.86988500
C	-4.13973500	-2.33117400	-1.49627000
C	-4.82066400	-1.86726100	0.76464200
C	-4.95515700	-2.60716300	-0.40285500
H	-4.25148900	-2.90322700	-2.41163900
H	-5.45726100	-2.08455600	1.61660700
H	-5.69428100	-3.39854500	-0.46230800
C	-2.31213300	-1.01756400	-2.63534700
H	-2.51026000	-0.01709200	-3.03270300
H	-1.24603800	-1.05355700	-2.38951800
H	-2.49272800	-1.73125900	-3.43988000
C	-3.78705900	-0.04379600	2.15166000
H	-2.78252200	0.33651400	2.34165900
H	-4.46701300	0.81482800	2.13778300
H	-4.07740100	-0.65709200	3.00628700
C	2.53310200	-0.90923400	-2.64305200
H	1.45312900	-0.86223100	-2.47326600
H	2.83700500	0.07997200	-3.00073900
H	2.71405400	-1.61765700	-3.45219000
C	3.63673900	-0.24189700	2.29516400
H	4.34355100	0.59005900	2.38714300
H	2.63387900	0.16851000	2.42299800
H	3.83357500	-0.91081400	3.13486900
C	0.02870000	-2.03638600	0.13522600
H	-0.93318800	-2.41073500	-0.20168900
H	0.88431600	-2.28718100	-0.48348100
C	0.21873900	-1.77822300	1.48949000
H	0.08540800	0.05767800	1.69604000
H	1.24299900	-1.73291400	1.84448000
C	-0.79780900	-2.11501900	2.54786500
H	-1.81665100	-2.07761000	2.16430000
H	-0.61024700	-3.14352900	2.87764700
H	-0.72092900	-1.47081200	3.42483300
Co	0.01789200	0.01932700	0.17324600

$^{1/2}$Co(+)-9

Atom	x	y	z
C	1.13729400	2.58467300	0.01901900
C	1.14811400	3.97732000	0.01433400
C	-0.06424900	4.66610900	-0.01998400

C	-1.26447600	3.95558000	-0.02928200
C	-1.22869100	2.56354700	-0.02267200
N	-0.03886700	1.91278500	-0.02884400
H	-0.07391100	5.74938800	-0.02456100
H	2.08552400	4.51854700	0.04166400
H	-2.21205800	4.47962800	-0.03575900
C	2.28313500	1.68586200	0.08853800
C	-2.36014900	1.64484700	0.01175400
N	-2.01697200	0.38395900	0.06995400
N	1.96410400	0.41680800	0.11505100
C	-3.76500400	2.16860200	-0.00850000
H	-3.91292100	2.90392100	0.78708000
H	-3.97484100	2.67363500	-0.95659000
H	-4.49475700	1.37338700	0.12227500
C	3.67544900	2.24050300	0.14184300
H	3.75716200	2.99235900	0.93123700
H	4.41374000	1.46519300	0.33093900
H	3.93248400	2.73434000	-0.80056500
C	-3.03592900	-0.63145300	0.12085800
C	-3.64299100	-1.07811500	-1.06791100
C	-3.37508000	-1.16952900	1.37699000
C	-4.58362300	-2.10822800	-0.97349600
C	-4.32479900	-2.19269500	1.41800500
C	-4.92033000	-2.66610000	0.25395600
H	-5.05860300	-2.47113800	-1.87942900
H	-4.60106200	-2.61806700	2.37741700
H	-5.65112300	-3.46580700	0.30461000
C	3.00842400	-0.57138800	0.17635200
C	3.28800700	-1.16445700	1.42265100
C	3.70782800	-0.92863300	-0.99029800
C	4.27239000	-2.15344500	1.47339000
C	4.68211000	-1.92670800	-0.88758900
C	4.96102700	-2.53935800	0.32797800
H	4.50385700	-2.61967700	2.42560700
H	5.22823100	-2.22153600	-1.77808700
H	5.71949600	-3.31244200	0.38508800
C	2.59249300	-0.71254200	2.68338500
H	2.89980800	0.29845100	2.97084700
H	1.50493000	-0.68861800	2.57383900
H	2.83131800	-1.37302400	3.51771200
C	3.45692200	-0.25501200	-2.31824500
H	2.41053100	0.02095400	-2.45510600
H	4.05206600	0.65947800	-2.41749700

H	3.74567000	-0.90781700	-3.14345000
C	-2.78907400	-0.62241800	2.65643400
H	-1.70717100	-0.47881900	2.59761600
H	-3.21960800	0.35328500	2.90637800
H	-2.99476700	-1.28893100	3.49484600
C	-3.33526600	-0.45783200	-2.41040300
H	-3.93649100	0.44291900	-2.57743600
H	-2.28810200	-0.16674500	-2.50887500
H	-3.57386900	-1.14928400	-3.22002300
C	-0.00104300	-2.03866500	0.40455000
H	0.97707900	-2.29219100	0.79726100
H	-0.82703900	-2.04421700	1.10628700
C	-0.24125500	-2.09522900	-0.93826200
H	-0.01399600	0.14495100	-1.61173300
H	-1.27169300	-2.02695800	-1.26846100
C	0.72828100	-2.57349500	-1.97457500
H	1.75795000	-2.57453600	-1.62087300
H	0.46326000	-3.60838700	-2.22391200
H	0.66189800	-1.99839600	-2.89912400
Co	-0.02029400	0.07003100	-0.11241800

$^{1/2}$Co(+)-10

Atom	x	y	z
C	-1.12754200	2.71011000	0.09644000
C	-1.14602300	4.10175800	0.19352300
C	0.07822700	4.77169200	0.26099400
C	1.28392500	4.06642600	0.23234100
C	1.22848400	2.67565400	0.13475800
N	0.04207100	2.06627700	0.07207100
H	0.09278100	5.85283500	0.33670000
H	-2.07718300	4.65398600	0.21654800
H	2.22931400	4.59173900	0.28558800
C	-2.27815200	1.76043100	0.01002500
C	2.35333200	1.69310000	0.08639800
N	1.98501000	0.45247300	-0.00322700
N	-1.94273100	0.51027800	-0.07343600
C	3.76316400	2.18946200	0.13431900
H	3.94299400	2.89708400	-0.68104700
H	3.94700200	2.72754200	1.06969700
H	4.48092400	1.37699700	0.05446100
C	-3.67476800	2.29457000	0.02478500
H	-3.82495300	2.98958800	-0.80737000
H	-4.41186300	1.49906400	-0.04935600
H	-3.85743400	2.85624200	0.94638900

C	2.95910300	-0.61205900	-0.04652400
C	3.47376400	-1.11444500	1.15839600
C	3.30317600	-1.14799500	-1.29676200
C	4.38615200	-2.16927600	1.08172700
C	4.22419900	-2.19688300	-1.32092200
C	4.76566900	-2.70316700	-0.14451300
H	4.79646300	-2.57829000	1.99930900
H	4.51083800	-2.62446600	-2.27617900
H	5.47564200	-3.52197500	-0.18270800
C	-2.94677800	-0.52425400	-0.16082900
C	-3.34942700	-0.96302300	-1.43085600
C	-3.43194100	-1.09482100	1.02532600
C	-4.29567500	-1.98825300	-1.49148600
C	-4.37570200	-2.11798700	0.91204600
C	-4.80957900	-2.55974500	-0.33284300
H	-4.62523100	-2.34427900	-2.46215900
H	-4.76706400	-2.57589600	1.81465500
H	-5.54164700	-3.35693400	-0.40015900
C	-2.76757700	-0.36866600	-2.68866500
H	-2.98577100	0.69968600	-2.78875800
H	-1.67815400	-0.48055700	-2.71272800
H	-3.16755000	-0.86426500	-3.57356100
C	-2.93642200	-0.64403400	2.37664900
H	-1.85138400	-0.76597100	2.46328400
H	-3.16137600	0.40853200	2.57759800
H	-3.39597700	-1.22952000	3.17328100
C	2.68637900	-0.62626700	-2.56931400
H	1.59646100	-0.73873400	-2.55145400
H	2.90124800	0.43406100	-2.73695100
H	3.05855500	-1.17389300	-3.43552100
C	3.04393900	-0.56241400	2.49531200
H	3.38994400	0.46411100	2.65710900
H	1.95416200	-0.55737800	2.59718100
H	3.44593300	-1.16619000	3.30922600
H	-0.00505100	-1.35241800	-0.17743100
Co	0.01580500	0.15182700	-0.06767300

$^{3/2}$Co(+)

$^{3/2}$Co(+)-1

Atom	x	y	z
C	1.16931800	2.44969700	-0.11223100
C	1.20663400	3.83274800	-0.29869000
C	0.00000100	4.52487500	-0.37661800
C	-1.20663300	3.83274800	-0.29868700
C	-1.16931600	2.44969700	-0.11222900
N	0.00000100	1.81281500	0.01430300
H	0.00000100	5.59953900	-0.51870300
H	2.14723800	4.36012300	-0.38996600
H	-2.14723700	4.36012300	-0.38996100
C	2.36487900	1.54917100	-0.09690600
C	-2.36487800	1.54917200	-0.09689900
N	-2.09945600	0.29100800	-0.07713700
N	2.09945600	0.29100800	-0.07713500
C	-3.73296600	2.16030800	-0.16208100
H	-3.90817100	2.81747300	0.69487000
H	-3.83301100	2.77336400	-1.06290500
H	-4.50808300	1.39810800	-0.18108300
C	3.73296700	2.16030600	-0.16210500
H	3.83300100	2.77336000	-1.06293200
H	3.90818300	2.81747200	0.69484200
H	4.50808300	1.39810500	-0.18111600
C	-3.12725000	-0.71108000	-0.07047700
C	-3.33903800	-1.43423700	-1.25702900
C	-3.81734300	-1.00460500	1.11886500
C	-4.29924600	-2.44669900	-1.24293300
C	-4.75977400	-2.03545100	1.08399000
C	-5.00680100	-2.74712100	-0.08412600
H	-4.48660000	-3.00889800	-2.15201900
H	-5.30040000	-2.28420800	1.99143100
H	-5.74321300	-3.54311500	-0.08864000
C	3.12724800	-0.71108200	-0.07048100
C	3.81736000	-1.00459700	1.11885300
C	3.33901400	-1.43425200	-1.25702900
C	4.75978800	-2.03544500	1.08397300
C	4.29922000	-2.44671600	-1.24293800
C	5.00679400	-2.74712800	-0.08414000
H	5.30042800	-2.28419500	1.99140700
H	4.48655800	-3.00892500	-2.15202200
H	5.74320400	-3.54312400	-0.08865800
C	3.54635600	-0.26268600	2.40545600

H	3.92451100	0.76485700	2.38400700
H	2.47701300	-0.21159100	2.63006900
H	4.03148500	-0.76100600	3.24512200
C	2.56456700	-1.11868400	-2.51202900
H	1.48362900	-1.17414400	-2.34438600
H	2.77665000	-0.11245800	-2.88767000
H	2.81007200	-1.82217800	-3.30806500
C	-3.54631600	-0.26270700	2.40547000
H	-2.47697000	-0.21162500	2.63007200
H	-3.92446100	0.76484000	2.38403300
H	-4.03144100	-0.76102800	3.24513900
C	-2.56461100	-1.11865700	-2.51203900
H	-2.77670300	-0.11242900	-2.88766900
H	-1.48367000	-1.17411400	-2.34441300
H	-2.81012600	-1.82214600	-3.30807600
Co	0.00000300	-0.25067100	0.40159600
C	0.00000900	-2.08618400	1.13530400
H	0.00005400	-2.79489200	0.29672400
H	0.88532400	-2.30064800	1.74192900
H	-0.88534000	-2.30068200	1.74186600

$^{3/2}$Co(+)-2

Atom	x	y	z
C	1.16488100	2.40490200	-0.36195900
C	1.20222900	3.78313200	-0.58877000
C	0.00003100	4.47749000	-0.68197000
C	-1.20218800	3.78324600	-0.58822600
C	-1.16488100	2.40499800	-0.36149100
N	-0.00000800	1.76260000	-0.21369100
H	0.00004700	5.54838000	-0.84988100
H	2.14403000	4.30463000	-0.69763200
H	-2.14399200	4.30483300	-0.69662500
C	2.37747400	1.52898500	-0.33132300
C	-2.37754200	1.52914700	-0.33057200
N	-2.15543000	0.28104100	-0.13306400
N	2.15538700	0.28093000	-0.13329000
C	-3.71978300	2.15126800	-0.59110300
H	-3.96493500	2.88774600	0.18008000
H	-3.72000800	2.67755400	-1.54996500
H	-4.50658700	1.40111300	-0.61284600
C	3.71965000	2.15089500	-0.59263500
H	3.71939000	2.67718100	-1.55149200
H	3.96536100	2.88734600	0.17839900
H	4.50634300	1.40063500	-0.61481200

C	-3.21620300	-0.68848900	-0.13952600
C	-3.36466900	-1.48536100	-1.28941900
C	-4.02453200	-0.86752100	0.99718400
C	-4.34927000	-2.47418300	-1.27991200
C	-4.98822600	-1.87923700	0.96081700
C	-5.15293100	-2.67799700	-0.16386800
H	-4.48117000	-3.09368200	-2.16104500
H	-5.61730400	-2.03670100	1.83103900
H	-5.90605900	-3.45817200	-0.17075900
C	3.21610600	-0.68870600	-0.13969300
C	4.02484400	-0.86719700	0.99681600
C	3.36407300	-1.48618100	-1.28922900
C	4.98839400	-1.87905900	0.96063900
C	4.34855600	-2.47512400	-1.27954100
C	5.15257400	-2.67845500	-0.16367100
H	5.61779400	-2.03611800	1.83070100
H	4.48008500	-3.09508700	-2.16040100
H	5.90559300	-3.45873600	-0.17041300
C	3.89240300	-0.00024100	2.22584200
H	4.28141600	1.01043200	2.06159300
H	2.85572700	0.10455200	2.55181700
H	4.45532400	-0.42361800	3.05823100
C	2.50928400	-1.26508000	-2.51157300
H	1.44392400	-1.33160100	-2.27494300
H	2.68000900	-0.28048900	-2.95967900
H	2.72553500	-2.01158500	-3.27641800
C	-3.89144900	-0.00126800	2.22663500
H	-2.85461300	0.10315000	2.55222600
H	-4.28033900	1.00957200	2.06309600
H	-4.45410700	-0.42499700	3.05902300
C	-2.51024800	-1.26372500	-2.51191900
H	-2.68164200	-0.27921300	-2.95995900
H	-1.44480800	-1.32958700	-2.27547600
H	-2.72620100	-2.01032600	-3.27675600
C	-0.00154800	-2.34604100	0.18630500
H	-0.00226200	-2.70930300	-0.84781500
H	0.88217000	-2.77367700	0.67210100
H	-0.88604000	-2.77161600	0.67251300
C	0.00080900	-0.59834100	2.77985500
H	0.91782600	-1.17242400	2.84633200
H	-0.91603000	-1.17259100	2.84716100
C	0.00067000	0.74106700	2.73549300
H	-0.91961500	1.31439800	2.75165000

H	0.92087800	1.31455000	2.75067100
Co	0.00050200	-0.34615200	0.27116600

$^{3/2}$Co(+)-TS-2/3

Atom	x	y	z
C	1.16915700	2.47857100	0.00930000
C	1.19915300	3.87447100	0.02595800
C	-0.00297100	4.57353700	0.06166900
C	-1.20409300	3.87101300	0.09295900
C	-1.16972100	2.47631800	0.07222200
N	0.00014600	1.81483800	0.02306800
H	-0.00420000	5.65739700	0.07137000
H	2.13980900	4.40886600	0.01209300
H	-2.14557800	4.40264900	0.13293300
C	2.39497300	1.62508000	0.01008900
C	-2.39189800	1.61806900	0.12305500
N	-2.19499100	0.35165100	0.03533500
N	2.19878300	0.35807000	-0.06117400
C	-3.72976800	2.28186800	0.28824000
H	-3.74116500	2.91862500	1.17716400
H	-3.95362900	2.92166900	-0.57081200
H	-4.52557700	1.54661900	0.38098300
C	3.73573100	2.29742600	0.11474600
H	3.89599300	2.97354700	-0.73031700
H	3.80307300	2.89820700	1.02625200
H	4.54229000	1.56807900	0.12380800
C	-3.28299100	-0.58577900	0.09357400
C	-3.98105700	-0.91890400	-1.08162000
C	-3.57570500	-1.19827800	1.32767800
C	-4.94529000	-1.92861100	-1.00621600
C	-4.55021100	-2.19800600	1.34965400
C	-5.22280000	-2.57367000	0.19220800
H	-5.48787300	-2.20350500	-1.90542400
H	-4.78599300	-2.68163300	2.29236700
H	-5.96999000	-3.35884700	0.22739800
C	3.29153200	-0.56991600	0.01629000
C	3.71991000	-1.00800300	1.28344700
C	3.86075900	-1.06539100	-1.17065100
C	4.71275700	-1.99019700	1.33615700
C	4.85338200	-2.04240500	-1.06392700
C	5.27221300	-2.51171200	0.17599100
H	5.05056500	-2.34429100	2.30497200
H	5.30491100	-2.43405200	-1.96991900
H	6.03896200	-3.27612900	0.23759900

C	3.17172800	-0.41304300	2.55877700
H	3.61715200	0.56640500	2.76690300
H	2.08953000	-0.27113800	2.52306800
H	3.39819400	-1.05184600	3.41346800
C	3.46622500	-0.52431200	-2.52304600
H	2.38435200	-0.48830600	-2.65845800
H	3.84032600	0.49461800	-2.67307400
H	3.88222000	-1.13761600	-3.32334000
C	-2.93168300	-0.74482200	2.61660100
H	-1.88688100	-0.45748900	2.49148900
H	-3.45386500	0.12561700	3.03016200
H	-2.97637200	-1.52970700	3.37329200
C	-3.77675800	-0.18351200	-2.38604400
H	-4.48556700	0.64709700	-2.47950800
H	-2.77607500	0.23546000	-2.49050600
H	-3.95269000	-0.84239100	-3.23832100
C	-0.21978200	-1.24780900	-2.04986000
H	0.09839400	-0.21798100	-2.30047100
H	0.39748100	-1.91438400	-2.64348600
H	-1.26717800	-1.37405100	-2.30311000
C	0.07624500	-2.53039600	-0.37830000
H	0.96828400	-2.94049400	-0.83320800
H	-0.84128600	-3.02837000	-0.66713600
C	0.19553500	-2.00954600	0.93391000
H	-0.66257900	-2.09167300	1.59267800
H	1.16635300	-2.05535900	1.41111900
Co	-0.01986700	-0.23888000	-0.14517800

$^{3/2}$Co(+)-3

Atom	x	y	z
C	-1.17002500	2.70667100	0.00355600
C	-1.20720600	4.09756100	0.11815200
C	0.00000000	4.79248000	0.15885100
C	1.20720600	4.09756100	0.11815200
C	1.17002500	2.70667100	0.00355600
N	0.00000000	2.06587300	-0.09461600
H	0.00000000	5.87303100	0.24535200
H	-2.14732600	4.62964700	0.18384600
H	2.14732500	4.62964700	0.18384600
C	-2.36165000	1.80377800	0.04307000
C	2.36165000	1.80377800	0.04307000
N	2.09363800	0.54582400	0.10675600
N	-2.09363800	0.54582400	0.10675600
C	3.73143100	2.41477800	0.06624300

H	3.91005300	3.00741800	-0.83588000
H	3.83097900	3.09162800	0.92013900
H	4.50534300	1.65504900	0.14302000
C	-3.73143100	2.41477800	0.06624300
H	-3.83097900	3.09162800	0.92013900
H	-3.91005400	3.00741800	-0.83588000
H	-4.50534300	1.65504900	0.14302000
C	3.12279100	-0.45302200	0.16286400
C	3.32276900	-1.10926400	1.39064500
C	3.82965500	-0.80982500	-0.99948900
C	4.28307500	-2.12021300	1.44399100
C	4.77045800	-1.83809500	-0.89648100
C	5.00307700	-2.48493800	0.31136500
H	4.46142300	-2.62957900	2.38545400
H	5.32282100	-2.13516200	-1.78210900
H	5.73904300	-3.27934600	0.36827300
C	-3.12279100	-0.45302200	0.16286400
C	-3.82965500	-0.80982500	-0.99948900
C	-3.32276900	-1.10926400	1.39064500
C	-4.77045800	-1.83809500	-0.89648100
C	-4.28307500	-2.12021300	1.44399100
C	-5.00307700	-2.48493800	0.31136500
H	-5.32282100	-2.13516200	-1.78210900
H	-4.46142300	-2.62958000	2.38545400
H	-5.73904300	-3.27934600	0.36827300
C	-3.58883400	-0.13207100	-2.32703300
H	-4.03308900	0.86816700	-2.36905700
H	-2.52363600	-0.02490100	-2.54799300
H	-4.03345800	-0.70925600	-3.13827100
C	-2.53971000	-0.72048600	2.61960900
H	-1.45975500	-0.77901300	2.44773700
H	-2.75463000	0.30434200	2.93893100
H	-2.77587800	-1.37913200	3.45586100
C	3.58883300	-0.13207100	-2.32703300
H	2.52363600	-0.02490100	-2.54799300
H	4.03308800	0.86816700	-2.36905700
H	4.03345700	-0.70925500	-3.13827100
C	2.53971000	-0.72048500	2.61960900
H	2.75463000	0.30434200	2.93893000
H	1.45975600	-0.77901300	2.44773700
H	2.77587800	-1.37913200	3.45586100
C	0.00000000	-1.80170000	-1.22287900
H	-0.87813900	-1.88695700	-1.87727500

H	0.87813900	-1.88695700	-1.87727500
C	0.00000000	-2.94115100	-0.19226000
H	-0.87760400	-2.85873300	0.46134000
H	0.87760400	-2.85873300	0.46134000
C	0.00000000	-4.33782200	-0.83227000
H	-0.88273800	-4.48103600	-1.46225800
H	0.88273800	-4.48103600	-1.46225800
H	0.00000000	-5.12637900	-0.07359800
Co	0.00000000	-0.00610700	-0.38126400

$^{3/2}$Co(+)-4

Atom	x	y	z
N	-0.11856100	2.00248500	-0.13863500
C	-1.30709700	2.60968200	-0.24096300
C	-2.49053300	1.69407600	-0.25435100
N	-2.23092700	0.44539900	-0.12506700
C	-3.26497400	-0.54817200	-0.20239100
C	-3.40516300	-1.25135000	-1.41269400
C	-2.57592000	-0.90039100	-2.62244700
H	-2.72882000	-1.62573600	-3.42223300
C	-4.36038600	-2.26685200	-1.47534100
C	-5.14539200	-2.58431300	-0.37270800
C	-4.99181500	-1.87425200	0.81171500
C	-4.05654300	-0.84154700	0.92202700
C	-3.93758000	-0.06801300	2.21303900
H	-2.90187600	0.03506900	2.54297000
H	-5.60775500	-2.11932300	1.67107100
H	-4.48429200	-2.81610100	-2.40308300
C	-3.85242100	2.28871200	-0.48057900
H	-4.11375500	2.98203300	0.32452600
H	-3.87513800	2.85725500	-1.41474300
H	-4.61681300	1.51719500	-0.53167800
C	-1.39650100	3.99612500	-0.39175100
C	-0.22248400	4.73951500	-0.45929400
C	1.00459900	4.08560900	-0.41790400
C	1.01910200	2.69670100	-0.26454000
C	2.26427100	1.86988100	-0.29797900
N	2.10233800	0.60642200	-0.13809300
C	3.21023900	-0.30662200	-0.22602100
C	3.37593400	-1.02015300	-1.42691600
C	4.40689900	-1.95850900	-1.49455200
C	5.24063100	-2.19022000	-0.40618300
C	5.05994900	-1.47053200	0.76848700
C	4.04834400	-0.51312800	0.88344100

H	5.71320900	-1.64924900	1.61647100
H	4.55202200	-2.51542700	-2.41454600
C	3.57208100	2.55533600	-0.57520700
H	3.81395200	3.26721000	0.21983000
H	4.38605200	1.83895200	-0.65378700
H	3.51971600	3.12227900	-1.50896700
H	1.92575600	4.64576500	-0.50950000
H	-0.26393100	5.81726000	-0.56767100
H	-2.35784900	4.48760300	-0.46278300
H	6.03070500	-2.92988600	-0.47405600
C	3.89668900	0.27417900	2.16254900
H	4.23679000	1.30943100	2.05012200
H	-5.87567500	-3.38342700	-0.43652000
C	2.48855600	-0.76617900	-2.61976500
H	2.71916900	-1.45936000	-3.42927800
C	-0.10936300	-2.12568300	0.04030600
H	-1.13151800	-2.41415000	0.32199600
H	-0.06287200	-2.26958100	-1.05141600
H	-1.50803300	-0.88023700	-2.39040200
H	-2.83620900	0.08525300	-3.02355300
H	-4.48771800	-0.56510900	3.01262200
H	-4.34857600	0.94377700	2.12612800
H	4.49150200	-0.16911500	2.96170700
H	2.86138100	0.31371500	2.50740200
H	2.61235500	0.24782700	-3.01460000
H	1.43084600	-0.88735300	-2.37069700
C	0.71784200	-4.54127700	0.27947700
C	0.89248100	-3.07720600	0.70739800
H	1.43469400	-5.19646300	0.78412600
H	0.86525100	-4.65754300	-0.79870500
H	-0.28752800	-4.90457300	0.51326400
H	1.92037500	-2.76788700	0.48895800
H	0.79034000	-3.02580800	1.79853200
C	-0.00090800	-0.42298600	2.75124700
C	-0.06594600	0.91639000	2.74223100
H	-0.88753300	-1.04372100	2.81091800
H	0.94434200	-0.95021700	2.81225500
H	-1.01289000	1.44385300	2.77146800
H	0.82675100	1.53125800	2.77196800
Co	-0.00162600	-0.13290900	0.28675800

$^{3/2}$Co(+)-TS-4/5

Atom	x	y	z
C	1.14469600	2.59804800	-0.32304700

C	1.16230400	3.98254400	-0.50016500
C	-0.04728700	4.66795900	-0.56539800
C	-1.24175600	3.95709900	-0.47841500
C	-1.19445000	2.57335300	-0.30332600
N	-0.01747200	1.93008600	-0.20882100
H	-0.05990800	5.74373500	-0.69525200
H	2.09805700	4.51895300	-0.58896300
H	-2.18887700	4.47546800	-0.55134400
C	2.35824900	1.74394500	-0.27662100
C	-2.39389400	1.69650000	-0.24491500
N	-2.18305600	0.44799700	0.00394400
N	2.16730200	0.49661500	-0.00087300
C	-3.74097700	2.31619800	-0.49563700
H	-3.95898100	3.07686900	0.26020400
H	-3.76679800	2.81443200	-1.46862400
H	-4.53467600	1.57404000	-0.46727500
C	3.69227400	2.37420400	-0.56304800
H	3.69191300	2.86345900	-1.54090400
H	3.91893500	3.14424600	0.18078000
H	4.49375200	1.64003600	-0.54417800
C	-3.27772600	-0.48853400	-0.03853100
C	-3.60221500	-1.07446000	-1.27807600
C	-3.97508500	-0.82216000	1.13657300
C	-4.60019500	-2.05128800	-1.30607000
C	-4.97068300	-1.80027700	1.05387200
C	-5.27439800	-2.42407200	-0.14957700
H	-4.85478500	-2.51570300	-2.25345600
H	-5.52006400	-2.06553200	1.95156900
H	-6.04677700	-3.18421900	-0.18952200
C	3.26736700	-0.43297900	-0.03938800
C	3.97270600	-0.74078000	1.13761100
C	3.57460100	-1.05125700	-1.26678600
C	4.97733800	-1.71027500	1.06625000
C	4.58159100	-2.01907800	-1.28371900
C	5.27561400	-2.35527000	-0.12743700
H	5.53452400	-1.95517000	1.96488400
H	4.82728000	-2.50611900	-2.22200000
H	6.05534400	-3.10824400	-0.15942900
C	3.69007200	-0.05294000	2.45126700
H	3.56258300	1.02671900	2.34092400
H	2.78325000	-0.43717000	2.92618300
H	4.51014200	-0.21438600	3.15191100
C	2.87632200	-0.66557500	-2.54861600

H	1.78978200	-0.63949800	-2.44219300
H	3.18512400	0.32643900	-2.89614000
H	3.11491100	-1.37020200	-3.34596100
C	-3.71616400	-0.13590600	2.45645900
H	-2.81146400	-0.50384500	2.94620200
H	-3.60648800	0.94620100	2.34961200
H	-4.54367400	-0.31116400	3.14499200
C	-2.94016900	-0.63775000	-2.56299200
H	-3.32617100	0.32940800	-2.90434600
H	-1.85871900	-0.53119700	-2.46360100
H	-3.13358300	-1.35526400	-3.36141400
C	0.34093000	-2.23301500	0.59368800
H	1.43084900	-2.25301200	0.59530900
H	-0.01487600	-3.06054800	1.20320200
C	-0.24163100	-2.37456500	-0.81280200
H	0.02682300	-1.52838700	-1.46189100
H	-1.33182400	-2.39540200	-0.76493700
C	0.25985700	-3.66284800	-1.49349500
H	1.34846500	-3.66586500	-1.58797500
H	-0.02754900	-4.54411300	-0.91435200
H	-0.16819300	-3.76639500	-2.49482200
Co	0.03097300	0.04125700	0.50541800
C	-0.06243200	-1.13734200	2.41002500
H	0.79056600	-1.69353300	2.78053200
H	-1.00205100	-1.65125400	2.57097700
C	-0.04494500	0.28544400	2.53545800
H	-0.96562300	0.81099000	2.76261700
H	0.85561300	0.77886800	2.88377300

$^{3/2}$Co(+)-5

Atom	x	y	z
C	1.17023100	-3.08644800	-0.02332000
C	1.20733500	-4.47837500	0.07772300
C	-0.00000200	-5.17357400	0.11139900
C	-1.20733900	-4.47837400	0.07772300
C	-1.17023400	-3.08644700	-0.02332000
N	-0.00000100	-2.44510600	-0.11613500
H	-0.00000300	-6.25491400	0.18740600
H	2.14736300	-5.01121000	0.13859400
H	-2.14736800	-5.01120800	0.13859400
C	2.36122400	-2.18342300	0.02644800
C	-2.36122600	-2.18342100	0.02644800
N	-2.09257400	-0.92622700	0.10586400
N	2.09257300	-0.92622900	0.10586400

C	-3.73138300	-2.79390400	0.04153500
H	-3.91045500	-3.37438100	-0.86837600
H	-3.83125300	-3.48199800	0.88634700
H	-4.50490600	-2.03488100	0.12858100
C	3.73138100	-2.79390700	0.04153600
H	3.83125000	-3.48200100	0.88634700
H	3.91045200	-3.37438400	-0.86837600
H	4.50490400	-2.03488500	0.12858100
C	-3.12109900	0.07242200	0.17314300
C	-3.31834400	0.71690400	1.40766800
C	-3.82993900	0.44122900	-0.98432700
C	-4.27770700	1.72802600	1.47275800
C	-4.76956500	1.46936500	-0.86948300
C	-4.99945900	2.10451000	0.34504800
H	-4.45412300	2.22797300	2.41962500
H	-5.32333900	1.77550300	-1.75114200
H	-5.73485500	2.89875500	0.41114300
C	3.12109900	0.07242000	0.17314300
C	3.82993900	0.44122600	-0.98432700
C	3.31834400	0.71690100	1.40766800
C	4.76956600	1.46936100	-0.86948300
C	4.27770800	1.72802200	1.47275800
C	4.99946000	2.10450600	0.34504800
H	5.32334000	1.77549900	-1.75114200
H	4.45412500	2.22797000	2.41962500
H	5.73485800	2.89875000	0.41114300
C	3.59293900	-0.22370300	-2.31904100
H	4.04477500	-1.22001800	-2.37216800
H	2.52850200	-0.33647500	-2.54048300
H	4.03274800	0.36558300	-3.12420300
C	2.53335900	0.31551800	2.63130700
H	1.45373000	0.37637000	2.45837900
H	2.74736900	-0.71274100	2.93997900
H	2.76857000	0.96521200	3.47480400
C	-3.59293900	-0.22370000	-2.31904100
H	-2.52850200	-0.33647400	-2.54048300
H	-4.04477700	-1.22001500	-2.37216800
H	-4.03274700	0.36558700	-3.12420300
C	-2.53335900	0.31552100	2.63130700
H	-2.74737000	-0.71273800	2.93997900
H	-1.45373000	0.37637100	2.45837900
H	-2.76856900	0.96521400	3.47480400
C	0.00000000	1.42257900	-1.21893200

H	0.87859800	1.51112400	-1.87174500
H	-0.87859800	1.51112500	-1.87174400
C	0.00000200	2.54964100	-0.17556800
H	0.87824000	2.46088200	0.47775100
H	-0.87823600	2.46088300	0.47775200
C	0.00000200	3.95972200	-0.79328000
H	0.87638400	4.06306100	-1.44562700
H	-0.87638000	4.06306200	-1.44562700
Co	0.00000000	-0.37255100	-0.37935100
C	0.00000300	5.08613800	0.24577600
H	0.87600400	4.97786900	0.89766900
H	-0.87599700	4.97787000	0.89766900
C	0.00000400	6.48338400	-0.37887000
H	-0.88199800	6.63925900	-1.00763400
H	0.00000400	7.26424000	0.38628400
H	0.88200500	6.63925800	-1.00763500

$^{3/2}$Co(+)-6

Atom	x	y	z
C	1.30679500	2.60941600	0.23650000
C	1.39691600	3.99601500	0.38610200
C	0.22315700	4.73970000	0.45383300
C	-1.00415500	4.08611500	0.41223800
C	-1.01933500	2.69718200	0.26027500
N	0.11821200	2.00235400	0.13568200
H	0.26479500	5.81745500	0.56195800
H	2.35861200	4.48686300	0.45614800
H	-1.92502800	4.64689200	0.50315400
C	2.49031300	1.69390200	0.24864000
C	-2.26498400	1.87109600	0.29326600
N	-2.10274000	0.60711500	0.13870300
N	2.23169800	0.44512000	0.11734000
C	-3.57348000	2.55839600	0.56263000
H	-3.52562600	3.12624600	1.49609500
H	-3.80955500	3.26965700	-0.23464200
H	-4.38906900	1.84341500	0.63755000
C	3.85187600	2.28974300	0.47360800
H	4.11183800	2.98215900	-0.33275800
H	3.87436400	2.85998000	1.40670100
H	4.61720400	1.51926900	0.52514300
C	-3.21024100	-0.30622000	0.22730000
C	-4.04696200	-0.51656400	-0.88226000
C	-3.37713200	-1.01662400	1.43021100
C	-5.05612600	-1.47678900	-0.76680600

C	-4.40601200	-1.95698400	1.49857000
C	-5.23677700	-2.19428300	0.40898500
H	-5.70738600	-1.65921300	-1.61559600
H	-4.55224700	-2.51105900	2.42010600
H	-6.02426000	-2.93667400	0.47704200
C	3.26848500	-0.54631200	0.19673000
C	3.42110200	-1.23677800	1.41280700
C	4.05087300	-0.84910800	-0.93125500
C	4.37953100	-2.24930300	1.47709300
C	4.99087300	-1.87720600	-0.81862700
C	5.15652900	-2.57518600	0.37131300
H	4.51253700	-2.78932300	2.40897200
H	5.60044200	-2.12851500	-1.68069400
H	5.89007300	-3.37112900	0.43706600
C	2.59884500	-0.87952100	2.62550400
H	2.83691400	0.12157400	3.00103700
H	1.52769400	-0.89443200	2.40797100
H	2.78178200	-1.58213800	3.43910600
C	3.91545900	-0.09033800	-2.22917600
H	2.87756200	-0.01673400	-2.56024300
H	4.30086000	0.93211900	-2.15131800
H	4.47813600	-0.58124800	-3.02378900
C	-2.49673400	-0.75318400	2.62619700
H	-1.43625600	-0.85185300	2.37987700
H	-2.64152500	0.25616800	3.02608300
H	-2.71616600	-1.45488900	3.43147700
C	-3.90159500	0.27155000	-2.16161800
H	-4.30609900	1.28520500	-2.06473500
H	-2.86084000	0.37145100	-2.47503800
H	-4.44543300	-0.20897500	-2.97559000
C	0.10154000	-2.12652900	-0.02099300
H	1.12942500	-2.41806300	-0.27723200
H	0.02943800	-2.26132200	1.07048600
C	-0.88555100	-3.08231400	-0.70399200
H	-0.75878400	-3.03813200	-1.79294600
H	-1.91833600	-2.77224900	-0.51073300
C	-0.72100400	-4.54351900	-0.26232500
H	0.28893200	-4.90906600	-0.47167500
H	-0.89196600	-4.65219000	0.81316300
H	-1.42716600	-5.20184100	-0.77788400
Co	0.00190600	-0.13505200	-0.28345300
C	-0.02277600	-0.43318600	-2.74231300
H	0.85088300	-1.07122900	-2.80972500

H	-0.97860900	-0.94165700	-2.79499100
C	0.06856200	0.90472600	-2.73409300
H	-0.81201700	1.53702600	-2.75690700
H	1.02527900	1.41336600	-2.77154800

$^{3/2}$Co(+)-TS-6/7

Atom	x	y	z
C	1.27119600	2.64747100	-0.03841100
C	1.34898800	4.04069500	-0.11154400
C	0.16542100	4.77210400	-0.16179500
C	-1.05783600	4.11058500	-0.09691300
C	-1.05978800	2.71512300	-0.02457200
N	0.08656100	2.02711500	-0.04498400
H	0.19646600	5.85374100	-0.22583600
H	2.30510100	4.54783400	-0.12161700
H	-1.98324000	4.67184600	-0.09517000
C	2.44605400	1.73801400	0.12666200
C	-2.28376200	1.87596500	0.15547600
N	-2.07517400	0.61241900	0.26208700
N	2.16361800	0.48930300	0.24016400
C	-3.61466800	2.56245200	0.27180100
H	-3.59163000	3.30665100	1.07303200
H	-3.86243000	3.09339600	-0.65225200
H	-4.41094500	1.85396800	0.48715200
C	3.81723600	2.34320300	0.21951800
H	4.08725200	2.84283600	-0.71578200
H	3.84871700	3.09983600	1.00856300
H	4.57034600	1.58993400	0.43815100
C	-3.13627500	-0.31966500	0.50937900
C	-4.01227900	-0.71346200	-0.51875900
C	-3.20757000	-0.88211300	1.79817300
C	-4.97572500	-1.68199400	-0.22065100
C	-4.19388900	-1.83690300	2.04841200
C	-5.07288200	-2.23881800	1.04865400
H	-5.65839600	-2.00019200	-1.00210200
H	-4.26863800	-2.27035800	3.04055300
H	-5.82917700	-2.98745300	1.25752200
C	3.16909500	-0.50636500	0.47059500
C	3.22164000	-1.07803600	1.75685300
C	4.00645800	-0.94867800	-0.56976900
C	4.14848100	-2.09416500	1.99006600
C	4.90932000	-1.97878400	-0.28862100
C	4.98641100	-2.54715900	0.97650900
H	4.20937100	-2.53558700	2.97963700

H	5.56001600	-2.33629200	-1.08039200
H	5.69534400	-3.34411800	1.17231000
C	2.32404100	-0.58631200	2.86418000
H	2.54335700	0.45015700	3.14018700
H	1.26881700	-0.61984800	2.57593300
H	2.44251000	-1.19535100	3.76098400
C	3.96064100	-0.34934000	-1.95467900
H	2.93974600	-0.16286300	-2.29148500
H	4.49823800	0.60354300	-2.00661900
H	4.43247200	-1.01601800	-2.67764500
C	-2.26341300	-0.44651500	2.89002800
H	-1.21747400	-0.54335900	2.58280600
H	-2.41519200	0.60094200	3.17006300
H	-2.40269100	-1.04845500	3.78862300
C	-3.93930000	-0.13131800	-1.90977200
H	-4.33403700	0.88920900	-1.95252900
H	-2.91617700	-0.09742200	-2.28875200
H	-4.53060700	-0.72688400	-2.60626500
C	-0.04346600	-2.18167300	-0.10685400
H	0.80120500	-2.35115200	0.56467100
H	-0.99106800	-2.34419200	0.41229600
C	0.05944100	-2.94493000	-1.34482500
H	1.04100100	-3.38932700	-1.52718900
H	0.09133700	-2.09680500	-2.30977300
C	-1.08920400	-3.84492600	-1.76097500
H	-1.12472600	-4.72352500	-1.10874100
H	-2.05044800	-3.33258100	-1.66535200
H	-0.98563700	-4.20187600	-2.78904000
Co	0.02521000	-0.07901200	-0.31664000
C	0.07495200	-1.08053200	-3.22050400
H	0.99555500	-1.36402900	-3.72745400
H	-0.81715400	-1.42007000	-3.74435400
C	0.02984900	0.15670700	-2.51288800
H	-0.89151100	0.72633400	-2.61764300
H	0.91360700	0.78522300	-2.60672700

$^{3/2}$Co(+)-7

Atom	x	y	z
C	1.24565000	2.60078600	0.09988700
C	1.31178700	3.99570800	0.12563900
C	0.12064000	4.71835900	0.14932900
C	-1.09832200	4.04432600	0.17839800
C	-1.08930500	2.64767000	0.15072700
N	0.06409400	1.97587300	0.07903800

H	0.14279400	5.80185200	0.16451000
H	2.26370300	4.51131700	0.13545200
H	-2.02751400	4.59760900	0.22858100
C	2.41395300	1.67873500	0.16635900
C	-2.28980600	1.77312900	0.26023000
N	-2.05995200	0.50472600	0.22431500
N	2.13090200	0.42102800	0.15981200
C	-3.63511600	2.41198500	0.45175600
H	-3.62053600	3.09546500	1.30513100
H	-3.90795400	3.00287100	-0.42813500
H	-4.41128000	1.66913900	0.62003700
C	3.79173900	2.26339900	0.28611300
H	4.01820300	2.89127400	-0.58080400
H	3.86624400	2.90101100	1.17181300
H	4.55076100	1.48797400	0.35732900
C	-3.11581700	-0.44980400	0.42569100
C	-3.92045000	-0.86442300	-0.64983500
C	-3.26213200	-0.99608300	1.71544400
C	-4.87127200	-1.86117800	-0.40879900
C	-4.22860100	-1.98593200	1.90592300
C	-5.02520400	-2.42298300	0.85303100
H	-5.50054000	-2.19466000	-1.22787800
H	-4.35744600	-2.41382100	2.89503700
H	-5.76780200	-3.19605000	1.01741400
C	3.15133900	-0.57324100	0.35433900
C	3.35959200	-1.04710900	1.66372500
C	3.86185300	-1.09226000	-0.74284300
C	4.28913400	-2.07247900	1.85288100
C	4.77984000	-2.11838100	-0.50127400
C	4.99172100	-2.61099500	0.78122500
H	4.46297600	-2.44763400	2.85639300
H	5.33816500	-2.53000600	-1.33602800
H	5.70683700	-3.40945900	0.94583000
C	2.63951700	-0.44185000	2.84506000
H	3.03199000	0.55086800	3.09127700
H	1.56854000	-0.31633100	2.66358600
H	2.75925000	-1.06315600	3.73338400
C	3.68053800	-0.54506100	-2.13702600
H	2.63074100	-0.48647800	-2.42765000
H	4.09092700	0.46622400	-2.23155200
H	4.19688800	-1.16833100	-2.86798700
C	-2.43390500	-0.50040800	2.87593100
H	-1.36819700	-0.45299700	2.63536900

H	-2.73048800	0.50886800	3.18121400
H	-2.55419400	-1.14812300	3.74515100
C	-3.80408000	-0.24285000	-2.01974000
H	-4.28188800	0.74252700	-2.05530400
H	-2.76725900	-0.10568700	-2.32788800
H	-4.29914600	-0.86138900	-2.76944800
C	-0.01507200	-2.28524400	0.53561800
H	0.83309900	-1.99866200	1.14804500
H	-0.98866400	-2.33014200	1.01280900
C	0.17023400	-2.78611500	-0.69923900
H	1.18181400	-2.80359100	-1.10246700
H	0.71877600	-1.21191800	-3.49314400
C	-0.88980800	-3.43507400	-1.53087400
H	-0.68817400	-4.51116300	-1.58563900
H	-1.88677000	-3.29984200	-1.10855200
H	-0.88214900	-3.06849400	-2.55871900
Co	0.00848500	-0.02204900	-0.47220600
C	-0.07265800	-0.45810300	-3.55899800
H	0.01948500	-0.00012700	-4.55254100
H	-1.02519100	-0.99553400	-3.55484400
C	0.00994400	0.58675600	-2.44429500
H	-0.81373600	1.30473800	-2.54437200
H	0.92775800	1.17812300	-2.55427800

$^{3/2}$Co(+)-8

Atom	x	y	z
C	1.16999400	2.55564700	-0.09686800
C	1.20722100	3.93892200	-0.28239100
C	0.00002200	4.63098600	-0.35781600
C	-1.20718300	3.93893300	-0.28242700
C	-1.16997800	2.55565400	-0.09690500
N	0.00000500	1.92087300	0.03429000
H	0.00002900	5.70578800	-0.49882100
H	2.14734200	4.46688900	-0.37581200
H	-2.14729700	4.46690800	-0.37587700
C	2.36123800	1.65136500	-0.09281200
C	-2.36124000	1.65139700	-0.09288400
N	-2.09229100	0.39194500	-0.08708100
N	2.09226600	0.39192000	-0.08699500
C	-3.73101200	2.25913700	-0.15847900
H	-3.91178800	2.91032100	0.70180900
H	-3.82908500	2.87778400	-1.05570000
H	-4.50429600	1.49544000	-0.18661500
C	3.73102600	2.25907000	-0.15837600

H	3.82916900	2.87763600	-1.05564600
H	3.91176300	2.91032500	0.70186500
H	4.50429500	1.49535100	-0.18639900
C	-3.12113600	-0.60884700	-0.09995500
C	-3.31499500	-1.32269200	-1.29604500
C	-3.83476600	-0.90912600	1.07420600
C	-4.27659700	-2.33394800	-1.30667900
C	-4.77661500	-1.93972100	1.01481100
C	-5.00360000	-2.64310900	-0.16222600
H	-4.45011700	-2.88747800	-2.22379800
H	-5.33433800	-2.19356600	1.91044100
H	-5.74050300	-3.43834000	-0.18529200
C	3.12113600	-0.60885700	-0.09988000
C	3.83465700	-0.90923400	1.07431800
C	3.31513900	-1.32255400	-1.29603000
C	4.77654400	-1.93979400	1.01490700
C	4.27676200	-2.33379300	-1.30667200
C	5.00365700	-2.64305700	-0.16218000
H	5.33419100	-2.19371200	1.91056400
H	4.45038700	-2.88722100	-2.22383300
H	5.74058300	-3.43826700	-0.18525600
C	3.59763700	-0.17077600	2.36977900
H	4.00491500	0.84561500	2.35030200
H	2.53375200	-0.09069300	2.60892000
H	4.07970800	-0.68852000	3.19950200
C	2.52459200	-0.99387200	-2.53781300
H	1.44564900	-1.04391400	-2.35703100
H	2.73722600	0.01415600	-2.90809900
H	2.75591600	-1.69245700	-3.34238900
C	-3.59791100	-0.17053700	2.36962500
H	-2.53404500	-0.09014800	2.60874300
H	-4.00547500	0.84573900	2.35010800
H	-4.07982300	-0.68837300	3.19938300
C	-2.52430700	-0.99415800	-2.53777800
H	-2.73676100	0.01388900	-2.90810900
H	-1.44538500	-1.04436400	-2.35690900
H	-2.75566700	-1.69273700	-3.34234900
C	-0.00013400	-1.89258100	1.34780700
H	0.87719400	-1.95186500	2.00392000
H	-0.87772300	-1.95170800	2.00359400
C	-0.00006000	-3.06367200	0.35477900
H	0.88415300	-3.05861300	-0.29081000
H	-0.88397900	-3.05840300	-0.29121100

Co	-0.00000400	-0.13265900	0.43452600
H	-0.00029600	-4.03155100	0.87101200

$^{3/2}$Co(+)-TS-3/9

Atom	x	y	z
C	-1.11049100	2.57971800	0.05199100
C	-1.12612100	3.97258200	0.13135500
C	0.08642500	4.65528500	0.18363400
C	1.28113100	3.94089700	0.15746600
C	1.23156400	2.54859600	0.07718400
N	0.05202000	1.90725500	0.02292300
H	0.09997900	5.73717000	0.24727800
H	-2.06056400	4.51777200	0.15520200
H	2.22887900	4.46142200	0.20122100
C	-2.33198200	1.72661700	-0.00081500
C	2.43177600	1.66468600	0.04876600
N	2.19324700	0.40106800	0.00843600
N	-2.13044700	0.45490300	-0.02252800
C	3.79534300	2.29368400	0.07571300
H	3.92971900	2.96914200	-0.77405900
H	3.92841300	2.88812800	0.98449700
H	4.57876200	1.54012600	0.04320800
C	-3.67679400	2.39505600	-0.02056900
H	-3.82112600	2.99842500	0.88058600
H	-3.76156800	3.07000800	-0.87709600
H	-4.48189400	1.66635200	-0.07537000
C	3.25496400	-0.56388500	-0.03983900
C	3.73081300	-1.11573300	1.16348300
C	3.73601100	-0.98082400	-1.29406600
C	4.70356400	-2.11539400	1.08222700
C	4.70642200	-1.98578700	-1.32085700
C	5.18600800	-2.55342300	-0.14618700
H	5.08582100	-2.55248400	1.99916900
H	5.08957800	-2.32204100	-2.27903100
H	5.93719500	-3.33448800	-0.18760800
C	-3.22907500	-0.46929900	-0.07965900
C	-3.67614400	-0.91417800	-1.33610300
C	-3.77757600	-0.94970800	1.12240000
C	-4.69170000	-1.87363600	-1.36556000
C	-4.79395800	-1.90459400	1.03910000
C	-5.24679000	-2.36878800	-0.19113000
H	-5.05078000	-2.23090500	-2.32544800
H	-5.23144700	-2.28835300	1.95522100
H	-6.03326800	-3.11422300	-0.23431100

C	-3.11277800	-0.35290200	-2.61912000
H	-3.46356100	0.66892600	-2.80182400
H	-2.02026800	-0.31681900	-2.61120900
H	-3.42144300	-0.95416800	-3.47508600
C	-3.29895400	-0.44779500	2.46238900
H	-2.20893200	-0.47098700	2.54079000
H	-3.61176800	0.58617800	2.64522500
H	-3.70837700	-1.05314200	3.27188600
C	3.25937600	-0.34435600	-2.57780100
H	2.17323400	-0.22574700	-2.60796800
H	3.69105200	0.65283700	-2.71903500
H	3.55331200	-0.94339600	-3.44050300
C	3.23733500	-0.62919300	2.50414800
H	3.61290000	0.37454200	2.73244200
H	2.14651000	-0.57921800	2.54530200
H	3.57736800	-1.28720600	3.30475100
C	0.03886400	-2.01922600	-0.98169100
H	-0.91725300	-2.18729500	-1.46698500
H	0.90631600	-1.96457600	-1.63094400
C	0.20505800	-2.39564700	0.35606400
H	0.10466000	-0.98140800	1.37920800
H	1.22665100	-2.54324500	0.69394500
C	-0.83070900	-3.19281700	1.10873600
H	-1.84693500	-2.92581600	0.81924900
H	-0.68308900	-4.25018000	0.86213600
H	-0.73153700	-3.08705600	2.18977100
Co	0.01815700	-0.12816600	0.01651900

$^{3/2}$Co(+)-9

Atom	x	y	z
C	1.12102400	2.61687400	-0.04985500
C	1.14208300	4.01314100	-0.07407100
C	-0.07206300	4.69565400	-0.10324500
C	-1.27026400	3.98453500	-0.09476600
C	-1.21706000	2.58937500	-0.06980000
N	-0.04017400	1.95617800	-0.06485000
H	-0.08471100	5.77925900	-0.12509300
H	2.07598900	4.56028100	-0.06834400
H	-2.21668700	4.50968300	-0.10517100
C	2.32912000	1.73886000	0.01203700
C	-2.40591100	1.68368000	-0.02584600
N	-2.15291000	0.42241400	0.02690600
N	2.10553300	0.47129800	0.05710100
C	-3.77598600	2.29587900	-0.03450900

H	-3.90402200	2.96921000	0.81811300
H	-3.92367700	2.89204300	-0.93994800
H	-4.55243100	1.53580300	0.00792700
C	3.68384900	2.38444700	0.02973000
H	3.77600400	3.06407100	0.88198500
H	4.47837300	1.64487100	0.09218700
H	3.83627900	2.98090700	-0.87475600
C	-3.20713500	-0.55169700	0.10710800
C	-3.74786600	-1.08221100	-1.07841700
C	-3.61113200	-0.99802700	1.37802000
C	-4.70818300	-2.09067800	-0.95987300
C	-4.57347400	-2.00884200	1.44157200
C	-5.11712700	-2.55576200	0.28507700
H	-5.13935800	-2.51300900	-1.86187000
H	-4.89889500	-2.36630200	2.41331700
H	-5.86053500	-3.34234400	0.35366800
C	3.18505100	-0.47419100	0.14372100
C	3.56160500	-0.94090400	1.41580600
C	3.78033500	-0.95461900	-1.03586000
C	4.55615200	-1.91940500	1.48626400
C	4.77041300	-1.93348200	-0.91109500
C	5.15570200	-2.41663500	0.33442400
H	4.86264800	-2.29067900	2.45896700
H	5.24334200	-2.31846800	-1.80888600
H	5.92415700	-3.17836600	0.40760500
C	2.94293900	-0.38154600	2.67405200
H	3.26747100	0.64742300	2.86348600
H	1.85028100	-0.36303500	2.62686300
H	3.22884200	-0.97325700	3.54439500
C	3.38787500	-0.42741000	-2.39415800
H	2.30361500	-0.38180500	-2.51901800
H	3.77416200	0.58443100	-2.56184100
H	3.79522600	-1.05777700	-3.18554600
C	-3.06461500	-0.38243500	2.64396300
H	-1.97971200	-0.25059000	2.61256700
H	-3.49567400	0.60750300	2.83042400
H	-3.30037500	-1.00119400	3.51059200
C	-3.33310200	-0.57184400	-2.43674400
H	-3.73531600	0.42885500	-2.63152000
H	-2.24722000	-0.50453600	-2.53750900
H	-3.70863700	-1.22460000	-3.22573800
C	0.04304000	-2.20772600	0.81777100
H	1.05537200	-2.29030500	1.20086000

H	-0.73680600	-1.95336300	1.52865100
C	-0.26960800	-2.63631700	-0.42271600
H	0.00275900	-0.27075000	-1.89516800
H	-1.31684400	-2.63047800	-0.71753900
C	0.68211100	-3.25890500	-1.39412100
H	1.72073600	-3.17229300	-1.07216200
H	0.44448600	-4.32447600	-1.49217400
H	0.57935200	-2.81929900	-2.38849500
Co	-0.01155500	-0.08094400	-0.31043500

$^{3/2}$Co(+)-10

Atom	x	y	z
C	1.17034100	2.38208200	0.07115200
C	1.20830900	3.76193100	0.27779700
C	0.00000000	4.45155800	0.36575500
C	-1.20830900	3.76193100	0.27779700
C	-1.17034100	2.38208200	0.07115200
N	0.00000000	1.75153600	-0.06282900
H	0.00000000	5.52391300	0.52434200
H	2.14864500	4.28841700	0.37826300
H	-2.14864500	4.28841700	0.37826200
C	2.35764100	1.46834500	0.04788500
C	-2.35764100	1.46834500	0.04788500
N	-2.07617200	0.21373900	0.01823900
N	2.07617200	0.21373900	0.01824000
C	-3.73328700	2.06028200	0.10753200
H	-4.49854700	1.28819300	0.08486000
H	-3.85947000	2.64270300	1.02547100
H	-3.89770300	2.74299800	-0.73141800
C	3.73328700	2.06028200	0.10753300
H	3.85947000	2.64270300	1.02547100
H	4.49854700	1.28819300	0.08486000
H	3.89770300	2.74299800	-0.73141800
C	-3.09522100	-0.80135600	0.02687000
C	-3.70264800	-1.18586600	-1.18003600
C	-3.38200000	-1.43276800	1.24822800
C	-4.64457100	-2.21601100	-1.13053900
C	-4.33427200	-2.45354500	1.24543200
C	-4.96403000	-2.84274700	0.06860100
H	-5.12579100	-2.53289500	-2.05002400
H	-4.57711000	-2.95075900	2.17893000
H	-5.69702600	-3.64173700	0.08415800
C	3.09522100	-0.80135600	0.02687000
C	3.38200000	-1.43276900	1.24822800

C	3.70264800	-1.18586500	-1.18003600
C	4.33427200	-2.45354500	1.24543200
C	4.64457100	-2.21601100	-1.13053900
C	4.96403000	-2.84274700	0.06860100
H	4.57711000	-2.95075900	2.17893000
H	5.12579100	-2.53289500	-2.05002400
H	5.69702700	-3.64173700	0.08415800
C	2.68960100	-1.02213000	2.52406300
H	2.93684900	0.00295600	2.81954000
H	1.59986100	-1.07224400	2.42761100
H	2.97617200	-1.67483400	3.34901800
C	3.33815800	-0.53818500	-2.49311800
H	2.26763400	-0.63325400	-2.70150500
H	3.58474900	0.52843600	-2.51942100
H	3.87274200	-1.01045300	-3.31757000
C	-2.68960100	-1.02212900	2.52406300
H	-1.59986100	-1.07224400	2.42761100
H	-2.93684900	0.00295700	2.81954000
H	-2.97617200	-1.67483300	3.34901800
C	-3.33815800	-0.53818500	-2.49311800
H	-3.58474900	0.52843600	-2.51942200
H	-2.26763400	-0.63325500	-2.70150500
H	-3.87274200	-1.01045400	-3.31757000
H	0.00000000	-1.71284700	-1.17537700
Co	0.00000000	-0.29218300	-0.48819600

^{1}Fe(+)

^{1}Fe(+)-1

Atom	x	y	z
C	-1.17707400	2.47433000	-0.02646800
C	-1.21051000	3.86594200	0.05524700
C	-0.00003400	4.56059400	0.08501700
C	1.21049300	3.86591100	0.05517700
C	1.17703000	2.47435600	-0.02652400
N	-0.00002200	1.82832500	-0.08520100
H	-0.00001700	5.64234100	0.14860600
H	-2.15102100	4.40035200	0.10525600
H	2.15099400	4.40034300	0.10510800
C	-2.32447100	1.53791700	-0.00828900
C	2.32449700	1.53791000	-0.00844000
N	1.99844100	0.27920000	-0.01345700
N	-1.99833400	0.27917400	-0.01334700
C	3.72070400	2.07567700	0.04415400
H	3.90632200	2.73916100	-0.80576200

H	3.86602400	2.67050400	0.95139800
H	4.46100900	1.27989700	0.03246000
C	-3.72072000	2.07559900	0.04416500
H	-3.86619800	2.67037600	0.95141800
H	-3.90630800	2.73909800	-0.80574600
H	-4.46097600	1.27977300	0.03235700
C	3.01615400	-0.74363200	0.02237200
C	3.42349700	-1.24365100	1.26885700
C	3.51583800	-1.24398900	-1.19041400
C	4.38068700	-2.26083500	1.27797000
C	4.47060900	-2.26154400	-1.12872900
C	4.90363200	-2.76547600	0.09269800
H	4.71315900	-2.66284300	2.22950400
H	4.87290500	-2.66390700	-2.05274400
H	5.64383800	-3.55749100	0.12050100
C	-3.01604500	-0.74366800	0.02253500
C	-3.51604400	-1.24375600	-1.19023500
C	-3.42310900	-1.24394200	1.26900700
C	-4.47078000	-2.26134200	-1.12853900
C	-4.38027100	-2.26115600	1.27813200
C	-4.90349100	-2.76555600	0.09288100
H	-4.87329600	-2.66351100	-2.05254500
H	-4.71248100	-2.66339400	2.22966000
H	-5.64365500	-3.55761100	0.12068900
C	-3.03484200	-0.71486200	-2.51854400
H	-3.25654300	0.34899600	-2.65078100
H	-1.95150500	-0.83417400	-2.63140500
H	-3.50816800	-1.24848500	-3.34307700
C	-2.85062900	-0.70892600	2.55796400
H	-1.75720400	-0.74972500	2.56142400
H	-3.13316200	0.33410100	2.73632100
H	-3.20609700	-1.28871400	3.41013200
C	3.03420600	-0.71545900	-2.51870900
H	1.95085500	-0.83500900	-2.63122700
H	3.25566900	0.34840900	-2.65125800
H	3.50739400	-1.24918500	-3.34325400
C	2.85117900	-0.70844900	2.55780600
H	3.13283300	0.33491900	2.73551400
H	1.75778400	-0.75023900	2.56174100
H	3.20751900	-1.28750000	3.41011000
C	-0.00014800	-2.09499500	-0.17042200
H	-0.00159900	-2.41671700	0.88095000
H	-0.89057500	-2.51825900	-0.64571300

H	0.89136400	-2.51848800	-0.64343900
Fe	-0.00006200	-0.12891900	-0.19746800

^{1}Fe(+)-2

Atom	x	y	z
C	1.17611500	2.43845100	-0.35472700
C	1.20584600	3.79352800	-0.68245100
C	-0.00010300	4.48134400	-0.81742900
C	-1.20602900	3.79359700	-0.68194700
C	-1.17622700	2.43851700	-0.35423700
N	-0.00003500	1.81236700	-0.12785000
H	-0.00012500	5.53546300	-1.06775300
H	2.14721000	4.30236100	-0.84818700
H	-2.14744100	4.30247000	-0.84729400
C	2.32444100	1.51722500	-0.31443200
C	-2.32455300	1.51733200	-0.31363300
N	-2.01155900	0.26863200	-0.12176000
N	2.01146200	0.26853200	-0.12246500
C	-3.70916700	2.03972200	-0.55686000
H	-4.00145100	2.73768700	0.23371600
H	-3.75161700	2.58903000	-1.50152000
H	-4.44136100	1.23709700	-0.59557300
C	3.70904500	2.03956400	-0.55780400
H	3.75118100	2.58986800	-1.50188800
H	4.00189000	2.73659700	0.23339300
H	4.44103200	1.23680400	-0.59768700
C	-3.02222200	-0.75985800	-0.14185200
C	-3.12950700	-1.54153300	-1.30833800
C	-3.82742300	-0.99775700	0.98494000
C	-4.05239900	-2.58707400	-1.31621500
C	-4.72831200	-2.06678200	0.93186100
C	-4.84068400	-2.85860700	-0.20253600
H	-4.15077100	-3.19637800	-2.20874800
H	-5.35130000	-2.27164300	1.79689000
H	-5.54403800	-3.68379700	-0.22219600
C	3.02210100	-0.75996400	-0.14224100
C	3.82764100	-0.99718800	0.98443100
C	3.12904200	-1.54236500	-1.30830600
C	4.72852200	-2.06626100	0.93173100
C	4.05192400	-2.58789000	-1.31583200
C	4.84055100	-2.85876300	-0.20220200
H	5.35177300	-2.27057300	1.79670500
H	4.15005900	-3.19771100	-2.20803700
H	5.54391100	-3.68395500	-0.22158900

C	3.79284600	-0.12442100	2.21656900
H	4.53746700	0.67704600	2.15445300
H	2.82488600	0.35036600	2.37395900
H	4.02939300	-0.70332700	3.11099200
C	2.30978200	-1.23780600	-2.53719800
H	1.24126200	-1.18662500	-2.31513100
H	2.58862800	-0.27683100	-2.98254900
H	2.45523600	-2.00321500	-3.30016500
C	-3.79222200	-0.12559200	2.21747700
H	-2.82260700	0.34483600	2.37790400
H	-4.53306100	0.67925200	2.15368200
H	-4.03381000	-0.70382700	3.11096000
C	-2.31057800	-1.23628100	-2.53728300
H	-2.58987600	-0.27527500	-2.98228900
H	-1.24203100	-1.18475100	-2.31541000
H	-2.45588600	-2.00149900	-3.30047000
C	-0.00044200	-2.07873200	0.35790700
H	-0.00124000	-2.41548200	-0.68528500
H	0.89150300	-2.48927400	0.83952600
H	-0.89206000	-2.48869000	0.84064000
C	0.00142200	-0.36579900	2.79162000
H	0.91935900	-0.93309400	2.88922100
H	-0.91567700	-0.93428100	2.89010900
C	0.00056500	0.97719200	2.72528500
H	-0.91849800	1.55236700	2.74106600
H	0.91895600	1.55345600	2.74032700
Fe	0.00000600	-0.09361500	0.34788300

^{1}Fe(+)-TS-2/3

Atom	x	y	z
C	1.18179700	2.48086100	0.27614500
C	1.20567400	3.84628200	0.55598100
C	-0.00011100	4.53996200	0.66056600
C	-1.20556500	3.84757300	0.54275100
C	-1.17946600	2.48270800	0.26192500
N	0.00183900	1.84528500	0.06045900
H	-0.00063400	5.60200800	0.87406300
H	2.14616200	4.36109500	0.70782600
H	-2.14736900	4.36263900	0.68565600
C	2.32877000	1.56557500	0.28522100
C	-2.32761300	1.56905600	0.25793400
N	-2.01559800	0.30811000	0.13042700
N	2.01479400	0.30481200	0.15903100
C	-3.71226100	2.10510600	0.47753400

H	-3.76017800	2.66233600	1.41752000
H	-3.99320100	2.79841000	-0.32045000
H	-4.45106000	1.30852600	0.51962900
C	3.71370200	2.09827800	0.50971400
H	4.03157900	2.72330500	-0.33014500
H	3.74288400	2.72434500	1.40538800
H	4.43723000	1.29600200	0.63357400
C	-3.02229400	-0.71917000	0.18472000
C	-3.84463100	-0.98544400	-0.92647500
C	-3.10538600	-1.48343700	1.36416700
C	-4.75367400	-2.04340500	-0.82950800
C	-4.03604400	-2.52253200	1.41501300
C	-4.85318000	-2.80708200	0.32678000
H	-5.39303000	-2.26547700	-1.67786600
H	-4.11745000	-3.11381200	2.32134400
H	-5.56621300	-3.62243900	0.37994500
C	3.01449900	-0.72750300	0.21019400
C	3.04576400	-1.53658400	1.36443700
C	3.87666900	-0.96411600	-0.87692400
C	3.96255000	-2.58633700	1.41323400
C	4.76787900	-2.03902500	-0.78495000
C	4.81589800	-2.84373800	0.34492300
H	4.00495000	-3.20929400	2.30077600
H	5.43474000	-2.23948200	-1.61765900
H	5.51626200	-3.67022400	0.39477900
C	2.13390400	-1.26310200	2.53299900
H	2.29834400	-0.26870600	2.95886700
H	1.07974500	-1.31050900	2.24305000
H	2.29096700	-1.99234100	3.32845200
C	3.89705200	-0.09797000	-2.11381200
H	2.92288500	0.33016300	-2.34747600
H	4.59990900	0.73530200	-2.00676800
H	4.22441800	-0.67256300	-2.98189300
C	-2.23352700	-1.17794300	2.55537600
H	-1.17041100	-1.22027900	2.30020600
H	-2.42098700	-0.17688600	2.95591900
H	-2.40983700	-1.89191900	3.36055000
C	-3.78525200	-0.16654500	-2.19365700
H	-4.21870500	0.83002300	-2.06055500
H	-2.76427100	-0.02472100	-2.55138000
H	-4.34937800	-0.65212600	-2.99068500
C	0.03854300	-1.56273000	-2.14226900
H	0.96225200	-1.66923300	-2.69739200

H	-0.85224600	-1.67917800	-2.74662000
C	0.00314800	-1.99768100	-0.79187600
H	-0.92597700	-2.41942000	-0.41901900
H	0.91221000	-2.41983500	-0.37307000
Fe	0.00211900	-0.00362900	-0.42260900
C	0.03419600	0.53219900	-2.62738500
H	0.05333000	0.12734600	-3.63332300
H	-0.86772100	1.13480500	-2.51882500
H	0.92221800	1.14951300	-2.49256400

^{1}Fe(+)-3

Atom	x	y	z
C	1.17763300	2.70403100	-0.05797300
C	1.20953700	4.09122800	-0.19182800
C	0.00004900	4.78581600	-0.25024600
C	-1.20943300	4.09120900	-0.19175000
C	-1.17751600	2.70401700	-0.05789700
N	0.00006800	2.05431300	0.02105800
H	0.00003300	5.86422000	-0.35526200
H	2.15049200	4.62309800	-0.25880200
H	-2.15039100	4.62307600	-0.25870000
C	2.32574300	1.77718500	-0.02547200
C	-2.32561300	1.77714800	-0.02534000
N	-2.00641700	0.51608700	0.03986000
N	2.00651300	0.51613700	0.03980500
C	-3.72119200	2.31729900	-0.09115000
H	-3.89704600	3.02148300	0.72739100
H	-3.87384300	2.86803500	-1.02448800
H	-4.46480900	1.52654500	-0.03362300
C	3.72131900	2.31734500	-0.09135600
H	3.87395200	2.86795700	-1.02477100
H	3.89718000	3.02164200	0.72708400
H	4.46494800	1.52660900	-0.03372900
C	-3.03230100	-0.49768100	0.05342000
C	-3.48304600	-1.01838200	-1.17032600
C	-3.50945500	-0.96310600	1.28998800
C	-4.44270600	-2.03298600	-1.13079400
C	-4.46945300	-1.97747400	1.27667500
C	-4.93331800	-2.51067600	0.07907600
H	-4.80552800	-2.45168700	-2.06392500
H	-4.85399100	-2.35197900	2.21978400
H	-5.67628500	-3.30056400	0.08905300
C	3.03230300	-0.49772700	0.05338700
C	3.50948200	-0.96309000	1.28997600

C	3.48290700	-1.01859800	-1.17032800
C	4.46936200	-1.97756200	1.27670100
C	4.44243000	-2.03333900	-1.13076000
C	4.93307300	-2.51095500	0.07912200
H	4.85393900	-2.35200300	2.21982000
H	4.80510800	-2.45220000	-2.06387400
H	5.67593500	-3.30094000	0.08913900
C	3.01765500	-0.38388100	2.59339300
H	3.26982000	0.67647600	2.69677200
H	1.93000400	-0.46506900	2.69268200
H	3.46139500	-0.90575500	3.44161800
C	2.97311700	-0.49192000	-2.48948100
H	1.88225500	-0.42027300	-2.51053900
H	3.36393800	0.50791300	-2.70798300
H	3.27883200	-1.14132300	-3.31034300
C	-3.01752200	-0.38405500	2.59343300
H	-1.92984700	-0.46509700	2.69256800
H	-3.26982900	0.67625000	2.69701500
H	-3.46107900	-0.90612800	3.44163100
C	-2.97324000	-0.49164100	-2.48944900
H	-3.36368300	0.50838400	-2.70772400
H	-1.88234800	-0.42042600	-2.51062100
H	-3.27930800	-1.14077700	-3.31039200
C	0.00003800	-1.85980300	0.50345900
H	0.88521000	-2.10098100	1.10775000
H	-0.88507900	-2.10092600	1.10785800
Fe	0.00006000	0.10289700	0.24318100
C	-0.00006900	-2.69008300	-0.78365000
H	0.87810300	-2.44377200	-1.39148900
H	-0.87833700	-2.44374100	-1.39133700
C	-0.00012300	-4.20407600	-0.51905700
H	0.88290700	-4.50414400	0.05205000
H	-0.88314200	-4.50406500	0.05211400
H	-0.00018300	-4.77036900	-1.45513200

^{1}Fe(+)-4

Atom	x	y	z
Fe	-0.03928400	0.07460100	0.38534600
N	-0.11123400	2.01772400	-0.03393400
C	-1.31018100	2.62237900	-0.19276500
C	-2.43570600	1.67470500	-0.19952700
N	-2.09987300	0.42385200	-0.08362800
C	-3.10066200	-0.60669600	-0.20601700
C	-3.23964100	-1.23813200	-1.45496700

C	-2.45415400	-0.78407600	-2.66017600
H	-2.55358300	-1.49665700	-3.47973300
C	-4.16288600	-2.27999600	-1.56551600
C	-4.92338800	-2.68470600	-0.47496700
C	-4.77792400	-2.03843100	0.74682100
C	-3.87065800	-0.98762900	0.90667500
C	-3.76404100	-0.28061300	2.23594400
H	-2.73278400	-0.20796600	2.58650300
H	-5.37871500	-2.34852900	1.59574100
H	-4.28370000	-2.77720400	-2.52258300
C	-3.83084100	2.18658000	-0.41454100
H	-4.10761000	2.89424600	0.37239300
H	-3.89962800	2.72283600	-1.36559400
H	-4.55978800	1.38046600	-0.42702700
C	-1.39252200	3.99471300	-0.42700900
C	-0.21555800	4.73284900	-0.54174300
C	1.01293900	4.07652000	-0.48339900
C	1.03479600	2.70184000	-0.24833200
C	2.22182500	1.83321700	-0.29619500
N	1.97852900	0.56184800	-0.16577200
C	3.05007800	-0.39369900	-0.27859000
C	3.14892400	-1.11470900	-1.48554700
C	4.13901100	-2.09067800	-1.59056900
C	5.00377300	-2.35382000	-0.53220200
C	4.89863100	-1.62245600	0.64226600
C	3.93060700	-0.62306700	0.79246600
H	5.57973200	-1.82091200	1.46403900
H	4.23162700	-2.65075100	-2.51541200
C	3.57088100	2.43943000	-0.55369500
H	3.87102400	3.07951600	0.28178200
H	4.33497100	1.67911700	-0.69314200
H	3.54535800	3.06872800	-1.44725800
H	1.93339100	4.62589500	-0.63540800
H	-0.25596600	5.80115200	-0.71751600
H	-2.35429200	4.47978600	-0.53700500
H	5.76105400	-3.12426000	-0.62732800
C	3.90241400	0.17975600	2.07176600
H	4.66678300	0.96435800	2.05962700
H	-5.63046500	-3.50054000	-0.57738600
C	2.24360400	-0.81593100	-2.65417600
H	2.40878800	-1.52639900	-3.46482200
C	-0.14412400	-1.92603200	0.26434500
H	-1.15623400	-2.16419900	0.61242000

H	-0.16007400	-2.02149500	-0.83352100
H	-1.38987400	-0.67143600	-2.44073400
H	-2.80536100	0.18551800	-3.03026400
H	-4.33354500	-0.80887400	3.00112800
H	-4.15928400	0.73987500	2.19116900
H	4.11856800	-0.45363800	2.93446900
H	2.94501600	0.66844800	2.24941400
H	2.41941100	0.18673300	-3.05791100
H	1.18767400	-0.86459400	-2.37735600
C	0.61853600	-4.34966000	0.41086000
C	0.86391300	-2.90054400	0.86337200
H	1.33747100	-5.03308700	0.87176300
H	0.71648600	-4.44798200	-0.67424500
H	-0.38534200	-4.68825400	0.68317000
H	1.88610200	-2.62032400	0.59647500
H	0.81281200	-2.87005100	1.95792800
C	0.14688100	-0.25918200	2.74156400
C	-0.03314900	1.07641800	2.71030400
H	-0.67482700	-0.94439600	2.91184600
H	1.13709400	-0.69781800	2.76914300
H	-1.01509700	1.52485500	2.81228000
H	0.80394700	1.76412900	2.67861200

^{1}Fe(+)-TS-4/5

Atom	x	y	z
C	1.11935000	2.57026700	-0.30245300
C	1.12043600	3.93441000	-0.59067700
C	-0.09017800	4.61276300	-0.69754000
C	-1.27775600	3.89635900	-0.56711900
C	-1.23147600	2.53264300	-0.28351000
N	-0.04411000	1.89960000	-0.08851700
H	-0.10920700	5.67419300	-0.91334200
H	2.05453100	4.45994000	-0.74214100
H	-2.22949800	4.39426500	-0.70063500
C	2.32261700	1.72594400	-0.27679400
C	-2.41287100	1.65144900	-0.26321300
N	-2.16562800	0.39132600	-0.10240600
N	2.10980100	0.45957700	-0.09060800
C	-3.77562900	2.24661800	-0.49489500
H	-4.02197100	2.97296800	0.28494000
H	-3.81217100	2.77584100	-1.45101400
H	-4.54654600	1.47980400	-0.50550900
C	3.66886500	2.35257900	-0.51742600
H	3.69876100	2.84814000	-1.49191000

H	3.88421000	3.11469200	0.23691800
H	4.46390700	1.61109500	-0.49276900
C	-3.21630200	-0.58316400	-0.19661100
C	-3.37958800	-1.24813300	-1.42964900
C	-4.01334800	-0.90531100	0.91703500
C	-4.32853300	-2.26809500	-1.51348600
C	-4.94420900	-1.94135300	0.78582100
C	-5.10002200	-2.62503100	-0.41264400
H	-4.46420500	-2.78496300	-2.45827700
H	-5.56071100	-2.20389300	1.64000900
H	-5.82656000	-3.42618200	-0.49269200
C	3.19668600	-0.47732300	-0.15713900
C	3.94372200	-0.78331500	0.99543600
C	3.45215400	-1.11073700	-1.38821700
C	4.93594500	-1.76316100	0.89804500
C	4.45736400	-2.07959200	-1.43682100
C	5.19078400	-2.41306300	-0.30372700
H	5.51985900	-2.01025600	1.77899000
H	4.66727300	-2.57348000	-2.38029500
H	5.96493000	-3.17045600	-0.35934900
C	3.72697800	-0.05334000	2.29864200
H	4.30981500	-0.50869500	3.10007400
H	4.03410100	0.99572200	2.23327300
H	2.67980400	-0.05462800	2.60832400
C	2.69768700	-0.73244500	-2.63957000
H	1.61498300	-0.74023700	-2.49106300
H	2.95930800	0.27479000	-2.98086200
H	2.92899200	-1.41850800	-3.45518800
C	-3.94662500	-0.13265700	2.21258700
H	-2.94366800	0.22339200	2.44427200
H	-4.59531100	0.75010200	2.18006300
H	-4.28880000	-0.74309700	3.05007000
C	-2.59247100	-0.84065800	-2.65131900
H	-2.93404600	0.12293400	-3.04506900
H	-1.52606200	-0.73082800	-2.44229100
H	-2.70741800	-1.57331800	-3.45121700
C	0.33621300	-1.94933700	1.24159100
H	1.42135900	-1.98784000	1.33434700
H	-0.09580600	-2.68967700	1.90862700
C	-0.13772200	-2.24785200	-0.17995000
H	0.05906900	-1.41467900	-0.88661600
H	-1.21557800	-2.40828800	-0.19071500
C	0.57984600	-3.48479100	-0.75219800

H	1.66034300	-3.34021900	-0.79699700
H	0.37990600	-4.36238400	-0.13298200
H	0.22059000	-3.70053200	-1.76143200
C	-0.19935900	-0.64334400	2.74644700
H	0.60760000	-1.08648600	3.31806000
H	-1.16250900	-1.09547100	2.95066800
C	-0.16597200	0.76396300	2.51742500
H	-1.08373300	1.33757200	2.58772400
H	0.72839800	1.31612400	2.79024700
Fe	0.01331100	0.09204900	0.60761700

^{1}Fe(+)-5

Atom	x	y	z
C	1.35817100	-2.98782200	0.26969400
C	1.46482400	-4.35446700	0.51903000
C	0.29462600	-5.10875100	0.62963000
C	-0.95024700	-4.49040900	0.50589200
C	-0.99419100	-3.11907500	0.25710400
N	0.14687400	-2.41226200	0.13238800
H	0.35345500	-6.17297600	0.82427700
H	2.43285400	-4.82626700	0.63348400
H	-1.86126300	-5.06658400	0.61001700
C	2.45374700	-2.00603600	0.15789600
C	-2.18952900	-2.26520900	0.13728900
N	-1.93867200	-0.99927500	-0.04509300
N	2.06751000	-0.77573600	-0.02562700
C	-3.55472700	-2.87120300	0.25293400
H	-3.69387000	-3.64568800	-0.50725700
H	-3.67773900	-3.35419300	1.22714200
H	-4.33933700	-2.12788700	0.13684300
C	3.87630900	-2.45953300	0.27969800
H	4.04646700	-2.92600800	1.25481800
H	4.10251300	-3.21471200	-0.47893900
H	4.57566200	-1.63512700	0.16632200
C	-3.01827200	-0.04761400	-0.14248200
C	-3.47477700	0.57254800	1.03199500
C	-3.54304000	0.26157300	-1.40820600
C	-4.48861100	1.52625100	0.91210700
C	-4.55429700	1.22282700	-1.47598000
C	-5.02455000	1.85214600	-0.32865300
H	-4.85777200	2.01816500	1.80621700
H	-4.97512400	1.47801800	-2.44312200
H	-5.80901600	2.59736000	-0.40180900
C	3.03606300	0.28802200	-0.12956800

C	3.52731100	0.63944500	-1.39773400
C	3.41508000	0.96949500	1.03853000
C	4.42657900	1.70553300	-1.47460200
C	4.31717500	2.02822200	0.90942600
C	4.81886800	2.39690900	-0.33377300
H	4.82004100	1.99454200	-2.44374100
H	4.62605500	2.56866300	1.79836500
H	5.51558100	3.22409200	-0.41376300
C	3.11286100	-0.11036400	-2.63964300
H	3.43859400	-1.15545800	-2.61983600
H	2.02570100	-0.11648500	-2.77012200
H	3.54515800	0.34578500	-3.53056400
C	2.88692500	0.56699300	2.39346100
H	1.79489800	0.50613100	2.40670400
H	3.26479600	-0.41202400	2.70693400
H	3.18702100	1.28648200	3.15579300
C	-3.05135900	-0.42835500	-2.65672600
H	-1.96804400	-0.33080400	-2.78054100
H	-3.27735900	-1.49971000	-2.65166500
H	-3.52064100	-0.00388400	-3.54461400
C	-2.91075600	0.21439700	2.38507600
H	-3.21961700	-0.78645000	2.70596200
H	-1.81727000	0.22763500	2.39126300
H	-3.25470400	0.91547300	3.14611200
C	-0.06183800	1.40863300	-0.80446100
H	0.83192500	1.62312200	-1.40557800
H	-0.93270400	1.50044300	-1.46809400
C	-0.17261400	2.40345600	0.35390100
H	0.69704400	2.31183200	1.01616800
H	-1.05478000	2.17656500	0.96441600
C	-0.27310800	3.86689900	-0.11459600
H	0.61074000	4.11180800	-0.71661500
H	-1.13517300	3.96802700	-0.78577800
C	-0.40259700	4.87023200	1.03663800
H	0.45802900	4.76540300	1.70927600
H	-1.28639500	4.62046500	1.63701300
C	-0.50339000	6.32163300	0.56179900
H	-1.37487900	6.47085700	-0.08297200
H	-0.59577500	7.01228300	1.40408800
H	0.38169600	6.61696900	-0.00985300
Fe	0.04190100	-0.49820000	-0.28585000

^{1}Fe(+)-6

Atom	x	y	z
C	1.03492700	2.70186500	0.24831600
C	1.01309800	4.07653800	0.48335600
C	-0.21539400	4.73290800	0.54155700
C	-1.39236600	3.99481700	0.42668700
C	-1.31004300	2.62246200	0.19251900
N	-0.11108900	2.01776200	0.03388100
H	-0.25578700	5.80121300	0.71732300
H	1.93355400	4.62587100	0.63550800
H	-2.35412800	4.47993200	0.53656900
C	2.22193900	1.83319800	0.29631700
C	-2.43557300	1.67481100	0.19926200
N	-2.09970300	0.42394500	0.08349700
N	1.97855700	0.56184700	0.16607400
C	-3.83073200	2.18667900	0.41407700
H	-3.89970900	2.72283400	1.36517300
H	-4.10732300	2.89443200	-0.37284200
H	-4.55970300	1.38058100	0.42631400
C	3.57092800	2.43946200	0.55400700
H	3.87018400	3.08145300	-0.28030600
H	3.54567900	3.06689000	1.44892300
H	4.33545800	1.67924100	0.69145200
C	-3.10054400	-0.60655400	0.20605800
C	-3.87053900	-0.98764300	-0.90658300
C	-3.23959300	-1.23771200	1.45511800
C	-4.77797000	-2.03825800	-0.74651100
C	-4.16299400	-2.27943700	1.56587900
C	-4.92356200	-2.68424300	0.47542700
H	-5.37877800	-2.34847900	-1.59537700
H	-4.28384900	-2.77643700	2.52304800
H	-5.63077700	-3.49993800	0.57799800
C	3.04999900	-0.39382500	0.27880400
C	3.14864400	-1.11506800	1.48564400
C	3.93058200	-0.62310600	-0.79222500
C	4.13861100	-2.09115300	1.59059500
C	4.89850400	-1.62261900	-0.64208800
C	5.00345900	-2.35418800	0.53226200
H	4.23106500	-2.65143400	2.51532800
H	5.57967500	-1.82098100	-1.46382500
H	5.76064600	-3.12472900	0.62733200
C	2.24334700	-0.81624800	2.65427800
H	2.42119500	0.18541000	3.05965300
H	1.18745400	-0.86211000	2.37688100

H	2.40660600	-1.52831900	3.46391000
C	3.90264400	0.17995900	-2.07137700
H	2.94526600	0.66864700	-2.24919300
H	4.66692900	0.96463000	-2.05885800
H	4.11905300	-0.45324100	-2.93416100
C	-2.45398800	-0.78359600	2.66023000
H	-1.38959400	-0.67178100	2.44088600
H	-2.80458200	0.18640100	3.02982800
H	-2.55399200	-1.49574500	3.48009100
C	-3.76368400	-0.28101700	-2.23603400
H	-4.15976400	0.73917500	-2.19183200
H	-2.73226900	-0.20769100	-2.58598700
H	-4.33231100	-0.80999600	-3.00137900
C	-0.14456600	-1.92611700	-0.26480800
H	-0.16111700	-2.02148900	0.83306100
H	-1.15649300	-2.16414100	-0.61348800
C	0.86382600	-2.90066600	-0.86315500
H	1.88577000	-2.62085500	-0.59492000
H	0.81405400	-2.86964600	-1.95776000
C	0.61750300	-4.34990600	-0.41157900
H	0.71406600	-4.44871300	0.67360700
H	-0.38612000	-4.68815000	-0.68527400
H	1.33683700	-5.03333000	-0.87186600
C	0.14788500	-0.25924500	-2.74183900
H	1.13843500	-0.69713600	-2.76916200
H	-0.67325600	-0.94505000	-2.91247300
C	-0.03307200	1.07622000	-2.71043300
H	-1.01530900	1.52398400	-2.81260700
H	0.80351500	1.76453500	-2.67845000
Fe	-0.03933000	0.07459200	-0.38537800

^{1}Fe(+)-TS-6/7

Atom	x	y	z
C	1.17047500	2.70558000	-0.03193000
C	1.19449700	4.09789300	-0.09274500
C	-0.01272800	4.79468200	-0.16185100
C	-1.22106500	4.09532200	-0.13706700
C	-1.19630100	2.70388500	-0.07564600
N	-0.01244200	2.04057100	-0.06463400
H	-0.01286200	5.87686400	-0.21034000
H	2.13497800	4.63499100	-0.07610500
H	-2.16268600	4.63045400	-0.15358300
C	2.30239800	1.79899900	0.13109900
C	-2.33253100	1.79492100	0.04722600

N	-2.00449400	0.52842600	0.11643000
N	1.97306700	0.53143500	0.18467300
C	-3.72822300	2.33797600	0.13656900
H	-3.81319000	3.04248800	0.96880400
H	-3.98682000	2.88619200	-0.77446900
H	-4.46200600	1.54923600	0.28123400
C	3.69438100	2.33952700	0.27195000
H	4.03218700	2.78262800	-0.67028600
H	3.72747700	3.12779500	1.02813300
H	4.40195500	1.56367600	0.55463000
C	-3.01624300	-0.46630700	0.37718100
C	-3.77520100	-1.01502000	-0.67126500
C	-3.18543100	-0.88446900	1.71024500
C	-4.71175500	-2.00346900	-0.35408600
C	-4.13317300	-1.87495200	1.97624500
C	-4.89091500	-2.43523900	0.95457800
H	-5.31053700	-2.43431800	-1.15015000
H	-4.27744400	-2.20528100	2.99984000
H	-5.62336100	-3.20312400	1.17828000
C	2.97107200	-0.47427400	0.44932400
C	3.04511100	-0.98643800	1.76071200
C	3.81347600	-0.94505500	-0.57329600
C	3.96033200	-2.00735700	2.02018800
C	4.70950300	-1.97445200	-0.26430200
C	4.78161000	-2.50839200	1.01534500
H	4.03063200	-2.40955000	3.02564000
H	5.36307800	-2.35263700	-1.04425300
H	5.48253000	-3.30678600	1.23324300
C	2.20517800	-0.41692800	2.87739900
H	2.50226300	0.60850600	3.12116400
H	1.14281900	-0.38173500	2.62340600
H	2.31265100	-1.01088800	3.78562700
C	3.82421400	-0.34997600	-1.96066200
H	4.55881200	0.45951200	-2.03502000
H	4.10892800	-1.09807600	-2.70285500
H	2.85929700	0.06235500	-2.25020000
C	-2.38313200	-0.27529100	2.83286000
H	-1.30730800	-0.35628800	2.65369600
H	-2.60210700	0.78928300	2.96375400
H	-2.60164800	-0.77112300	3.77914800
C	-3.60442900	-0.57894100	-2.10554000
H	-3.62611400	0.50761100	-2.22210100
H	-2.65407600	-0.92569400	-2.51931500

H	-4.40020500	-0.98810900	-2.72889700
C	-0.04085900	-1.93472300	0.04343800
H	0.61360100	-1.93772700	0.91960000
H	-1.06598800	-2.18371900	0.31721600
C	0.47818100	-2.78114300	-1.01412800
H	1.55821400	-2.93526300	-1.00542400
H	0.46525900	-2.00470300	-2.13211200
C	-0.31222800	-3.97381500	-1.50048600
H	-0.25736200	-4.77253200	-0.75206100
H	-1.36915400	-3.72906200	-1.63254100
H	0.07730800	-4.37777700	-2.43821000
C	0.32816600	-1.13752300	-3.06535000
H	1.28541400	-1.27789900	-3.56574700
H	-0.48407100	-1.62613200	-3.60449400
C	0.05942300	0.14615100	-2.46820100
H	-0.93150200	0.55379900	-2.65493100
H	0.83641200	0.89670700	-2.60587900
Fe	-0.00773500	0.14870300	-0.26640600

^{1}Fe(+)-7

Atom	x	y	z
C	-1.25857400	2.56805300	-0.12196200
C	-1.31212000	3.95474800	-0.25243600
C	-0.12508100	4.68027000	-0.32872700
C	1.09267200	4.00305100	-0.31591800
C	1.10155100	2.61564600	-0.18289800
N	-0.06179600	1.93254900	-0.02628800
H	-0.14944900	5.75847100	-0.43010600
H	-2.26775800	4.46083000	-0.31002500
H	2.02289900	4.54706000	-0.42179400
C	-2.38716900	1.64348800	-0.16553400
C	2.26321900	1.73673000	-0.26733400
N	1.96757300	0.46298900	-0.25625300
N	-2.03918900	0.38420000	-0.19064800
C	3.64091200	2.31336700	-0.41342700
H	3.67939700	3.00816600	-1.25674100
H	3.92246200	2.87754400	0.48070500
H	4.38589300	1.53890300	-0.57915400
C	-3.79303700	2.16339700	-0.23889800
H	-4.03681100	2.74834800	0.65270900
H	-3.91512000	2.82523200	-1.10098600
H	-4.51572000	1.35597600	-0.32907000
C	3.00191700	-0.52330400	-0.42716100
C	3.80819500	-0.92057600	0.65437100

C	3.14323400	-1.09842400	-1.70573200
C	4.75148400	-1.92932800	0.43270400
C	4.10275900	-2.09798600	-1.87774800
C	4.89892800	-2.51786100	-0.81736400
H	5.38026600	-2.25039600	1.25714400
H	4.22732200	-2.54712000	-2.85785000
H	5.63627400	-3.29893000	-0.96712400
C	-3.03050900	-0.64565500	-0.36622000
C	-3.20047800	-1.16172700	-1.66712500
C	-3.76208500	-1.14586300	0.72641400
C	-4.10245500	-2.21198500	-1.84868200
C	-4.64793400	-2.20268300	0.49361700
C	-4.81607600	-2.73776600	-0.77747200
H	-4.24589500	-2.61793500	-2.84488600
H	-5.21693000	-2.60331000	1.32657800
H	-5.50701000	-3.55870900	-0.93485800
C	-2.47081300	-0.57203500	-2.84993100
H	-2.85280700	0.42274700	-3.10274900
H	-1.39953000	-0.45388900	-2.66527400
H	-2.59278700	-1.19926300	-3.73368600
C	-3.65543300	-0.54728100	2.10758100
H	-2.63334700	-0.28015600	2.37269300
H	-4.25578300	0.36540400	2.19204700
H	-4.02996700	-1.24136900	2.86141700
C	2.31722000	-0.62231900	-2.87521500
H	1.24983900	-0.58579900	-2.64065600
H	2.60233800	0.38869800	-3.18473900
H	2.45096400	-1.27548700	-3.73829600
C	3.70567100	-0.27288400	2.01324500
H	4.24775100	0.67859500	2.04458700
H	2.67468400	-0.06389600	2.29746800
H	4.14510300	-0.91120600	2.78107400
C	0.01022400	-2.13758300	-0.27222600
H	-0.85524800	-1.96285600	-0.90028000
H	0.96034000	-2.30596400	-0.76725600
C	-0.14252600	-2.44882400	1.03294000
H	-1.13883300	-2.39087100	1.46586500
H	-0.78996000	-0.93791100	3.51938600
C	0.92324900	-3.07117900	1.87840800
H	0.70895100	-4.14444800	1.95349500
H	1.91551800	-2.96300500	1.43872200
H	0.93236100	-2.68784000	2.89759900
Fe	-0.01469700	0.10755900	0.34164700

C	-0.00886400	-0.17325200	3.54166800
H	-0.14938800	0.38375600	4.47748300
H	0.95015800	-0.68679900	3.63380800
C	-0.05356800	0.77482400	2.34882300
H	0.77777800	1.48600600	2.41315900
H	-0.96905000	1.37637000	2.38254600

^{1}Fe(+)-8

Atom	x	y	z
C	1.17757100	2.56068800	-0.00653600
C	1.20957600	3.95066400	-0.10763700
C	-0.00000700	4.64636300	-0.14941400
C	-1.20958900	3.95066100	-0.10763800
C	-1.17758000	2.56068500	-0.00653600
N	-0.00000400	1.90971100	0.05759700
H	-0.00000800	5.72695200	-0.22890500
H	2.15049000	4.48401600	-0.16255600
H	-2.15050400	4.48401100	-0.16255600
C	2.32553100	1.63265200	0.00137400
C	-2.32553900	1.63264600	0.00137400
N	-2.00588500	0.37056100	0.03612000
N	2.00587900	0.37056600	0.03611900
C	-3.72120700	2.17347400	-0.05486800
H	-3.89799200	2.86132400	0.77721200
H	-3.87328800	2.74241100	-0.97736000
H	-4.46448700	1.38135300	-0.01374300
C	3.72119800	2.17348000	-0.05486800
H	3.87328200	2.74240900	-0.97736400
H	3.89798000	2.86133800	0.77720700
H	4.46447900	1.38136000	-0.01373400
C	-3.03057900	-0.64435200	0.02018900
C	-3.47323800	-1.13707200	-1.21801300
C	-3.51343800	-1.14006000	1.24270200
C	-4.43050300	-2.15465800	-1.20785900
C	-4.47060700	-2.15621100	1.19999500
C	-4.92631900	-2.66217900	-0.01244700
H	-4.78692000	-2.55221300	-2.15263800
H	-4.85910100	-2.55422100	2.13178200
H	-5.66678500	-3.45435300	-0.02525500
C	3.03057400	-0.64434600	0.02018800
C	3.51343700	-1.14004900	1.24270100
C	3.47323300	-1.13706700	-1.21801400
C	4.47060700	-2.15619900	1.19999500
C	4.43049800	-2.15465100	-1.20785900

C	4.92631700	-2.66217000	-0.01244600
H	4.85910400	-2.55420600	2.13178300
H	4.78691500	-2.55220900	-2.15263800
H	5.66678400	-3.45434400	-0.02525500
C	3.03039600	-0.59072800	2.56226200
H	3.28972300	0.46513800	2.69103100
H	1.94270200	-0.66745300	2.66433700
H	3.47441400	-1.13637800	3.39523900
C	2.95728600	-0.57859800	-2.52166400
H	1.86698100	-0.49687100	-2.53249700
H	3.35501900	0.42220800	-2.72270000
H	3.25079700	-1.21320000	-3.35842000
C	-3.03038900	-0.59074700	2.56226300
H	-1.94269600	-0.66749100	2.66433700
H	-3.28969800	0.46512300	2.69103300
H	-3.47441600	-1.13639100	3.39523900
C	-2.95729400	-0.57860000	-2.52166200
H	-3.35501900	0.42221100	-2.72269000
H	-1.86698800	-0.49688200	-2.53250000
H	-3.25081400	-1.21319400	-3.35842000
C	0.00001400	-2.01507600	0.44635400
H	0.88485400	-2.26869500	1.04395100
H	-0.88484000	-2.26871800	1.04391800
C	0.00004700	-2.80513900	-0.86360100
H	0.88531500	-2.59865700	-1.47158300
H	-0.88519600	-2.59866700	-1.47162200
H	0.00004900	-3.88526800	-0.67330600
Fe	-0.00000200	-0.04718400	0.23268600

^{1}Fe(+)-TS-3/9

Atom	x	y	z
C	-1.13922000	2.56650900	-0.08699000
C	-1.15995000	3.95121700	-0.24155600
C	0.04606600	4.64950900	-0.24190600
C	1.24287000	3.94350000	-0.16362000
C	1.20772700	2.55541800	-0.01972800
N	0.02659700	1.90822100	0.11325600
H	0.05323200	5.72753800	-0.35012200
H	-2.09656000	4.47743000	-0.37399300
H	2.18920900	4.46424600	-0.23373300
C	-2.30255400	1.67058800	-0.20163900
C	2.37033100	1.65566600	-0.10554900
N	2.06620100	0.39700600	-0.18825300
N	-2.01386000	0.40202900	-0.21927600

C	3.75550800	2.23168200	-0.16511600
H	3.82416800	2.98112700	-0.95812000
H	4.01451600	2.73023000	0.77363300
H	4.49836000	1.46271500	-0.36368000
C	-3.67507000	2.25563800	-0.35792900
H	-3.96688600	2.81318200	0.53680000
H	-3.69240300	2.96001600	-1.19421300
H	-4.42103200	1.48755500	-0.54610900
C	3.06606800	-0.62226300	-0.28379800
C	3.88799800	-0.94492100	0.81460800
C	3.13228200	-1.34627100	-1.49268400
C	4.77940200	-2.01413200	0.67126100
C	4.04950500	-2.39169500	-1.58943200
C	4.86647600	-2.73018300	-0.51484200
H	5.41453400	-2.28243300	1.50976000
H	4.12219000	-2.94679900	-2.51912900
H	5.56763100	-3.55284700	-0.60284600
C	-3.04930100	-0.58970100	-0.29935700
C	-3.14377300	-1.33759300	-1.48928100
C	-3.87911600	-0.85069800	0.80750300
C	-4.10343000	-2.34694600	-1.55920600
C	-4.81384400	-1.88529800	0.69301300
C	-4.93197900	-2.62513100	-0.47614500
H	-4.19832600	-2.92311400	-2.47388900
H	-5.45748600	-2.10726700	1.53841200
H	-5.66611900	-3.42046800	-0.54378000
C	-2.25002800	-1.04120500	-2.66605200
H	-2.40701400	-0.03109900	-3.05658300
H	-1.19180400	-1.11349600	-2.39591100
H	-2.43365200	-1.74137400	-3.48165500
C	-3.80507300	-0.05812300	2.09183300
H	-2.79908800	0.30398400	2.31223300
H	-4.46418700	0.81614400	2.06252500
H	-4.13150100	-0.66523000	2.93772300
C	2.27033100	-0.97042100	-2.67160400
H	1.21066200	-0.91677800	-2.40431800
H	2.53978800	0.01079800	-3.07516700
H	2.37496800	-1.69666800	-3.47848400
C	3.85141300	-0.18890100	2.12261100
H	4.58739900	0.62212000	2.13613100
H	2.87601100	0.25329700	2.33068800
H	4.10221700	-0.84956600	2.95455500
C	-0.12728400	-2.06404000	0.50015300

H	-1.15147700	-2.40096000	0.37426200
H	0.58114200	-2.40518600	-0.25161100
C	0.34574600	-1.75269900	1.77794700
H	0.53218600	0.01096300	1.86950900
H	1.41681400	-1.81835600	1.93891100
C	-0.49296300	-1.92428300	3.02036400
H	-1.55343000	-1.76253900	2.82436200
H	-0.37933100	-2.95635700	3.36955900
H	-0.18063600	-1.26465600	3.83113800
Fe	-0.00982700	0.00045100	0.37792000

^{1}Fe(+)-9

Atom	x	y	z
C	1.12850900	2.58646500	0.05678400
C	1.14041300	3.97670500	0.16639200
C	-0.06763200	4.66888900	0.15744100
C	-1.26324200	3.95635300	0.09863500
C	-1.22200900	2.56720100	-0.00655800
N	-0.03719800	1.91943600	-0.10892500
H	-0.07892800	5.74937000	0.23599200
H	2.07634700	4.51052400	0.27086300
H	-2.21221800	4.47474100	0.15046700
C	2.29018000	1.69728000	0.16319300
C	-2.37259800	1.65762700	0.05439600
N	-2.05136000	0.39949600	0.13936400
N	1.99300000	0.42975700	0.19597100
C	-3.76727900	2.20876200	0.06667500
H	-3.87684700	2.95558100	0.85769200
H	-3.99632700	2.70679400	-0.88034300
H	-4.50555700	1.42787400	0.23296200
C	3.66828700	2.27828900	0.27743800
H	3.70616500	3.01059500	1.08846400
H	4.41230200	1.51111800	0.47777700
H	3.94886000	2.80144200	-0.64158200
C	-3.05682500	-0.62162600	0.21864500
C	-3.78379000	-1.00587600	-0.92415500
C	-3.23080400	-1.26456500	1.46072500
C	-4.69282100	-2.06112500	-0.79332300
C	-4.15867500	-2.30341000	1.54077400
C	-4.88304300	-2.70472900	0.42274700
H	-5.25842100	-2.37727900	-1.66416000
H	-4.31332300	-2.80166000	2.49237800
H	-5.59424200	-3.51977500	0.50024400
C	3.02398700	-0.56523100	0.28203300

C	3.14554200	-1.27301600	1.49441300
C	3.83187000	-0.85955300	-0.83277600
C	4.10172700	-2.28565600	1.57397500
C	4.76611400	-1.89328400	-0.70574100
C	4.90483900	-2.60013700	0.48184200
H	4.21607900	-2.83266800	2.50424200
H	5.39339800	-2.14090900	-1.55630800
H	5.63746100	-3.39617700	0.55763200
C	2.29469300	-0.92249700	2.68906200
H	2.52904300	0.07429700	3.07606100
H	1.22810600	-0.91981600	2.44437800
H	2.45011600	-1.63365400	3.50109500
C	3.73300300	-0.10013100	-2.13491900
H	2.72125400	0.25109500	-2.34269500
H	4.39116100	0.77558600	-2.13658300
H	4.04700900	-0.72706100	-2.97097000
C	-2.47350300	-0.81516600	2.68585300
H	-1.39739200	-0.74037000	2.50280900
H	-2.80033600	0.17363000	3.02398700
H	-2.62526600	-1.50866000	3.51373700
C	-3.62881600	-0.31610300	-2.25973000
H	-4.31011600	0.53710100	-2.34935700
H	-2.61777700	0.05801700	-2.43018400
H	-3.87586400	-0.99791000	-3.07528800
C	0.01557200	-2.14435100	-0.15172200
H	0.99797800	-2.44091300	0.20087800
H	-0.80877800	-2.24072300	0.54771600
C	-0.22678900	-2.00147800	-1.48509800
H	-0.04175800	0.40140800	-1.90200400
H	-1.25776800	-1.88791600	-1.80814200
C	0.76603400	-2.28227900	-2.57290500
H	1.79082400	-2.29729400	-2.20147200
H	0.55028000	-3.27457200	-2.98695500
H	0.69041000	-1.56751700	-3.39304900
Fe	-0.01710100	0.04541300	-0.36806600

^{1}Fe(+)-10

Atom	x	y	z
C	-1.15317300	2.41713500	0.04565800
C	-1.18407000	3.80681400	0.04008500
C	0.03528600	4.49699500	0.08233000
C	1.24161600	3.80407800	0.12018600
C	1.20297600	2.40477800	0.12178200
N	0.02216200	1.77471200	0.09276500

H	0.03721200	5.58077000	0.07834100
H	-2.11965200	4.35040200	-0.00000300
H	2.18289900	4.33899900	0.14130700
C	-2.31246200	1.47051500	-0.01487700
C	2.33991000	1.45376500	0.12256800
N	1.99425200	0.19817600	0.07768100
N	-2.00027000	0.21429600	-0.02707900
C	3.74231600	1.97387200	0.17330600
H	3.96870700	2.56589800	-0.71910900
H	3.87011200	2.63424500	1.03625700
H	4.46770100	1.16708000	0.24345300
C	-3.70100600	2.02305500	-0.06924700
H	-3.81932300	2.66375000	-0.94876400
H	-4.44727600	1.23381100	-0.11020300
H	-3.89643900	2.64705200	0.80831300
C	2.98871300	-0.84620100	0.02230100
C	3.23919100	-1.58297500	1.19122300
C	3.61737400	-1.13561400	-1.19984000
C	4.18205600	-2.60945100	1.12337500
C	4.54482200	-2.18025100	-1.21822000
C	4.83343900	-2.90661500	-0.06881200
H	4.39871600	-3.18621800	2.01659800
H	5.03905400	-2.42836800	-2.15189500
H	5.55768500	-3.71293900	-0.10475700
C	-3.01486800	-0.81094900	-0.08461000
C	-3.38408900	-1.31738400	-1.33994000
C	-3.54125700	-1.30954100	1.11677200
C	-4.33969000	-2.33513700	-1.37120600
C	-4.49175000	-2.32917400	1.03247400
C	-4.89357000	-2.83593800	-0.19836300
H	-4.64420800	-2.74223500	-2.32987900
H	-4.91432900	-2.73226600	1.94707500
H	-5.63178900	-3.62902100	-0.24297500
C	-2.75961800	-0.79913000	-2.61071400
H	-2.97602200	0.26047400	-2.78307500
H	-1.66995200	-0.90779500	-2.59032400
H	-3.12872600	-1.34881100	-3.47684800
C	-3.08228600	-0.78769200	2.45537100
H	-2.00047500	-0.90726700	2.58010700
H	-3.30876500	0.27462800	2.59396600
H	-3.56642100	-1.32843700	3.26887200
C	3.29449700	-0.37825600	-2.46519600
H	2.21584900	-0.29088100	-2.62386200

H	3.70640500	0.63663300	-2.46265800
H	3.71291100	-0.88715100	-3.33392500
C	2.50522000	-1.28712700	2.47359800
H	2.64736900	-0.25548800	2.81040000
H	1.42706000	-1.44760900	2.35207900
H	2.84287800	-1.94275200	3.27673100
H	0.02469600	-1.72980400	0.06468900
Fe	0.01744800	-0.17632400	0.10678800

^{2}Fe(+)

^{2}Fe(+)-1

Atom	x	y	z
C	1.16956000	2.43390000	0.11743100
C	1.20659700	3.82339900	0.25057700
C	0.00097100	4.51904700	0.29785300
C	-1.20435800	3.82415500	0.23379600
C	-1.16597200	2.43468400	0.10149200
N	0.00215600	1.78943900	0.01873900
H	0.00064200	5.59847200	0.39725400
H	2.14703400	4.35433200	0.31940200
H	-2.14543000	4.35551200	0.28972200
C	2.37579300	1.54560000	0.10796600
C	-2.37236300	1.54685000	0.07752700
N	-2.12978800	0.28471000	0.08248500
N	2.13179200	0.28362400	0.10013600
C	-3.73295300	2.17759400	0.09316000
H	-3.85291300	2.80149000	0.98404600
H	-3.87124100	2.82765200	-0.77578100
H	-4.51889900	1.42642300	0.09460200
C	3.73595800	2.17536200	0.15736900
H	3.89991300	2.82109500	-0.71033700
H	3.83118100	2.80342500	1.04825200
H	4.52050100	1.42319500	0.18482400
C	-3.17789000	-0.69871200	0.06865400
C	-3.81958300	-1.02161700	-1.13981900
C	-3.45816100	-1.37177600	1.27025000
C	-4.78565300	-2.03047200	-1.11029100
C	-4.43867300	-2.36492500	1.24870800
C	-5.10015500	-2.69324900	0.07052300
H	-5.29111600	-2.30076000	-2.03168900
H	-4.67872500	-2.88905100	2.16808900
H	-5.85377100	-3.47298800	0.07046400
C	3.17437000	-0.70398600	0.08838200
C	3.39331300	-1.43073600	1.27211400

C	3.87000900	-0.98291900	-1.10156900
C	4.36780300	-2.42925500	1.25565900
C	4.82637600	-2.00099800	-1.06872200
C	5.08166400	-2.71407200	0.09665800
H	4.56167500	-2.99246700	2.16272900
H	5.37120800	-2.23881000	-1.97655200
H	5.82928900	-3.49956100	0.09893400
C	2.60955100	-1.13452800	2.52612100
H	2.78012900	-0.11711800	2.89206400
H	1.53095700	-1.23728000	2.36110800
H	2.88416700	-1.82053900	3.32784800
C	3.59185100	-0.24049800	-2.38610100
H	2.52109400	-0.17519600	-2.59662600
H	3.98517300	0.78152400	-2.37069100
H	4.06069200	-0.74702200	-3.23011500
C	-2.73105700	-1.02936500	2.54661700
H	-1.64663500	-1.13999300	2.43575000
H	-2.91480900	0.00133800	2.86632100
H	-3.04489300	-1.68364000	3.36038800
C	-3.47171700	-0.33168900	-2.43630600
H	-3.80695400	0.71071100	-2.45734900
H	-2.39336000	-0.33152200	-2.61925700
H	-3.94682900	-0.83507200	-3.27865600
C	0.02933400	-2.06618700	-1.35056500
H	0.39154900	-1.92213700	-2.37371800
H	0.69513500	-2.79148700	-0.86880300
H	-0.96417800	-2.52158000	-1.41107600
Fe	0.00163900	-0.35027000	-0.28829100

^{2}Fe(+)-2

Atom	x	y	z
C	1.16911000	2.40603800	-0.27191200
C	1.21109400	3.79750900	-0.35879700
C	0.01388700	4.50794600	-0.31936200
C	-1.18678600	3.81689500	-0.22053500
C	-1.15929000	2.42042400	-0.13767300
N	0.00373800	1.75180400	-0.14563800
H	0.01903400	5.59035000	-0.37734000
H	2.15288200	4.32111400	-0.45574600
H	-2.12603400	4.35378500	-0.21100400
C	2.38886900	1.53954300	-0.33300100
C	-2.38885700	1.57562200	-0.09515600
N	-2.20046900	0.31680800	0.07737600
N	2.19572900	0.28474500	-0.14803300

C	-3.72197300	2.24351100	-0.29034700
H	-3.91138500	2.96310300	0.51224800
H	-3.75242400	2.79679800	-1.23312200
H	-4.53056900	1.51683400	-0.29017200
C	3.71269200	2.18446600	-0.62857500
H	3.65359000	2.78654700	-1.53930400
H	4.00878000	2.85581400	0.18341400
H	4.49453300	1.43958600	-0.75650100
C	-3.29814800	-0.61078500	-0.02611700
C	-3.66551000	-1.06138100	-1.30875400
C	-3.93317500	-1.08688500	1.13267300
C	-4.67946700	-2.01610000	-1.40448600
C	-4.94962500	-2.03452400	0.98265500
C	-5.31901400	-2.50397900	-0.27112900
H	-4.96955700	-2.37746700	-2.38582800
H	-5.45611000	-2.40500100	1.86823400
H	-6.10598000	-3.24406100	-0.36552400
C	3.27540900	-0.66386200	-0.18559500
C	4.11996100	-0.82277400	0.92804700
C	3.40857300	-1.46248900	-1.33835300
C	5.08902400	-1.83033000	0.87514400
C	4.40096900	-2.44254600	-1.34608400
C	5.23016800	-2.63663400	-0.24598500
H	5.74288700	-1.97418900	1.72954500
H	4.52092400	-3.06233800	-2.22866200
H	5.98763000	-3.41238800	-0.26601200
C	4.04811100	0.06927400	2.14560800
H	4.69673000	0.94541800	2.03555300
H	3.04225300	0.43951500	2.34699400
H	4.38865500	-0.46147700	3.03614300
C	2.53949900	-1.24018500	-2.55068900
H	1.47668100	-1.30977800	-2.30675600
H	2.70788700	-0.25386800	-2.99627100
H	2.75031700	-1.98377300	-3.31983700
C	-3.55788000	-0.61100500	2.51492000
H	-2.65222700	-1.10763700	2.87773500
H	-3.38258800	0.46689100	2.55727000
H	-4.35042100	-0.83940100	3.22865000
C	-3.00598700	-0.52966000	-2.55797000
H	-3.29807200	0.50520200	-2.76858100
H	-1.91606500	-0.55070400	-2.48634000
H	-3.29216600	-1.12335800	-3.42673300
C	-0.30982000	-2.31865500	-0.49347400

H	-0.59155100	-2.37667800	-1.55026900
H	0.60061300	-2.91539200	-0.36437900
H	-1.10911800	-2.81149000	0.07096200
C	0.48223600	-1.16448700	2.43023600
H	1.52522200	-1.43198700	2.30572900
H	-0.21539700	-1.99407200	2.47079100
C	0.08626100	0.10135600	2.66065600
H	-0.93992700	0.34661300	2.89992000
H	0.79778300	0.91929600	2.70384600
Fe	0.00147000	-0.41704400	0.16537500

^{2}Fe(+)-TS-2/3

Atom	x	y	z
C	1.17218400	2.51798700	0.04555500
C	1.20765000	3.91337800	0.05886200
C	0.00571400	4.61514400	0.05434000
C	-1.19751500	3.91571400	0.04820200
C	-1.16474700	2.52016800	0.03521100
N	0.00315000	1.85614500	0.02722700
H	0.00673600	5.69903700	0.06070400
H	2.15024900	4.44468900	0.07276200
H	-2.13912700	4.44891700	0.05391000
C	2.38635200	1.65257300	0.07356100
C	-2.38079800	1.65723600	0.05501200
N	-2.16298200	0.39231400	-0.01288700
N	2.16631800	0.38824800	0.00266300
C	-3.72981300	2.30744000	0.16969900
H	-3.78838900	2.92741000	1.06892500
H	-3.91774000	2.96250400	-0.68634500
H	-4.52386400	1.56547600	0.21162900
C	3.73608700	2.29944900	0.19713800
H	3.93752000	2.94210700	-0.66533400
H	3.78529000	2.93117500	1.08860200
H	4.52663000	1.55515000	0.25910100
C	-3.23930300	-0.55881000	0.04738800
C	-3.84729900	-0.99067200	-1.14488800
C	-3.61115200	-1.07742800	1.30182600
C	-4.81399000	-1.99617900	-1.05912300
C	-4.58271100	-2.08084700	1.33368000
C	-5.17401400	-2.54719400	0.16514400
H	-5.29244900	-2.34385300	-1.96926400
H	-4.87929400	-2.49570600	2.29178000
H	-5.92169800	-3.33144800	0.20958700
C	3.24027200	-0.56600200	0.05872400

C	3.59020000	-1.11157800	1.30844100
C	3.86737600	-0.97427300	-1.13177600
C	4.55718600	-2.11902500	1.33560200
C	4.82760700	-1.98683700	-1.05079800
C	5.16491700	-2.56471200	0.16706900
H	4.83747200	-2.55378300	2.28977300
H	5.31902500	-2.31827700	-1.96016800
H	5.90802800	-3.35352800	0.20740400
C	2.99947500	-0.58818300	2.59585500
H	3.45465300	0.36695600	2.88122700
H	1.92291000	-0.41876300	2.52672000
H	3.17784400	-1.28341100	3.41729900
C	3.58339500	-0.30837300	-2.45700000
H	2.53962600	-0.01428500	-2.56811900
H	4.18846400	0.59735100	-2.57942500
H	3.83516900	-0.96944200	-3.28782700
C	-3.03742100	-0.53288300	2.58822900
H	-1.96082300	-0.35997600	2.52909100
H	-3.49973600	0.42425800	2.85481400
H	-3.22252300	-1.21689400	3.41755700
C	-3.53155100	-0.35392100	-2.47676900
H	-4.06106800	0.59835100	-2.59557400
H	-2.46869700	-0.14624200	-2.60317600
H	-3.84765200	-0.99600600	-3.30020800
C	-0.06637800	-2.65822400	-0.35165100
H	0.81020400	-3.14406600	-0.75906000
H	-1.00708700	-3.04213200	-0.72351900
C	-0.01735100	-2.13584400	0.95925000
H	-0.92647200	-2.15996600	1.54979400
H	0.91405000	-2.22290500	1.50774700
Fe	0.00318600	-0.28475700	-0.10899300
C	0.03449800	-1.32011200	-2.05851700
H	-0.80885000	-1.78727000	-2.55824800
H	-0.02083800	-0.23459200	-2.27388100
H	0.97099300	-1.69206100	-2.46308500

^{2}Fe(+)-3

Atom	x	y	z
C	1.10750400	2.71721900	0.07080500
C	1.12220300	4.11342800	0.05728200
C	-0.09483000	4.79153700	0.06804500
C	-1.29033700	4.07668900	0.05738700
C	-1.23233000	2.68147000	0.07173000
N	-0.05232700	2.05060900	0.12517600

H	-0.11136000	5.87541500	0.06153400
H	2.05376400	4.66351100	0.03134000
H	-2.23835600	4.59793700	0.03126300
C	2.32019200	1.84665000	-0.02877400
C	-2.41642200	1.77380700	-0.02652500
N	-2.13877600	0.52260400	-0.15942800
N	2.08270000	0.58897100	-0.17123700
C	-3.79080900	2.37446200	-0.02761100
H	-4.00349400	2.86963700	0.92463800
H	-3.87277900	3.13400800	-0.81046200
H	-4.55402400	1.62032700	-0.20405300
C	3.67419400	2.49278000	-0.02178300
H	3.73477800	3.25615500	-0.80293100
H	3.86555700	2.99302500	0.93235400
H	4.46323500	1.76519400	-0.19591000
C	-3.14547400	-0.49175000	-0.25803700
C	-3.24804500	-1.17390400	-1.48647800
C	-3.91948100	-0.85453900	0.86019500
C	-4.18176700	-2.20362800	-1.59235000
C	-4.82821300	-1.90612800	0.70677800
C	-4.96878700	-2.57004900	-0.50499500
H	-4.28717200	-2.72709000	-2.53704700
H	-5.42872500	-2.20806800	1.55887400
H	-5.68270900	-3.38076400	-0.60007700
C	3.12503700	-0.38809100	-0.27265000
C	3.90228200	-0.73524900	0.84834300
C	3.26489000	-1.05110800	-1.50785100
C	4.84803300	-1.75341600	0.69301800
C	4.23371600	-2.04777500	-1.61495600
C	5.02204800	-2.39986600	-0.52380900
H	5.45150600	-2.04263600	1.54748200
H	4.36594800	-2.55656200	-2.56430100
H	5.76401600	-3.18483600	-0.62032300
C	3.73910100	-0.06729600	2.19286100
H	4.32126900	0.85772500	2.26365600
H	2.69904500	0.18242300	2.41165900
H	4.09221400	-0.72289300	2.98979500
C	2.41052100	-0.67696600	-2.69253300
H	1.34159400	-0.75501900	-2.46278000
H	2.58734200	0.35165700	-3.02170700
H	2.61088400	-1.33241900	-3.54058300
C	-3.78625400	-0.17106600	2.20011200
H	-2.75302300	0.09694000	2.43060200

H	-4.38371600	0.74519100	2.25460100
H	-4.13991200	-0.82485300	2.99820800
C	-2.39157000	-0.78645300	-2.66580100
H	-2.58216500	0.23839000	-2.99838000
H	-1.32190400	-0.84824800	-2.43140600
H	-2.57435200	-1.44692300	-3.51390300
C	0.03564400	-1.68811600	1.47908500
H	0.81272300	-1.53419000	2.23997700
H	-0.91850800	-1.73640200	2.02072200
Fe	-0.02718700	-0.08556400	0.24478900
C	0.28215400	-3.01126200	0.73228100
H	1.23681700	-2.96875300	0.19424500
H	-0.49086600	-3.16047300	-0.03317500
C	0.29337800	-4.23711100	1.65732200
H	1.07916900	-4.15071700	2.41362200
H	-0.66026700	-4.34257300	2.18288500
H	0.46966200	-5.16035500	1.09695300

^{2}Fe(+)-4

Atom	x	y	z
Fe	-0.05268300	-0.18170800	0.22486200
N	-0.17140800	1.97715700	-0.16930800
C	-1.36812700	2.57146800	-0.30622900
C	-2.54511200	1.64831700	-0.33364700
N	-2.29323000	0.40888100	-0.11975300
C	-3.32809600	-0.58889600	-0.15151600
C	-3.46041000	-1.36249900	-1.32096400
C	-2.65854600	-1.05467300	-2.56128400
H	-2.80231200	-1.82702400	-3.31746100
C	-4.39860500	-2.39506800	-1.32130200
C	-5.17970100	-2.65854500	-0.20075400
C	-5.04808900	-1.86852000	0.93328800
C	-4.13103900	-0.81333100	0.98076500
C	-4.08057500	0.07004600	2.20560200
H	-3.09186000	0.49093500	2.39084800
H	-5.66972900	-2.06292400	1.80168700
H	-4.51523400	-2.99929900	-2.21510500
C	-3.90153800	2.22230500	-0.63048000
H	-4.20764900	2.91976700	0.15520800
H	-3.88918000	2.78066600	-1.57051000
H	-4.65348800	1.44018100	-0.70314300
C	-1.47874400	3.95544900	-0.43955400
C	-0.31826900	4.72516100	-0.43796100
C	0.91495300	4.09622700	-0.33070200

C	0.95665400	2.70355200	-0.19927000
C	2.22757300	1.92672600	-0.14324600
N	2.11179400	0.66451300	0.07228100
C	3.26543500	-0.19499600	-0.01387600
C	3.65470900	-0.65839900	-1.28546000
C	4.72425100	-1.55312900	-1.35962500
C	5.39924300	-1.96542600	-0.21692700
C	5.01143600	-1.47817400	1.02470600
C	3.93864000	-0.59183000	1.15386000
H	5.54699100	-1.78735900	1.91664200
H	5.03154200	-1.92486200	-2.33184000
C	3.52120500	2.65908000	-0.37388000
H	3.67379800	3.41935500	0.39836700
H	4.36963800	1.97996600	-0.35085100
H	3.51623800	3.17554900	-1.33774600
H	1.82728400	4.67713400	-0.35200300
H	-0.37707500	5.80334900	-0.53258700
H	-2.44611500	4.42847500	-0.54440500
H	6.22916900	-2.65902600	-0.29476500
C	3.54509300	-0.09144200	2.52211200
H	3.33845400	0.98186400	2.53407900
H	-5.89475000	-3.47366400	-0.21563500
C	2.97057300	-0.19367000	-2.54854000
H	3.26468200	-0.81354900	-3.39616500
C	0.23407300	-2.07836100	-0.49827400
H	-0.78360800	-2.46237400	-0.66012000
H	0.67225800	-1.96791300	-1.50088300
H	-1.58770800	-0.98952300	-2.35597200
H	-2.96096200	-0.10176800	-3.00950100
H	-4.37779400	-0.48313000	3.09801400
H	-4.77439500	0.91319900	2.11286500
H	4.34252900	-0.27604400	3.24286700
H	2.65353300	-0.60360000	2.89767800
H	3.23848600	0.83846800	-2.80090600
H	1.88222300	-0.23501200	-2.46918500
C	1.22705700	-4.44481400	-0.46725500
C	1.04006400	-3.12166200	0.28837700
H	1.78919200	-5.17131400	0.12777300
H	1.77312700	-4.28974700	-1.40263800
H	0.26269700	-4.89614700	-0.71955100
H	2.02834800	-2.72737600	0.54928600
H	0.53798000	-3.33850200	1.23950200
C	-0.43297300	-0.78715000	2.50557800

C	-0.12832400	0.51817000	2.65054600
H	-1.45489300	-1.14165600	2.43694300
H	0.32679400	-1.55631000	2.58957600
H	-0.89725700	1.28331600	2.66694000
H	0.88185300	0.85096800	2.84922500

^{2}Fe(+)-TS-4/5

Atom	x	y	z
C	1.14132100	2.60994100	-0.29078900
C	1.16055400	3.99897300	-0.42146300
C	-0.04734400	4.68922400	-0.46286500
C	-1.24286900	3.97890200	-0.39396900
C	-1.19867400	2.59041600	-0.26628500
N	-0.02243900	1.93682200	-0.20608200
H	-0.05746000	5.76884600	-0.55692800
H	2.09730400	4.53593100	-0.49216900
H	-2.18921800	4.50113900	-0.44353500
C	2.36560400	1.76619200	-0.25773300
C	-2.40962200	1.72671500	-0.21908500
N	-2.20746600	0.47723900	0.02020500
N	2.18585500	0.51843700	0.01010000
C	-3.75109000	2.36160000	-0.46166100
H	-3.96980000	3.10262800	0.31347100
H	-3.77132200	2.88472500	-1.42151000
H	-4.54806200	1.62228100	-0.45366600
C	3.69253300	2.41512400	-0.53856600
H	3.68275000	2.93065300	-1.50266700
H	3.92133300	3.16515500	0.22502100
H	4.49854100	1.68568000	-0.54388400
C	-3.30167800	-0.45874400	-0.03530400
C	-3.63606400	-1.01184500	-1.28879600
C	-3.98398900	-0.83232800	1.13589500
C	-4.62753600	-1.99351300	-1.33505800
C	-4.97564200	-1.81381600	1.03420900
C	-5.28821800	-2.40407700	-0.18276200
H	-4.88945200	-2.43148900	-2.29298500
H	-5.51452300	-2.10750400	1.92964600
H	-6.05715200	-3.16681100	-0.23739800
C	3.29404500	-0.40011100	-0.02776300
C	3.98045200	-0.72669500	1.15476200
C	3.62811700	-0.99210500	-1.26192000
C	4.99654700	-1.68468200	1.08133600
C	4.64460700	-1.94923300	-1.28070300
C	5.32276500	-2.30158200	-0.11928300

H	5.54051100	-1.94191500	1.98477700
H	4.91121800	-2.41496600	-2.22410000
H	6.11149500	-3.04504700	-0.15317600
C	3.66465200	-0.07805600	2.48110600
H	4.52526700	-0.13384800	3.14924100
H	3.39290900	0.97464000	2.38272100
H	2.83538700	-0.57947800	2.98913800
C	2.94343600	-0.59063600	-2.54617900
H	1.85471700	-0.59957000	-2.45910500
H	3.22877000	0.41906500	-2.86094200
H	3.21709400	-1.26584900	-3.35758500
C	-3.71543300	-0.19698400	2.47964200
H	-2.94235300	-0.73085900	3.03985900
H	-3.39736000	0.84370800	2.39820600
H	-4.61670300	-0.21514600	3.09460700
C	-2.99110100	-0.53388300	-2.56786800
H	-3.38773100	0.43968100	-2.87713700
H	-1.90936300	-0.42212700	-2.47776600
H	-3.18860100	-1.22967200	-3.38430600
C	0.36575100	-2.30145600	0.47179700
H	1.45722800	-2.29758000	0.45988000
H	0.03915300	-3.19955800	0.99167200
C	-0.23524200	-2.31662500	-0.93851600
H	-0.01674700	-1.39329700	-1.49855600
H	-1.32302000	-2.38943300	-0.87919600
C	0.30654300	-3.49694600	-1.76725400
H	1.39238500	-3.44354900	-1.87486900
H	0.06575000	-4.44776100	-1.28530500
H	-0.13489700	-3.50718700	-2.76824600
C	-0.08854300	-1.42123300	2.42936000
H	0.77027800	-2.00468100	2.73713400
H	-1.02674400	-1.95849900	2.49639500
C	-0.08666000	-0.02265600	2.64296200
H	-1.01706400	0.47696200	2.88408200
H	0.81163200	0.44857800	3.02598600
Fe	0.01341800	-0.04079300	0.52654500

^{2}Fe(+)-5

Atom	x	y	z
C	1.13042600	-3.09187900	-0.23269200
C	1.15134000	-4.48546300	-0.31839200
C	-0.06260800	-5.16658400	-0.37569800
C	-1.26115700	-4.45938600	-0.31511300
C	-1.20942500	-3.06644100	-0.22997700

N	-0.03234300	-2.42772900	-0.23713400
H	-0.07442800	-6.24831100	-0.44528500
H	2.08541600	-5.03175000	-0.33290500
H	-2.20691600	-4.98528900	-0.32691800
C	2.33966500	-2.22541000	-0.07805800
C	-2.39831000	-2.17374400	-0.07289600
N	-2.12800000	-0.93494100	0.15536100
N	2.09769800	-0.98226100	0.15564800
C	-3.76964800	-2.77908900	-0.12978900
H	-3.96813700	-3.20947400	-1.11591100
H	-3.85682100	-3.59068400	0.59845100
H	-4.53920100	-2.04254700	0.08854100
C	3.69663000	-2.86220700	-0.14239000
H	3.76918000	-3.67590000	0.58515500
H	3.88011100	-3.29654700	-1.12970800
H	4.48407200	-2.14376800	0.07229600
C	-3.14334800	0.06331600	0.31525400
C	-3.27609300	0.64471200	1.59122100
C	-3.89679100	0.50911600	-0.78699300
C	-4.21841400	1.65868800	1.75812100
C	-4.81616700	1.53988600	-0.57024300
C	-4.98565200	2.10572900	0.68696900
H	-4.34645700	2.10543100	2.73875100
H	-5.40162500	1.90451300	-1.40815800
H	-5.70712500	2.90245900	0.83085500
C	3.13727400	-0.00953400	0.31557600
C	3.89481100	0.42417000	-0.78876700
C	3.29340900	0.56001000	1.59417100
C	4.84049400	1.43089000	-0.57232400
C	4.26096100	1.55015900	1.76042300
C	5.03164000	1.98524400	0.68689300
H	5.42964700	1.78564300	-1.41190500
H	4.40652200	1.98736000	2.74292600
H	5.77333300	2.76322700	0.83064800
C	3.70606200	-0.14025100	-2.17667200
H	4.24582900	-1.08301600	-2.31494800
H	2.65566600	-0.32674900	-2.41083900
H	4.08886000	0.55372600	-2.92586200
C	2.45599700	0.09696100	2.75961800
H	1.38409600	0.21435400	2.56125400
H	2.61960000	-0.95941900	2.99341600
H	2.68513400	0.67200900	3.65724500
C	-3.72904600	-0.06603400	-2.17310600

H	-2.68505900	-0.28221400	-2.41029500
H	-4.29537100	-0.99397500	-2.30526500
H	-4.09558700	0.63522800	-2.92364700
C	-2.44016100	0.16992200	2.75315800
H	-2.62090900	-0.88254300	2.99151600
H	-1.36701300	0.26811300	2.54954300
H	-2.65306500	0.75208100	3.65016900
C	0.02969400	1.43233400	-1.24924300
H	0.90833200	1.43186200	-1.90702400
H	-0.84922900	1.46378100	-1.90626900
C	0.05280700	2.67212200	-0.33773400
H	0.93465700	2.64416200	0.31601300
H	-0.82060100	2.66850000	0.32849200
C	0.06435700	4.00323600	-1.11003900
H	0.93726200	4.02161900	-1.77499300
H	-0.81519800	4.04247300	-1.76531500
C	0.08383800	5.23955700	-0.20463100
H	0.96284200	5.19544000	0.45060300
H	-0.78879700	5.21579500	0.46012500
C	0.09492500	6.55720800	-0.98328300
H	-0.79000900	6.65182400	-1.62009900
H	0.10950800	7.41924300	-0.31112600
H	0.97395300	6.63043600	-1.63099000
Fe	-0.01380800	-0.28715400	-0.18560900

^{2}Fe(+)-6

Atom	x	y	z
C	0.95661300	2.70370600	0.19935900
C	0.91487800	4.09635300	0.33104300
C	-0.31836700	4.72523100	0.43838600
C	-1.47881900	3.95548100	0.43983400
C	-1.36814300	2.57152200	0.30631800
N	-0.17141600	1.97727200	0.16929200
H	-0.37720700	5.80340600	0.53318100
H	1.82719900	4.67727600	0.35245700
H	-2.44621400	4.42845800	0.54469800
C	2.22757700	1.92692500	0.14313500
C	-2.54512300	1.64831900	0.33360900
N	-2.29313700	0.40887700	0.11999400
N	2.11184900	0.66479100	-0.07276500
C	-3.90164500	2.22229700	0.63004000
H	-3.88945500	2.78110200	1.56980600
H	-4.20776000	2.91932100	-0.15604000
H	-4.65349600	1.44009300	0.70299800

C	3.52116800	2.65929100	0.37399900
H	3.67376000	3.41971500	-0.39810300
H	3.51611900	3.17556500	1.33797200
H	4.36963000	1.98020600	0.35086500
C	-3.32795100	-0.58891400	0.15148900
C	-4.13085500	-0.81316000	-0.98083800
C	-3.46031100	-1.36274600	1.32080900
C	-5.04790100	-1.86838200	-0.93358000
C	-4.39847900	-2.39531600	1.32093900
C	-5.17954700	-2.65860400	0.20030800
H	-5.66949400	-2.06263300	-1.80205000
H	-4.51512500	-2.99972200	2.21462500
H	-5.89459100	-3.47373300	0.21502500
C	3.26542600	-0.19479100	0.01344900
C	3.65466700	-0.65809900	1.28508600
C	3.93852800	-0.59191500	-1.15424500
C	4.72397600	-1.55309800	1.35934000
C	5.01111900	-1.47849600	-1.02500000
C	5.39883300	-1.96571200	0.21667400
H	5.03121000	-1.92476300	2.33160100
H	5.54660100	-1.78789900	-1.91690900
H	6.22859800	-2.65950300	0.29457200
C	2.97059300	-0.19315200	2.54812300
H	3.23785300	0.83928500	2.79993300
H	1.88224100	-0.23529900	2.46905400
H	3.26534100	-0.81243100	3.39596700
C	3.54514000	-0.09170900	-2.52261600
H	2.65465300	-0.60519200	-2.89896700
H	3.33686200	0.98127100	-2.53440700
H	4.34336500	-0.27488200	-3.24287400
C	-2.65864300	-1.05498200	2.56127300
H	-1.58792900	-0.98822300	2.35587600
H	-2.96230400	-0.10285800	3.01032500
H	-2.80130200	-1.82816800	3.31681400
C	-4.08036300	0.07034900	-2.20558900
H	-4.77474000	0.91306900	-2.11309400
H	-3.09181400	0.49184900	-2.39036400
H	-4.37683900	-0.48295000	-3.09817900
C	0.23414500	-2.07793400	0.49880800
H	0.67195800	-1.96702500	1.50153700
H	-0.78354000	-2.46201200	0.66048800
C	1.04054000	-3.12149700	-0.28706100
H	2.02893800	-2.72728200	-0.54763600

H	0.53896400	-3.33872100	-1.23837400
C	1.22717600	-4.44436500	0.46914100
H	1.77275900	-4.28896000	1.40475900
H	0.26269600	-4.89563900	0.72110800
H	1.78963600	-5.17106200	-0.12534300
C	-0.43374500	-0.78829700	-2.50478900
H	0.32540900	-1.55809900	-2.58850600
H	-1.45591300	-1.14204700	-2.43585600
C	-0.12811200	0.51674100	-2.65058400
H	-0.89648400	1.28245800	-2.66732100
H	0.88226100	0.84863900	-2.84972500
Fe	-0.05258300	-0.18151700	-0.22525900

^{2}Fe(+)-TS-6/7

Atom	x	y	z
C	1.27987500	2.64778900	-0.07639800
C	1.35762500	4.04041700	-0.15188500
C	0.17793900	4.77671300	-0.20719800
C	-1.04567200	4.11533200	-0.14632400
C	-1.05401300	2.72121400	-0.06982600
N	0.09211500	2.02103200	-0.08044700
H	0.21152700	5.85794800	-0.27331200
H	2.31572200	4.54370400	-0.16073600
H	-1.97044800	4.67756500	-0.15087300
C	2.45603600	1.74954200	0.08327300
C	-2.28327800	1.89791900	0.10288600
N	-2.09368900	0.62714400	0.19126600
N	2.18718500	0.49296200	0.17213900
C	-3.60903500	2.59352900	0.22803200
H	-3.58641300	3.31871200	1.04638600
H	-3.84620700	3.14728800	-0.68527800
H	-4.41253500	1.88671700	0.42074500
C	3.82484000	2.35961700	0.19214500
H	4.08739100	2.89377800	-0.72591400
H	3.85816400	3.08718400	1.00798600
H	4.58332200	1.60314000	0.37879200
C	-3.17050100	-0.28623600	0.45549400
C	-4.02419100	-0.71440800	-0.57718300
C	-3.28411900	-0.78622000	1.76624700
C	-5.00517000	-1.65988600	-0.26395400
C	-4.28448200	-1.72371200	2.02970900
C	-5.13905400	-2.16250600	1.02484700
H	-5.67307000	-2.00244000	-1.04780800
H	-4.39043300	-2.11223700	3.03747400

H	-5.90761200	-2.89511700	1.24536800
C	3.20922500	-0.48633300	0.41666600
C	3.31566200	-0.99579200	1.72465900
C	4.01560200	-0.96433500	-0.63185000
C	4.25794200	-1.99671300	1.96740500
C	4.93837600	-1.97284300	-0.33921600
C	5.06287600	-2.48750100	0.94551100
H	4.35775000	-2.39398100	2.97240000
H	5.56770200	-2.35563300	-1.13631900
H	5.78556000	-3.26977100	1.15006500
C	2.46116200	-0.45779300	2.84539600
H	2.69842000	0.58608900	3.07559100
H	1.39556800	-0.49180700	2.59941600
H	2.61018000	-1.03429700	3.75897700
C	3.91636700	-0.41668400	-2.03481800
H	4.30828300	0.60325700	-2.10852000
H	4.49397900	-1.02861600	-2.72850200
H	2.88605300	-0.39065700	-2.39404900
C	-2.37275900	-0.30583000	2.86816100
H	-1.31716400	-0.42153900	2.60408700
H	-2.52721400	0.75418400	3.09466300
H	-2.54783400	-0.86412600	3.78837900
C	-3.90785400	-0.18637500	-1.98631600
H	-4.15345900	0.87825300	-2.05367600
H	-2.89922600	-0.30837100	-2.38667500
H	-4.59239900	-0.71319800	-2.65182300
C	-0.00658300	-2.19616300	0.12023600
H	0.87627400	-2.29311300	0.75573400
H	-0.92404500	-2.30432200	0.70436300
C	0.03183400	-3.04598500	-1.05915900
H	0.99723100	-3.52121000	-1.24797000
H	0.04575600	-2.27413500	-2.10888500
C	-1.15109700	-3.94619300	-1.36393000
H	-1.17766500	-4.77693400	-0.65135900
H	-2.09748100	-3.40687700	-1.26802300
H	-1.09653400	-4.37512500	-2.36785800
C	0.02681700	-1.35771500	-3.11580500
H	0.93261200	-1.70253000	-3.61175100
H	-0.87933300	-1.72589000	-3.59468100
C	0.01530100	-0.05342900	-2.53954600
H	-0.89606500	0.52619800	-2.67787900
H	0.90975200	0.54819800	-2.69347900
Fe	0.02371500	-0.09364500	-0.31305000

^{2}Fe(+)-7

Atom	x	y	z
C	-1.25857400	2.56805300	-0.12196200
C	-1.31212000	3.95474800	-0.25243600
C	-0.12508100	4.68027000	-0.32872700
C	1.09267200	4.00305100	-0.31591800
C	1.10155100	2.61564600	-0.18289800
N	-0.06179600	1.93254900	-0.02628800
H	-0.14944900	5.75847100	-0.43010600
H	-2.26775800	4.46083000	-0.31002500
H	2.02289900	4.54706000	-0.42179400
C	-2.38716900	1.64348800	-0.16553400
C	2.26321900	1.73673000	-0.26733400
N	1.96757300	0.46298900	-0.25625300
N	-2.03918900	0.38420000	-0.19064800
C	3.64091200	2.31336700	-0.41342700
H	3.67939700	3.00816600	-1.25674100
H	3.92246200	2.87754400	0.48070500
H	4.38589300	1.53890300	-0.57915400
C	-3.79303700	2.16339700	-0.23889800
H	-4.03681100	2.74834800	0.65270900
H	-3.91512000	2.82523200	-1.10098600
H	-4.51572000	1.35597600	-0.32907000
C	3.00191700	-0.52330400	-0.42716100
C	3.80819500	-0.92057600	0.65437100
C	3.14323400	-1.09842400	-1.70573200
C	4.75148400	-1.92932800	0.43270400
C	4.10275900	-2.09798600	-1.87774800
C	4.89892800	-2.51786100	-0.81736400
H	5.38026600	-2.25039600	1.25714400
H	4.22732200	-2.54712000	-2.85785000
H	5.63627400	-3.29893000	-0.96712400
C	-3.03050900	-0.64565500	-0.36622000
C	-3.20047800	-1.16172700	-1.66712500
C	-3.76208500	-1.14586300	0.72641400
C	-4.10245500	-2.21198500	-1.84868200
C	-4.64793400	-2.20268300	0.49361700
C	-4.81607600	-2.73776600	-0.77747200
H	-4.24589500	-2.61793500	-2.84488600
H	-5.21693000	-2.60331000	1.32657800
H	-5.50701000	-3.55870900	-0.93485800
C	-2.47081300	-0.57203500	-2.84993100
H	-2.85280700	0.42274700	-3.10274900

H	-1.39953000	-0.45388900	-2.66527400
H	-2.59278700	-1.19926300	-3.73368600
C	-3.65543300	-0.54728100	2.10758100
H	-2.63334700	-0.28015600	2.37269300
H	-4.25578300	0.36540400	2.19204700
H	-4.02996700	-1.24136900	2.86141700
C	2.31722000	-0.62231900	-2.87521500
H	1.24983900	-0.58579900	-2.64065600
H	2.60233800	0.38869800	-3.18473900
H	2.45096400	-1.27548700	-3.73829600
C	3.70567100	-0.27288400	2.01324500
H	4.24775100	0.67859500	2.04458700
H	2.67468400	-0.06389600	2.29746800
H	4.14510300	-0.91120600	2.78107400
C	0.01022400	-2.13758300	-0.27222600
H	-0.85524800	-1.96285600	-0.90028000
H	0.96034000	-2.30596400	-0.76725600
C	-0.14252600	-2.44882400	1.03294000
H	-1.13883300	-2.39087100	1.46586500
H	-0.78996000	-0.93791100	3.51938600
C	0.92324900	-3.07117900	1.87840800
H	0.70895100	-4.14444800	1.95349500
H	1.91551800	-2.96300500	1.43872200
H	0.93236100	-2.68784000	2.89759900
Fe	-0.01469700	0.10755900	0.34164700
C	-0.00886400	-0.17325200	3.54166800
H	-0.14938800	0.38375600	4.47748300
H	0.95015800	-0.68679900	3.63380800
C	-0.05356800	0.77482400	2.34882300
H	0.77777800	1.48600600	2.41315900
H	-0.96905000	1.37637000	2.38254600

^{2}Fe(+)-8

Atom	x	y	z
C	1.18333000	2.52179500	-0.01730800
C	1.22643700	3.91765200	-0.02874800
C	0.02713900	4.62362000	-0.02351500
C	-1.17859000	3.92858400	-0.00100800
C	-1.14814700	2.53258800	0.00897100
N	0.01451400	1.86632800	-0.00990800
H	0.03195800	5.70743200	-0.03228500
H	2.17097300	4.44575800	-0.03987700
H	-2.11812600	4.46550700	0.00969200
C	2.39391100	1.64566900	0.00277200

C	-2.36645600	1.66744000	0.05296800
N	-2.14589700	0.40268100	0.10810500
N	2.16327700	0.38356200	0.07303500
C	-3.71787700	2.31922400	0.05630100
H	-3.80986200	3.00036900	0.90748800
H	-3.86647000	2.91445100	-0.84944900
H	-4.51396800	1.58154500	0.12028400
C	3.75186000	2.28275700	-0.03840600
H	3.87304100	2.88212900	-0.94549000
H	3.88443100	2.95697300	0.81299800
H	4.54086900	1.53524900	-0.00932700
C	-3.21039200	-0.56174900	0.14083100
C	-3.85764800	-0.92600200	-1.05239600
C	-3.50451400	-1.17594600	1.37020000
C	-4.83985900	-1.91716100	-0.98160300
C	-4.50065000	-2.15320700	1.39010700
C	-5.16559400	-2.52307000	0.22605000
H	-5.34955500	-2.21816500	-1.89113200
H	-4.75045900	-2.63261300	2.33101700
H	-5.93119700	-3.29032400	0.25872700
C	3.22522100	-0.58518500	0.10220300
C	3.59234700	-1.12771000	1.34483000
C	3.79479600	-1.02301500	-1.10507100
C	4.58414800	-2.11012200	1.36001500
C	4.77746600	-2.01354800	-1.03790100
C	5.17521800	-2.55072800	0.18101000
H	4.88876200	-2.53716700	2.30998400
H	5.22992300	-2.36912800	-1.95793100
H	5.93928100	-3.31961000	0.21136100
C	2.93950000	-0.66593300	2.62387400
H	3.12160900	0.39454800	2.82559500
H	1.85294900	-0.80442300	2.59542100
H	3.31644500	-1.22868100	3.47824800
C	3.35911200	-0.46192500	-2.43677400
H	2.27314300	-0.51043200	-2.56385900
H	3.65318900	0.58521400	-2.56570500
H	3.80790800	-1.02260900	-3.25705200
C	-2.77479500	-0.78863600	2.63202800
H	-1.69411200	-0.94456100	2.53718800
H	-2.92528000	0.26335500	2.89416300
H	-3.11483700	-1.38721600	3.47753100
C	-3.50872600	-0.28954100	-2.37614600
H	-3.87535800	0.73980200	-2.45252000

H	-2.42876700	-0.26176700	-2.54726500
H	-3.95471200	-0.84678200	-3.20034900
C	-0.00128200	-2.33563600	-0.23390500
H	0.95919100	-2.70111400	0.15454600
H	-0.75845300	-2.73501200	0.45509100
C	-0.23818900	-2.92110300	-1.63761600
H	0.52278500	-2.59680700	-2.35584100
H	-1.21128400	-2.62830400	-2.04542000
H	-0.21839800	-4.01753100	-1.63659200
Fe	0.00478900	-0.30164500	-0.05224800

^{2}Fe(+)-3/9

Atom	x	y	z
C	-1.10261900	2.60071700	0.05342700
C	-1.11721300	3.99489400	0.12477500
C	0.09407300	4.67871200	0.17395600
C	1.28895400	3.96287900	0.14809200
C	1.23719000	2.57140000	0.07592000
N	0.05921300	1.92473100	0.03145400
H	0.10770300	5.76083100	0.23191000
H	-2.05218600	4.53959700	0.14272100
H	2.23764300	4.48256300	0.18476800
C	-2.32068000	1.75166900	-0.00490500
C	2.43042600	1.68415400	0.04209400
N	2.17836600	0.42127100	0.00301700
N	-2.11474700	0.47883100	-0.02236600
C	3.79993100	2.29771500	0.05840700
H	3.93492400	2.96899700	-0.79457700
H	3.94377900	2.89464200	0.96388100
H	4.57590100	1.53664100	0.02376500
C	-3.66825000	2.41329500	-0.03944600
H	-3.82538400	3.01623600	0.85985500
H	-3.74774100	3.08727400	-0.89719400
H	-4.46921500	1.68064500	-0.10236700
C	3.23236700	-0.55519200	-0.04390000
C	3.71168300	-1.09732200	1.16224800
C	3.70287600	-0.98620100	-1.29698500
C	4.68071300	-2.10094200	1.08530200
C	4.67028900	-1.99413100	-1.31945600
C	5.15500300	-2.55138900	-0.14182300
H	5.06622700	-2.53134600	2.00398900
H	5.04653000	-2.34153100	-2.27634100
H	5.90362500	-3.33508200	-0.17999500
C	-3.20897400	-0.45236700	-0.08564500

C	-3.63362300	-0.91257400	-1.34471600
C	-3.77540000	-0.92119700	1.11287400
C	-4.64670400	-1.87400000	-1.38044100
C	-4.78811600	-1.87972800	1.02272500
C	-5.21977100	-2.35767800	-0.20962400
H	-4.98958400	-2.24229500	-2.34203500
H	-5.23977100	-2.25478800	1.93552300
H	-6.00412300	-3.10508500	-0.25760200
C	-3.04655700	-0.36651400	-2.62331600
H	-3.36212300	0.66669800	-2.80532500
H	-1.95331400	-0.36731600	-2.60856200
H	-3.36974900	-0.95607600	-3.48198500
C	-3.32242400	-0.40420200	2.45613000
H	-2.23425900	-0.42777700	2.55593700
H	-3.63817900	0.63181500	2.62113600
H	-3.74840200	-1.00034300	3.26389300
C	3.21629000	-0.36332800	-2.58336200
H	2.12925800	-0.25188600	-2.60741600
H	3.64186300	0.63488300	-2.73540100
H	3.50877400	-0.96842400	-3.44228500
C	3.22513400	-0.59905100	2.50144800
H	3.59701400	0.40867700	2.71728800
H	2.13425000	-0.55468600	2.55293900
H	3.57405100	-1.24749400	3.30593600
C	0.04860500	-2.08288400	-0.94981500
H	-0.88933900	-2.30515100	-1.44927200
H	0.92845600	-2.06076900	-1.58417000
C	0.19654500	-2.43076800	0.41140900
H	-0.01591400	-1.08321700	1.41901000
H	1.21524800	-2.57540000	0.76110000
C	-0.83756200	-3.26427200	1.13464500
H	-1.85409900	-2.99152500	0.84944600
H	-0.68423700	-4.31130800	0.85168700
H	-0.74587400	-3.19136300	2.21926100
Fe	0.01558900	-0.17502500	0.02983300

^{2}Fe(+)-9

Atom	x	y	z
C	1.18824300	2.58062200	-0.03904100
C	1.23391600	3.97648400	-0.02958200
C	0.03602900	4.68491000	-0.01821900
C	-1.17280000	3.99536600	-0.01090700
C	-1.14649600	2.59934300	-0.02433800
N	0.01525600	1.93394700	-0.04451800

H	0.04471400	5.76884800	-0.01096100
H	2.17890700	4.50347800	-0.02962800
H	-2.10989300	4.53613400	0.00563200
C	2.40264400	1.70531200	-0.02766500
C	-2.36885600	1.73809800	-0.00484800
N	-2.16103700	0.47081400	0.00570000
N	2.18378600	0.44081600	-0.00884100
C	-3.71512500	2.40332400	0.00456700
H	-3.82309800	3.05023800	0.88008600
H	-3.83769100	3.03534500	-0.87995800
H	-4.51934000	1.67157700	0.01703700
C	3.75541400	2.35804400	-0.02960900
H	3.87592200	3.00801900	0.84197500
H	4.55162100	1.61754900	-0.01804400
H	3.87958900	2.98372900	-0.91844400
C	-3.25612500	-0.46063200	0.05251000
C	-3.77790500	-0.96937600	-1.15053900
C	-3.71715900	-0.89329700	1.30882100
C	-4.77608900	-1.94374300	-1.06491700
C	-4.71540100	-1.87049400	1.33967100
C	-5.24004900	-2.39723400	0.16498500
H	-5.19333500	-2.34866100	-1.98127800
H	-5.08386400	-2.21726500	2.29986300
H	-6.01231300	-3.15741500	0.20775700
C	3.26720500	-0.50348000	0.04766200
C	3.71627000	-0.92940200	1.31133300
C	3.79774700	-1.02314400	-1.14693500
C	4.70534500	-1.91517000	1.35822900
C	4.78635400	-2.00601100	-1.04439000
C	5.23461900	-2.45597300	0.19227500
H	5.06372700	-2.25625500	2.32428800
H	5.20972900	-2.41933500	-1.95417000
H	5.99946400	-3.22287100	0.24713000
C	3.18334800	-0.32158500	2.58669600
H	3.56605800	0.69317300	2.74251600
H	2.09255400	-0.25181800	2.59176500
H	3.48403800	-0.91172700	3.45320800
C	3.35279300	-0.52343900	-2.49955800
H	2.26621700	-0.54140500	-2.60741300
H	3.67882500	0.50801700	-2.67541200
H	3.78182600	-1.13354700	-3.29531400
C	-3.18239800	-0.30694400	2.59327000
H	-2.09156200	-0.23633900	2.59719400

H	-3.56409800	0.70531800	2.76668000
H	-3.48050300	-0.91138100	3.45064500
C	-3.30244100	-0.47199400	-2.49366800
H	-3.60637100	0.56581200	-2.67068600
H	-2.21403200	-0.50762000	-2.58401600
H	-3.72806900	-1.07112600	-3.29949700
C	0.22607600	-2.08276100	1.13832200
H	1.30007200	-2.23408000	1.15886500
H	-0.21337700	-1.56294500	1.98562100
C	-0.55192300	-2.70062100	0.22693600
H	0.07643200	-0.62665600	-1.98331800
H	-1.63178000	-2.60520300	0.31230000
C	-0.05388100	-3.60385900	-0.85630200
H	1.03571500	-3.62622700	-0.90837000
H	-0.41087500	-4.62267800	-0.66781200
H	-0.44477700	-3.30708300	-1.83234800
Fe	0.00605400	-0.18341200	-0.40541600

^{2}Fe(+)-10

Atom	x	y	z
C	-1.16931800	2.37214300	-0.13257400
C	-1.20761400	3.75477100	-0.32190000
C	-0.00008700	4.44580500	-0.40475200
C	1.20747200	3.75474300	-0.32254400
C	1.16921900	2.37213300	-0.13312900
N	-0.00003000	1.73759600	-0.01424700
H	-0.00011300	5.52029300	-0.54776300
H	-2.14804000	4.28363800	-0.40725100
H	2.14786900	4.28357300	-0.40844000
C	-2.36338800	1.46812000	-0.08622100
C	2.36328800	1.46811700	-0.08698200
N	2.09849700	0.20965300	-0.04453500
N	-2.09856700	0.20965500	-0.04444400
C	3.73346300	2.07283500	-0.13471200
H	3.85432600	2.67088100	-1.04306200
H	3.89103000	2.74371100	0.71508200
H	4.50597900	1.30785000	-0.12276400
C	-3.73355400	2.07293300	-0.13323100
H	-3.85480800	2.67107300	-1.04147200
H	-4.50612100	1.30800800	-0.12102400
H	-3.89067600	2.74373800	0.71670000
C	3.12768900	-0.79526100	-0.00683400
C	3.76464800	-1.09924000	1.20897700
C	3.39392700	-1.50047700	-1.19318500

C	4.71508600	-2.12316800	1.20047000
C	4.35806400	-2.50866100	-1.14970200
C	5.01659800	-2.81850000	0.03511200
H	5.21768600	-2.38012800	2.12712500
H	4.58786400	-3.05852800	-2.05656200
H	5.75793300	-3.60973600	0.05254600
C	-3.12770000	-0.79528600	-0.00698000
C	-3.39374400	-1.50027600	-1.19351700
C	-3.76483600	-1.09955500	1.20866500
C	-4.35786800	-2.50848100	-1.15039600
C	-4.71527200	-2.12349000	1.19979500
C	-5.01659000	-2.81858100	0.03425000
H	-4.58752300	-3.05815700	-2.05740800
H	-5.21800300	-2.38065000	2.12632300
H	-5.75791800	-3.60983100	0.05140100
C	-2.67012700	-1.17580300	-2.47682000
H	-2.86711100	-0.15493100	-2.81935800
H	-1.58405300	-1.27001400	-2.36462500
H	-2.97467300	-1.85179500	-3.27616600
C	-3.42436500	-0.37875100	2.48978200
H	-2.35002800	-0.40835300	2.69291600
H	-3.72791800	0.67336800	2.47184200
H	-3.93151700	-0.84171900	3.33654700
C	2.67048900	-1.17628400	-2.47666500
H	1.58440900	-1.27061500	-2.36465100
H	2.86741600	-0.15544400	-2.81932900
H	2.97525200	-1.85236100	-3.27585600
C	3.42397700	-0.37813600	2.48987300
H	3.72734900	0.67403000	2.47165100
H	2.34963600	-0.40784800	2.69299100
H	3.93115900	-0.84078100	3.33679600
H	-0.00142600	-1.46076300	1.59134100
Fe	0.00023000	-0.35602800	0.39709100

$^{1/2}$Fe(0)

$^{1/2}$Fe(0)-1

C	-1.20038500	2.47476700	-0.00726300
C	-1.21535600	3.86892200	-0.00597700
C	0.00013900	4.56144000	-0.00496600
C	1.21556600	3.86887800	-0.00594700
C	1.20056100	2.47469800	-0.00722700
N	0.00011100	1.81608700	-0.00722000
H	0.00016500	5.64582600	-0.00391400
H	-2.14917800	4.41790500	-0.00557200

H	2.14942400	4.41780000	-0.00554500
C	-2.31147000	1.54773600	-0.00674900
C	2.31136200	1.54751500	-0.00663500
N	1.95920200	0.26336800	-0.01140200
N	-1.95974600	0.26345800	-0.01145200
C	3.74336900	2.00434800	0.00236100
H	4.29334700	1.60528300	-0.85445300
H	3.82027200	3.09044200	-0.02576600
H	4.26817900	1.65344900	0.89573200
C	-3.74338200	2.00485600	0.00212600
H	-3.82012400	3.09092400	-0.02731000
H	-4.29366700	1.60481100	-0.85402600
H	-4.26797800	1.65515000	0.89610400
C	2.98691900	-0.73317400	0.00314500
C	3.45431200	-1.22393800	1.23488100
C	3.46692900	-1.24581100	-1.21477100
C	4.43945500	-2.21407600	1.22605900
C	4.45234400	-2.23521900	-1.17831300
C	4.94328000	-2.71499200	0.03083000
H	4.80794300	-2.60045700	2.17200000
H	4.83077500	-2.63797700	-2.11342100
H	5.70718200	-3.48592700	0.04171300
C	-2.98737500	-0.73315300	0.00301000
C	-3.46677000	-1.24624800	-1.21495100
C	-3.45501600	-1.22377800	1.23470800
C	-4.45209900	-2.23574100	-1.17860000
C	-4.44006100	-2.21401000	1.22578000
C	-4.94346200	-2.71521800	0.03049000
H	-4.83010500	-2.63881800	-2.11374200
H	-4.80877500	-2.60026400	2.17168400
H	-5.70731200	-3.48620600	0.04129300
C	-2.90790500	-0.76400300	-2.52999400
H	-3.04174600	0.31261500	-2.67291000
H	-1.83229200	-0.95712200	-2.59004700
H	-3.38865200	-1.27255400	-3.36792800
C	-2.88742700	-0.71622000	2.53688400
H	-1.80823600	-0.88897100	2.58777200
H	-3.03868600	0.35945700	2.66962900
H	-3.34912000	-1.22279600	3.38660000
C	2.90875200	-0.76311200	-2.52994500
H	1.83316500	-0.95610200	-2.59066300
H	3.04274600	0.31354100	-2.67244700
H	3.38991900	-1.27141500	-3.36779000

C	2.88666800	-0.71635600	2.53702700
H	3.03864300	0.35919300	2.67005000
H	1.80736000	-0.88834000	2.58764200
H	3.34782800	-1.22342300	3.38674000
Fe	-0.00065000	-0.09731900	-0.02753600
C	0.00247800	-2.10815200	-0.05484700
H	0.00582300	-2.45461000	0.99214600
H	-0.88562300	-2.55749500	-0.51469900
H	0.89011100	-2.55377000	-0.51910600

$^{1/2}$Fe(0)-2

C	-1.19110600	2.46133800	-0.18117800
C	-1.21238600	3.83412000	-0.38899200
C	-0.00277700	4.53595500	-0.47481600
C	1.20384700	3.84431100	-0.37969000
C	1.19986100	2.46344300	-0.17331900
N	0.00197100	1.80316600	-0.02909800
H	-0.00479000	5.60704500	-0.64077400
H	-2.15576700	4.35671600	-0.49896500
H	2.13994100	4.38011300	-0.48312400
C	-2.31899900	1.56485900	-0.16227700
C	2.31371500	1.56375600	-0.14406200
N	1.96941500	0.28128500	-0.01914200
N	-1.99271900	0.28785800	-0.04411000
C	3.73811000	2.02160700	-0.29714500
H	3.81615300	3.10811900	-0.29200300
H	4.37024400	1.63824800	0.50727900
H	4.17420600	1.66002900	-1.23396400
C	-3.72616800	2.08275600	-0.30291800
H	-3.98132800	2.75487500	0.52210400
H	-3.84519600	2.65196200	-1.22956500
H	-4.45187900	1.27189000	-0.31396300
C	2.99548500	-0.71251900	-0.12118800
C	3.68797300	-1.16657300	1.01788200
C	3.27046100	-1.24959400	-1.39590100
C	4.64657400	-2.17150100	0.85675000
C	4.23809900	-2.25033700	-1.50923700
C	4.92295900	-2.71457200	-0.39224100
H	5.18330300	-2.52930500	1.73062700
H	4.45094900	-2.67040100	-2.48804500
H	5.66808000	-3.49715200	-0.49443700
C	-3.00443300	-0.72032700	-0.14412400
C	-3.23867100	-1.29628800	-1.40948300
C	-3.71422100	-1.15403000	0.99127200

C	-4.17542300	-2.32680800	-1.51333800
C	-4.64008100	-2.19069600	0.84013800
C	-4.86967100	-2.78001900	-0.39726100
H	-4.35760400	-2.77814900	-2.48429300
H	-5.18832800	-2.53539600	1.71209900
H	-5.58846200	-3.58767300	-0.49213000
C	-2.51039700	-0.79834700	-2.63314000
H	-2.82458700	0.21505000	-2.90498200
H	-1.43119600	-0.75312400	-2.46911900
H	-2.70401100	-1.44415400	-3.49178400
C	-3.52692500	-0.49922600	2.33724100
H	-2.47537600	-0.37050600	2.58971700
H	-3.98004100	0.49845600	2.36206600
H	-4.00146000	-1.08892400	3.12413100
C	2.53858400	-0.75395000	-2.61864800
H	1.45543100	-0.78846300	-2.47782800
H	2.78468700	0.28791300	-2.84861100
H	2.79318900	-1.35386400	-3.49458200
C	3.43920600	-0.57800100	2.38495600
H	3.77521900	0.46267500	2.44791000
H	2.38121500	-0.57379000	2.64474400
H	3.97876100	-1.13975700	3.15007100
C	-0.02057800	-1.95603900	1.31348400
H	-0.94790000	-2.07650300	1.86051600
H	0.87985400	-2.08694900	1.90075800
C	0.00986200	-2.05660400	-0.06253000
H	0.93765900	-2.27267000	-0.57829700
H	-0.89714700	-2.26366800	-0.61782700
Fe	0.00371600	0.01097300	0.46912600
C	-0.02438300	0.61570000	2.46040700
H	-0.05978400	-0.15327900	3.23615400
H	0.87347500	1.22424800	2.60872600
H	-0.88591100	1.28044300	2.58271400

$^{1/2}$Fe(0)-TS2/3

C	1.18235100	2.49005100	0.13091500
C	1.21889200	3.85642400	0.36010700
C	0.00546400	4.56417700	0.44513800
C	-1.19924300	3.87926600	0.35654900
C	-1.20657000	2.49382000	0.13872100
N	-0.00474400	1.83988900	-0.04868500
H	0.01148500	5.63459300	0.61663600
H	2.16277800	4.37250300	0.48861900
H	-2.13159000	4.41906100	0.47317900

C	2.32767700	1.58736700	0.15254200
C	-2.32190200	1.59757300	0.15942900
N	-1.99984800	0.30194400	0.03618100
N	2.04002800	0.31463700	0.03100300
C	-3.73281000	2.06666100	0.39124200
H	-3.80459000	3.15372000	0.38773600
H	-4.41780500	1.68665300	-0.37051800
H	-4.11444800	1.71082400	1.35436000
C	3.71276900	2.13524700	0.38144400
H	3.97450100	2.86721600	-0.38773000
H	3.76994600	2.64913200	1.34549400
H	4.46340700	1.34802000	0.37493600
C	-3.03576900	-0.67637600	0.14910800
C	-3.80626000	-1.04612900	-0.97090100
C	-3.24418400	-1.29424100	1.39855100
C	-4.78355900	-2.03341000	-0.81490000
C	-4.22835900	-2.27880000	1.50879100
C	-4.99781400	-2.65011400	0.41201500
H	-5.38314700	-2.32008300	-1.67434900
H	-4.39004300	-2.75810900	2.47015900
H	-5.76015700	-3.41622800	0.51265300
C	3.05412600	-0.68438500	0.17941600
C	3.15740800	-1.32980900	1.42838500
C	3.88544000	-1.05232700	-0.89593400
C	4.09913400	-2.34916300	1.58030800
C	4.81499500	-2.07742000	-0.69582100
C	4.92429800	-2.72713800	0.52743400
H	4.18247900	-2.85016100	2.54027600
H	5.46244100	-2.36552500	-1.51893700
H	5.65054300	-3.52259000	0.66019900
C	2.27703100	-0.92273400	2.58243300
H	2.47853500	0.10291800	2.90828400
H	1.21993400	-0.96082500	2.30637400
H	2.43207000	-1.57903200	3.44088400
C	3.79626000	-0.38213400	-2.24563600
H	2.90745000	-0.70221200	-2.79470200
H	3.74360100	0.70635500	-2.17134800
H	4.66731400	-0.63026300	-2.85530700
C	-2.41044200	-0.90850500	2.59368800
H	-1.34740900	-1.07078900	2.39513700
H	-2.52014600	0.15026200	2.84785500
H	-2.69111800	-1.49416800	3.47158500
C	-3.59034100	-0.41737000	-2.32666600

H	-3.49705100	0.66952700	-2.27543700
H	-2.67430600	-0.78471800	-2.79666200
H	-4.42052600	-0.65102800	-2.99665900
C	0.06338800	-1.85285900	-1.71534300
H	1.00096400	-2.13195100	-2.18673800
H	-0.79224300	-2.12306300	-2.32573000
C	-0.05898300	-2.05521700	-0.30050300
H	-0.99849400	-2.45889900	0.06542900
H	0.81935700	-2.43458300	0.21820200
Fe	-0.03870000	-0.02821400	-0.37412200
C	0.14749300	0.00248900	-2.60749700
H	0.13130500	-0.55588100	-3.54238800
H	-0.72973300	0.65431600	-2.60581100
H	1.04990900	0.61360300	-2.59608200

$^{1/2}$Fe(0)- 3

C	-1.24781500	2.69031100	0.09812500
C	-1.25820100	4.09303000	0.18150700
C	-0.05869700	4.79132500	0.21575300
C	1.17014700	4.10373900	0.16531200
C	1.14155100	2.71899400	0.08490900
N	-0.03456800	2.04565600	0.05676500
H	-0.06765400	5.87375100	0.28089400
H	-2.19578400	4.63501300	0.22043100
H	2.10718800	4.64666200	0.18952300
C	-2.34337100	1.77021200	0.04386600
C	2.28420400	1.81004800	0.02068800
N	1.97622600	0.53532400	-0.04805100
N	-1.98621100	0.47537900	-0.04283800
C	3.68437200	2.35691400	0.03300500
H	3.82452300	3.06900800	-0.78545300
H	3.87809300	2.89994300	0.96321900
H	4.42918900	1.57022500	-0.06505600
C	-3.77900500	2.21416900	0.06685200
H	-3.86362300	3.29858300	0.13278000
H	-4.31132100	1.89223500	-0.83357400
H	-4.32187800	1.78568300	0.91452700
C	3.01512900	-0.45192500	-0.10166600
C	3.55418200	-0.94934000	1.09721800
C	3.43312800	-0.93720800	-1.35284000
C	4.52889800	-1.94723100	1.02007900
C	4.41198400	-1.93293600	-1.38228200
C	4.95811500	-2.43848900	-0.20755900
H	4.95010200	-2.34454300	1.93884100

H	4.74337800	-2.31786300	-2.34213900
H	5.71263800	-3.21739300	-0.24879100
C	-3.01219300	-0.51829300	-0.07937200
C	-3.48278800	-0.98254600	-1.32147400
C	-3.50291100	-1.05312800	1.12644300
C	-4.46519500	-1.97551300	-1.33600500
C	-4.48369100	-2.04617200	1.06723900
C	-4.96806600	-2.50517000	-0.15272900
H	-4.83374700	-2.33996300	-2.29072300
H	-4.86654900	-2.46632400	1.99302200
H	-5.72861100	-3.27913500	-0.18125300
C	-2.92524200	-0.43370100	-2.61038700
H	-3.08823100	0.64411800	-2.70710600
H	-1.84415200	-0.59165400	-2.66766900
H	-3.38626400	-0.91907800	-3.47305000
C	-2.97722200	-0.57389100	2.45678800
H	-1.88731500	-0.64653800	2.50249900
H	-3.22661500	0.47484300	2.64805300
H	-3.39166700	-1.16589600	3.27529000
C	2.84931100	-0.39113800	-2.63161400
H	1.75975400	-0.48141700	-2.64393000
H	3.08037000	0.67053400	-2.76719500
H	3.24118500	-0.92709200	-3.49791400
C	3.10412200	-0.41675000	2.43540500
H	3.45996100	0.60465400	2.60930400
H	2.01471400	-0.38919000	2.51449600
H	3.48586200	-1.03722100	3.24811800
C	-0.01810400	-1.88433200	-0.35623300
H	-0.95145900	-2.21021000	-0.83384600
H	0.78749400	-2.12037200	-1.07114700
C	0.19513500	-2.73081700	0.90940700
H	-0.61428200	-2.53854000	1.62560100
H	1.12240100	-2.43696500	1.41695800
C	0.25412700	-4.24293700	0.64307600
H	-0.67067300	-4.59229700	0.17282300
H	1.07944400	-4.48881200	-0.03298800
H	0.39697500	-4.81743600	1.56612400
Fe	-0.03396100	0.11710900	-0.08972600

$^{1/2}$Fe(0)- 4

C	1.19748800	2.61239300	-0.30122500
C	1.20174000	3.97721900	-0.62829000
C	0.00302100	4.64857000	-0.81648100
C	-1.21153800	3.94800100	-0.69387700

C	-1.17905000	2.60367400	-0.35751000
N	-0.00132000	1.95721800	-0.13598200
H	0.00037700	5.70153800	-1.07431200
H	2.14197700	4.50327100	-0.74816800
H	-2.15335400	4.45232700	-0.87302100
C	2.32504200	1.73992300	-0.17921800
C	-2.33513300	1.71399500	-0.26698800
N	-2.06802800	0.47511500	0.04929200
N	2.02248200	0.46735200	0.09944000
C	-3.70966800	2.24275900	-0.58458200
H	-3.93504000	3.11848300	0.02996500
H	-3.77264800	2.56091200	-1.62954200
H	-4.47964900	1.49394300	-0.41159400
C	3.72260200	2.24105100	-0.43652800
H	3.93304500	2.32266200	-1.50932200
H	3.87090500	3.23344800	-0.00430400
H	4.47170000	1.57566800	-0.01015800
C	-3.10569000	-0.51278200	-0.01938300
C	-3.36430800	-1.12611200	-1.26040600
C	-3.82755200	-0.87614600	1.13229200
C	-4.31414400	-2.14905500	-1.31387500
C	-4.77430200	-1.89816500	1.02938300
C	-5.01065600	-2.54409800	-0.17858100
H	-4.50787800	-2.63705600	-2.26459800
H	-5.33432200	-2.18618000	1.91423200
H	-5.74129700	-3.34442100	-0.23612600
C	3.05970300	-0.51466200	-0.01916700
C	3.81203700	-0.93053900	1.09366900
C	3.31159800	-1.06553500	-1.29606900
C	4.76229800	-1.94390500	0.92373700
C	4.26450300	-2.07644700	-1.41887200
C	4.98211300	-2.52739200	-0.31538400
H	5.34157100	-2.26847500	1.78428500
H	4.44755300	-2.51222400	-2.39696800
H	5.71692600	-3.31852500	-0.42637300
C	3.68176400	-0.28570700	2.45421700
H	4.65669100	0.06791500	2.80443200
H	3.00550300	0.56679500	2.44498100
H	3.31945600	-0.99659200	3.20325000
C	2.60206500	-0.55186800	-2.52615100
H	1.54029100	-0.37941100	-2.34606300
H	3.02598400	0.40089300	-2.86315200
H	2.69798400	-1.25828900	-3.35321300

C	-3.63733200	-0.15587900	2.44382500
H	-2.62903100	-0.27979900	2.84036900
H	-3.80812600	0.92081400	2.34511500
H	-4.33577500	-0.53047600	3.19434200
C	-2.67901600	-0.66706500	-2.52496200
H	-3.14191100	0.24513400	-2.91942300
H	-1.62299200	-0.44542600	-2.36701500
H	-2.75208000	-1.42754400	-3.30456100
C	0.03133200	-1.92601400	0.49410800
H	0.88666700	-2.30105000	1.07331800
H	-0.86584100	-2.27265400	1.02979500
C	0.05196900	-2.64023000	-0.86656600
H	0.95700700	-2.37673900	-1.42199100
H	-0.79174500	-2.31947000	-1.48719800
C	-0.00355000	-4.17221600	-0.74826500
H	0.84728300	-4.55021600	-0.17215800
H	-0.91603300	-4.49372600	-0.23548800
H	0.01640100	-4.66044900	-1.73034000
C	0.12687200	-0.25942500	2.64599400
H	1.11278800	-0.66443900	2.81493900
H	-0.68701200	-0.94204700	2.85039700
C	-0.08426800	1.08347700	2.50214500
H	-1.07323800	1.51984200	2.57581900
H	0.73927100	1.78884200	2.51261700
Fe	0.02873100	0.13338500	0.47984700

$^{1/2}$Fe(0)-TS4/5

C	1.23140700	2.55638000	-0.30320000
C	1.26945600	3.92495400	-0.53384900
C	0.07525800	4.64983800	-0.62545400
C	-1.13717200	3.97983600	-0.47991900
C	-1.15971200	2.60353900	-0.25184800
N	0.02854100	1.89188100	-0.16777100
H	0.09384600	5.71831000	-0.80667500
H	2.22210000	4.42992600	-0.64565300
H	-2.06739100	4.53130400	-0.55036500
C	2.36396900	1.67920700	-0.21497100
C	-2.30396900	1.76401700	-0.11948800
N	-2.01870900	0.47702600	0.09710000
N	2.06732100	0.41009000	0.01928900
C	-3.70674500	2.28763100	-0.28187300
H	-3.76201500	3.35522900	-0.06849200
H	-4.07832300	2.13957300	-1.30219500
H	-4.40481400	1.77816900	0.38399500

C	3.76028800	2.20872300	-0.42600800
H	3.89388000	2.56685600	-1.45191100
H	3.96432800	3.05437400	0.23637900
H	4.51476100	1.44710300	-0.23999600
C	-3.10365500	-0.45722600	0.04704700
C	-3.49764900	-0.98160200	-1.20246100
C	-3.76365600	-0.86382700	1.22609500
C	-4.50336700	-1.95206200	-1.24274200
C	-4.77020400	-1.82875100	1.13780600
C	-5.13399900	-2.38435900	-0.08342300
H	-4.79723000	-2.36506300	-2.20392200
H	-5.28000900	-2.14059100	2.04505600
H	-5.91314700	-3.13851000	-0.13144400
C	3.12609800	-0.55689000	-0.00791600
C	3.83026000	-0.90333200	1.16464600
C	3.45963800	-1.16027100	-1.24013300
C	4.78226000	-1.92573300	1.09717800
C	4.41304000	-2.18123900	-1.25841600
C	5.05986200	-2.58141600	-0.09578300
H	5.32369000	-2.19704700	1.99913100
H	4.65571400	-2.65753600	-2.20420300
H	5.79577600	-3.37866900	-0.12399400
C	3.65088800	-0.15849300	2.46756100
H	4.53899600	-0.27590800	3.09234800
H	3.49421700	0.90985900	2.31002500
H	2.79886300	-0.51745000	3.04842100
C	2.86343600	-0.67909600	-2.54220000
H	1.84033400	-0.32530700	-2.42597300
H	3.44509800	0.15656900	-2.94853500
H	2.87306700	-1.47091600	-3.29468800
C	-3.43575900	-0.25815900	2.56924400
H	-2.52482700	-0.68035300	2.99936000
H	-3.27980800	0.82042000	2.50573100
H	-4.24554600	-0.44067900	3.27909300
C	-2.89651400	-0.49240700	-2.49925000
H	-3.49000100	0.32651900	-2.92201400
H	-1.88373100	-0.11400400	-2.36948600
H	-2.87591400	-1.28851100	-3.24717000
C	-0.27957600	-2.07218400	0.52507000
H	0.21230600	-2.90971900	1.01926500
H	-1.35297400	-2.20665100	0.64789400
C	0.10531000	-2.15398200	-0.95996900
H	1.18700500	-2.24035600	-1.05319500

H	-0.18672100	-1.25560600	-1.52474700
C	-0.55455300	-3.36831100	-1.63682100
H	-0.24776800	-4.29741500	-1.14693100
H	-1.64420700	-3.31063900	-1.58670700
H	-0.26525600	-3.43666700	-2.69063100
C	0.18324200	-1.04746800	2.20488800
H	1.15386000	-1.50620200	2.34978300
H	-0.60158800	-1.62896100	2.67946000
C	0.11235600	0.38527100	2.31029900
H	-0.79109600	0.82724000	2.71842900
H	1.01657000	0.92715400	2.56765400
Fe	-0.00436700	0.12098600	0.34430400

$^{1/2}$Fe(0)-5

C	-1.59245500	2.86757200	0.36872700
C	-1.76197500	4.23649900	0.62943100
C	-0.64693500	5.05680600	0.74612400
C	0.64950500	4.52303300	0.60290100
C	0.77576200	3.16466600	0.34712100
N	-0.31825800	2.37188700	0.23826500
H	-0.77381700	6.11469100	0.94805800
H	-2.75753700	4.65211800	0.73928600
H	1.52042600	5.16113600	0.69189100
C	-2.58732000	1.85340400	0.20485800
C	2.00889100	2.40285800	0.16349100
N	1.83841800	1.12023900	-0.06365400
N	-2.10014400	0.62525300	-0.05296500
C	3.34215700	3.09300800	0.23962500
H	3.37909700	3.93264800	-0.46026100
H	3.50646700	3.50563400	1.24003900
H	4.16392700	2.41797800	0.01038700
C	-4.05195600	2.18325100	0.30176700
H	-4.29184100	2.65741400	1.25932700
H	-4.35357100	2.88454100	-0.48447100
H	-4.67172000	1.29361000	0.20564400
C	2.97584000	0.26581300	-0.24171400
C	3.58871800	-0.30835700	0.88533100
C	3.41853800	-0.01987700	-1.54481000
C	4.66461600	-1.17634400	0.68253800
C	4.49939100	-0.89067700	-1.70007200
C	5.12054000	-1.46811700	-0.59801900
H	5.14460400	-1.63086000	1.54419400
H	4.85152900	-1.12035700	-2.70136100
H	5.95486600	-2.14800000	-0.73728000

C	-2.99877800	-0.47298600	-0.21461400
C	-3.40413600	-0.85008000	-1.50826300
C	-3.42877600	-1.19181200	0.91656400
C	-4.24910300	-1.95322800	-1.64989800
C	-4.27192700	-2.29014800	0.73068600
C	-4.68296100	-2.67240100	-0.54153300
H	-4.56594200	-2.25124500	-2.64533200
H	-4.60609600	-2.85227400	1.59819900
H	-5.33572100	-3.53025600	-0.66901200
C	-2.92986100	-0.08413800	-2.71682400
H	-3.23707600	0.96561100	-2.68375900
H	-1.83768200	-0.08891700	-2.78095300
H	-3.32674500	-0.51980900	-3.63605300
C	-2.99504100	-0.78369100	2.30225700
H	-1.90869900	-0.68034000	2.36621400
H	-3.41857000	0.18262600	2.59542800
H	-3.31163600	-1.52063600	3.04311600
C	2.75211000	0.60459100	-2.74486100
H	1.67812800	0.39980900	-2.75653100
H	2.86686900	1.69347300	-2.75729100
H	3.17865400	0.21743900	-3.67195200
C	3.10769100	0.00535800	2.28073300
H	3.35120400	1.03154600	2.57704000
H	2.02365100	-0.09989200	2.36815500
H	3.57088600	-0.66208100	3.00958500
C	0.11660500	-1.45234100	-0.64560400
H	-0.77331900	-1.81767800	-1.17414900
H	0.94809100	-1.51828900	-1.36615200
C	0.40841700	-2.40743600	0.52359100
H	-0.42171400	-2.37889700	1.24280300
H	1.29812000	-2.07863800	1.07732700
C	0.62670600	-3.87041300	0.10109200
H	-0.25356600	-4.21325200	-0.45848300
H	1.46787600	-3.91577500	-0.60328400
C	0.88995400	-4.82700500	1.26934100
H	1.76737300	-4.48104700	1.83106300
H	0.04763800	-4.78115000	1.97168300
C	1.10724800	-6.27823600	0.83270100
H	1.28898700	-6.93644100	1.68805800
H	0.23449700	-6.66674400	0.29786900
H	1.96692100	-6.36672600	0.16047700
Fe	-0.11590200	0.49115100	-0.14873300

$^{1/2}$Fe(0)-6

C	-1.05787400	2.68836000	-0.23919500
C	-1.01229400	4.07392500	-0.44785200
C	0.21138000	4.71764600	-0.55496600
C	1.39611800	3.96321500	-0.47561800
C	1.31355400	2.59684300	-0.25882300
N	0.10984000	1.97307100	-0.11032600
H	0.25645000	5.78848800	-0.71731200
H	-1.93429900	4.63807600	-0.53224500
H	2.35835800	4.44664300	-0.59359900
C	-2.22596200	1.86276400	-0.19167600
C	2.44607500	1.67345600	-0.22079600
N	2.14478600	0.41983600	-0.02017500
N	-1.98697600	0.56537100	0.00082100
C	3.84032300	2.19871300	-0.44952400
H	3.91196300	2.69631300	-1.42078900
H	4.10274000	2.94101300	0.30987400
H	4.58098200	1.40288500	-0.41934700
C	-3.59231600	2.46334000	-0.40591700
H	-3.82184700	3.21025800	0.36111500
H	-3.65551300	2.97086400	-1.37393600
H	-4.37390300	1.70676500	-0.37752900
C	3.17523100	-0.57664900	-0.07438100
C	3.90386300	-0.92509800	1.07807800
C	3.41432700	-1.21973400	-1.30476600
C	4.84844600	-1.95141300	0.98193800
C	4.36700200	-2.23928200	-1.35237200
C	5.07669100	-2.61392100	-0.21765300
H	5.41420700	-2.22756600	1.86694600
H	4.55078800	-2.74328600	-2.29654600
H	5.81001700	-3.41218900	-0.26980300
C	-3.08751500	-0.34886900	-0.06680600
C	-3.39431400	-0.94898900	-1.30435400
C	-3.84406400	-0.64939100	1.08290900
C	-4.41128700	-1.90499700	-1.35395800
C	-4.85418400	-1.61066800	0.98701700
C	-5.13049300	-2.24974200	-0.21572600
H	-4.64074600	-2.38104700	-2.30294500
H	-5.43429400	-1.85371000	1.87266400
H	-5.91200600	-3.00102500	-0.26865800
C	-2.68224800	-0.53869300	-2.56975200
H	-2.99393800	0.46034300	-2.89532900
H	-1.60089000	-0.50305000	-2.43765500

H	-2.90524000	-1.23107400	-3.38404700
C	-3.62816400	0.07897100	2.38743000
H	-2.61157100	-0.02796100	2.76597100
H	-3.81231200	1.15317900	2.28411300
H	-4.30891300	-0.29604500	3.15423900
C	2.67980300	-0.80565300	-2.55523200
H	1.59791300	-0.85463000	-2.42011700
H	2.91970100	0.22250300	-2.84665900
H	2.94511300	-1.45403900	-3.39227700
C	3.71237800	-0.21093100	2.39418300
H	3.76410200	0.87596700	2.28658100
H	2.74622700	-0.43868200	2.84880200
H	4.48579200	-0.50652300	3.10557500
C	0.01005700	-1.86708100	-0.26111300
H	-0.24501700	-1.74354400	-1.33036300
H	1.05940300	-2.19018200	-0.24441000
C	-0.83665600	-3.01418200	0.29612200
H	-1.88817100	-2.72209900	0.37516900
H	-0.51349600	-3.24812600	1.31861500
C	-0.74901600	-4.30408000	-0.53360700
H	-1.11624400	-4.14361700	-1.55289200
H	0.28561500	-4.65520600	-0.61167200
H	-1.34307200	-5.11314100	-0.09290500
C	-0.01305800	-0.74477400	2.24263900
H	-0.96836500	-1.23313500	2.37714000
H	0.84225400	-1.40688500	2.31221200
C	0.13137100	0.62114300	2.38274100
H	1.09728800	1.07983000	2.55352800
H	-0.72184200	1.26155100	2.57660000
Fe	0.00600700	0.09764400	0.29407100

$^{1/2}$Fe(0)-TS6/7

C	-1.07185100	2.72080800	-0.13729800
C	-1.06297200	4.10860800	-0.24037600
C	0.15084700	4.79573400	-0.29691700
C	1.33989000	4.06626200	-0.25065200
C	1.30011000	2.67957800	-0.14728000
N	0.10058200	1.99823000	-0.08798500
H	0.16943400	5.87644200	-0.37660800
H	-1.99870000	4.65453000	-0.27691700
H	2.29499800	4.57735100	-0.29519200
C	-2.23964400	1.88241200	-0.07533200
C	2.43227300	1.79561800	-0.09104000
N	2.11629700	0.51834600	0.00172600

N	-1.99385700	0.58946800	0.01816100
C	3.83598400	2.33965100	-0.13852200
H	4.00570100	2.90535800	-1.05984100
H	4.01924600	3.02371900	0.69587500
H	4.57820100	1.54563600	-0.09029300
C	-3.61312700	2.50362500	-0.12618100
H	-4.40165500	1.75631600	-0.07688500
H	-3.75716800	3.20137600	0.70435200
H	-3.74785400	3.07515000	-1.04951800
C	3.16996200	-0.45083200	0.07125000
C	3.68795700	-0.82583800	1.32715900
C	3.66811100	-1.02630200	-1.11416700
C	4.64231000	-1.84509700	1.37934200
C	4.62352800	-2.04147500	-1.01388700
C	5.09860400	-2.46452500	0.22167700
H	5.03520400	-2.14825500	2.34579600
H	5.00129700	-2.49921600	-1.92392400
H	5.83235700	-3.26220600	0.28133700
C	-3.12255700	-0.29623800	0.07314700
C	-3.67305400	-0.79860900	-1.12147900
C	-3.68186200	-0.63784600	1.31991800
C	-4.73186900	-1.70774800	-1.04235700
C	-4.74079300	-1.54877500	1.35317900
C	-5.25683700	-2.09641900	0.18412500
H	-5.15075500	-2.10835000	-1.96120200
H	-5.16762600	-1.82417400	2.31334500
H	-6.07436800	-2.80897400	0.22833700
C	-3.19050600	-0.32459600	-2.47051000
H	-3.63558200	0.64398800	-2.72671300
H	-2.11014000	-0.19165000	-2.49904800
H	-3.47337400	-1.02703800	-3.25729800
C	-3.20378500	0.00658100	2.59774900
H	-3.60379100	-0.51388100	3.47020600
H	-2.11716200	0.01745400	2.67457300
H	-3.53356200	1.04964400	2.66175200
C	3.26076000	-0.51862000	-2.47736100
H	3.93122500	0.28482300	-2.80588400
H	3.32092500	-1.31219300	-3.22547800
H	2.24847300	-0.11903200	-2.48735100
C	3.30332500	-0.09801500	2.59390400
H	3.95448400	0.77017100	2.75218400
H	2.27887100	0.26920800	2.56975800
H	3.41336300	-0.74530600	3.46671600

C	0.12953900	-1.52264100	-1.27099200
H	-0.19430400	-0.89627800	-2.11302000
H	1.17542200	-1.80187700	-1.38557600
C	-0.72599500	-2.67439800	-1.04878100
H	-1.75682300	-2.57890600	-1.38812900
H	-0.94054400	-2.66366000	0.25956000
C	-0.16654200	-4.07296000	-1.23478900
H	-0.02439600	-4.29155600	-2.29983600
H	0.80989800	-4.17474000	-0.75174600
H	-0.83175100	-4.84112200	-0.82694600
C	-0.71071700	-2.45429700	1.56151100
H	-1.73167100	-2.36966500	1.92506500
H	-0.27744900	-3.43391300	1.77032900
C	0.14943400	-1.30154500	1.61845800
H	1.19737500	-1.54716300	1.76089300
H	-0.17903400	-0.52024900	2.31528200
Fe	0.08757400	0.12051200	0.04376000

$^{1/2}$Fe(0)- 7

C	-1.25796700	2.52191400	-0.11554800
C	-1.30736500	3.90526500	-0.23263900
C	-0.11549600	4.63567000	-0.31209600
C	1.10179100	3.95660600	-0.31194400
C	1.12169200	2.56650800	-0.19406200
N	-0.05329600	1.87151000	-0.03627900
H	-0.14043300	5.71512800	-0.40627800
H	-2.26289200	4.41464800	-0.28235500
H	2.02926600	4.50761500	-0.41447100
C	-2.38369100	1.62056200	-0.15327500
C	2.26292900	1.70372100	-0.28334600
N	1.97079400	0.40692500	-0.23753500
N	-2.05870000	0.34203300	-0.15401700
C	3.65520100	2.25660900	-0.43773900
H	4.32983200	1.52346500	-0.87815100
H	3.66203500	3.14343400	-1.07400100
H	4.07728800	2.54877500	0.53030200
C	-3.79163900	2.15099600	-0.24309000
H	-4.00967500	2.82887400	0.58690600
H	-3.94012400	2.71652700	-1.16832800
H	-4.52400600	1.34655700	-0.22577700
C	3.02383900	-0.54313800	-0.42236400
C	3.84774900	-0.93193000	0.65085900
C	3.20268600	-1.09592300	-1.70746400
C	4.83122400	-1.89857500	0.42116000

C	4.19711200	-2.05933700	-1.89102100
C	5.00597400	-2.46595000	-0.83539300
H	5.46487400	-2.20969500	1.24687700
H	4.33740400	-2.49150300	-2.87764900
H	5.77050400	-3.22023300	-0.99244800
C	-3.07413000	-0.64709300	-0.34820900
C	-3.31584800	-1.09805300	-1.66228000
C	-3.78433900	-1.18577200	0.74171300
C	-4.25507300	-2.11254400	-1.86086200
C	-4.71328500	-2.20072100	0.49590600
C	-4.94724700	-2.66921100	-0.79155700
H	-4.44192000	-2.46786400	-2.87010700
H	-5.26119700	-2.62438300	1.33262100
H	-5.66820600	-3.46253600	-0.96127100
C	-2.59906800	-0.48142400	-2.83834200
H	-2.93503500	0.54492300	-3.02159300
H	-1.52028500	-0.42772600	-2.67521700
H	-2.78235900	-1.05395700	-3.74965100
C	-3.59080000	-0.65744500	2.14041900
H	-4.04029400	0.33513700	2.25858400
H	-4.06053200	-1.31555300	2.87403600
H	-2.53752900	-0.55342000	2.39540200
C	2.37155900	-0.62553000	-2.87521400
H	1.30915500	-0.58869300	-2.62713800
H	2.65252300	0.38806300	-3.18202200
H	2.50597200	-1.27956900	-3.73920600
C	3.70253900	-0.31521400	2.01985800
H	4.23404300	0.64104500	2.08386900
H	2.66033100	-0.12017700	2.26907600
H	4.12431200	-0.96806500	2.78691200
C	-0.05009000	-1.95708000	-0.39134600
H	-0.95156700	-1.95942700	-0.99027800
H	0.86715000	-2.19677200	-0.91921300
C	-0.10221300	-2.11143900	0.97776700
H	-1.07933800	-2.15305900	1.45043300
H	-0.74248200	-1.09780300	3.64947700
C	1.00958100	-2.77943400	1.74676200
H	0.77513300	-3.84703000	1.85376300
H	1.96265500	-2.71306500	1.22145800
H	1.13993700	-2.38413400	2.75229400
C	-0.04780200	-0.25144500	3.67379100
H	-0.31624600	0.34459900	4.55851500
H	0.94405500	-0.66425400	3.87820400

C	-0.07366500	0.59600700	2.40233300
H	0.73297700	1.33918200	2.45743300
H	-0.99837100	1.18741800	2.38464600
Fe	0.00294200	0.03733200	0.35778800

$^{1/2}$Fe(0)- 8

C	-1.17222700	2.56372500	0.01841700
C	-1.21328700	3.95004900	0.05848600
C	0.00951300	4.64957300	0.08592900
C	1.21526400	3.96131000	0.07148400
C	1.21743200	2.55663700	0.02945400
N	0.00981600	1.90072400	0.00604900
H	0.00898300	5.73350600	0.11923100
H	-2.15517600	4.48507400	0.07014700
H	2.14781600	4.51283500	0.09531100
C	-2.30640300	1.64268100	-0.01262500
C	2.32078300	1.64457300	0.00717700
N	1.97529800	0.34406600	-0.03670100
N	-1.98646000	0.36900900	-0.04172500
C	3.75245800	2.10143700	0.02213700
H	3.82760800	3.18851800	0.03183300
H	4.28889400	1.72283400	0.89739000
H	4.29766300	1.73695600	-0.85371900
C	-3.71161000	2.17627100	-0.00963600
H	-3.90884100	2.73612700	0.90990500
H	-3.85999000	2.87004300	-0.84214900
H	-4.44880000	1.38043500	-0.08998500
C	3.01005400	-0.64089000	-0.03909400
C	3.49774900	-1.13664500	1.18444100
C	3.49122800	-1.13794400	-1.26447500
C	4.48785900	-2.12179900	1.16000300
C	4.48264500	-2.12184100	-1.24430200
C	4.98367400	-2.61157300	-0.04320800
H	4.86843500	-2.51173400	2.09985700
H	4.85942500	-2.51134600	-2.18584400
H	5.75133500	-3.37902500	-0.04484800
C	-3.01609800	-0.62861300	-0.06148100
C	-3.43153800	-1.15722100	-1.29587900
C	-3.54941900	-1.09180700	1.15340900
C	-4.40222500	-2.16114400	-1.29202500
C	-4.51583000	-2.09977300	1.10979600
C	-4.94260500	-2.63331100	-0.10078500
H	-4.73146400	-2.57949400	-2.23855200
H	-4.93231000	-2.47109800	2.04153000

H	-5.69054500	-3.41949900	-0.11596200
C	-2.85341400	-0.64681700	-2.59184700
H	-3.10002000	0.40608100	-2.76412100
H	-1.76260500	-0.72066300	-2.59890500
H	-3.23540800	-1.21791600	-3.43992600
C	-3.10308000	-0.51235600	2.47331000
H	-2.01497000	-0.43766400	2.53556800
H	-3.49965800	0.49686000	2.63084700
H	-3.44783400	-1.12994100	3.30461500
C	2.93449700	-0.63463900	-2.57226100
H	1.85630800	-0.81075500	-2.63219100
H	3.08136300	0.44230400	-2.69938000
H	3.40870500	-1.13764700	-3.41755100
C	2.95677700	-0.62591300	2.49682300
H	3.20273500	0.42747400	2.66602100
H	1.86647100	-0.69879900	2.53109500
H	3.36236100	-1.19752100	3.33408700
C	0.03049100	-2.04052000	-0.26652500
H	-0.76044700	-2.30962100	-0.98445800
H	0.97345300	-2.37656500	-0.71410200
C	-0.19891400	-2.83189400	1.03271100
H	-1.14592100	-2.57520000	1.51889600
H	0.59979100	-2.65545700	1.76170700
H	-0.22696100	-3.91725600	0.86118300
Fe	0.02640000	-0.03260700	-0.07451900

$^{1/2}$Fe(0)- TS3/9

C	1.14556200	2.57139800	0.00522100
C	1.14749500	3.96442600	0.00843600
C	-0.06356900	4.65774900	-0.03115500
C	-1.26483600	3.94119100	-0.04224200
C	-1.23424900	2.55092100	-0.04365100
N	-0.03802900	1.87540300	-0.05956800
H	-0.07360400	5.74171900	-0.03210000
H	2.08506500	4.50734600	0.04545200
H	-2.21312300	4.46640600	-0.04231000
C	2.28214900	1.69477700	0.08963100
C	-2.36216200	1.65359900	0.00616300
N	-2.03498600	0.37476900	0.04819300
N	1.97463600	0.40530600	0.09166500
C	-3.77053400	2.18435900	0.02013200
H	-3.88799400	2.96317100	0.77855200
H	-4.03070000	2.63440000	-0.94400300
H	-4.49480200	1.39876100	0.22762900

C	3.67790600	2.25054400	0.18755300
H	4.00111900	2.68494900	-0.76497600
H	3.72910700	3.04633900	0.93537100
H	4.39940200	1.48343800	0.46322400
C	-3.06814700	-0.61175600	0.11143500
C	-3.69126400	-1.05783400	-1.06955600
C	-3.41445700	-1.15394900	1.36464000
C	-4.65017900	-2.07084800	-0.97461300
C	-4.38169000	-2.15994000	1.41265200
C	-4.99448800	-2.62344200	0.25309600
H	-5.13089300	-2.42696100	-1.88138100
H	-4.65462400	-2.58375800	2.37476500
H	-5.73829900	-3.41202600	0.30715900
C	3.03340600	-0.55270400	0.16739400
C	3.31776100	-1.15683900	1.40797800
C	3.75647300	-0.89951200	-0.98944900
C	4.31860100	-2.12907100	1.46410200
C	4.74848100	-1.87941300	-0.88753500
C	5.02884500	-2.49636000	0.32575400
H	4.54272000	-2.60078100	2.41652000
H	5.30463900	-2.15961100	-1.77774700
H	5.79943400	-3.25843900	0.38549600
C	2.58436500	-0.73776100	2.65726800
H	2.80010700	0.30323300	2.91982900
H	1.50178200	-0.80960300	2.52808300
H	2.87254200	-1.36039200	3.50673700
C	3.49052300	-0.22509900	-2.31370400
H	2.43018000	-0.01176100	-2.45413100
H	4.02377500	0.72922200	-2.38963000
H	3.83041800	-0.84931800	-3.14292600
C	-2.78417300	-0.63373000	2.63270900
H	-1.69363900	-0.62711100	2.56768000
H	-3.09059900	0.39694600	2.84095700
H	-3.07342200	-1.24356900	3.49090100
C	-3.36422700	-0.44564500	-2.41057700
H	-3.91795200	0.48709600	-2.56840500
H	-2.30429400	-0.20414900	-2.50157800
H	-3.63713800	-1.12194900	-3.22358300
C	-0.01469800	-2.02019400	0.39832400
H	0.93855700	-2.39054400	0.76548700
H	-0.86741100	-2.23815800	1.03455200
C	-0.21657300	-1.95772400	-0.99750500
H	-0.06690900	-0.41816500	-1.55162900

H	-1.24745700	-2.03364100	-1.33046100
C	0.75655000	-2.57948200	-1.97765300
H	1.78956900	-2.48143000	-1.64599900
H	0.53823800	-3.65116000	-2.05357800
H	0.67076000	-2.15046900	-2.97984800
Fe	-0.02012000	0.00521800	-0.05827800

$^{1/2}$Fe(0)-9

C	1.14655800	2.57287200	-0.02507900
C	1.15212200	3.96407300	-0.06984400
C	-0.06055000	4.65663200	-0.12341000
C	-1.26042100	3.94108200	-0.11955800
C	-1.23034400	2.55008800	-0.07279700
N	-0.03490700	1.87836800	-0.03862500
H	-0.07008700	5.73999900	-0.16112300
H	2.09060200	4.50642200	-0.06495500
H	-2.20902600	4.46492700	-0.15061900
C	2.28810900	1.69620000	0.04660200
C	-2.35823500	1.65496900	-0.03051500
N	-2.03266600	0.37457400	0.02441400
N	1.98357700	0.41006500	0.07135500
C	-3.76489800	2.19059900	-0.04325100
H	-3.92146300	2.90577400	0.76999100
H	-3.97369200	2.72000100	-0.97882600
H	-4.50041200	1.39547200	0.06148000
C	3.68510500	2.25571500	0.08431200
H	3.76744000	3.05399800	0.82684900
H	4.42065900	1.49109100	0.32694900
H	3.96184100	2.68851100	-0.88340200
C	-3.07546600	-0.60274200	0.09100900
C	-3.62414100	-1.11718500	-1.10026000
C	-3.50749300	-1.06646300	1.34813900
C	-4.59257100	-2.12015800	-1.00861600
C	-4.47718100	-2.07182700	1.39211600
C	-5.01576900	-2.60191700	0.22530800
H	-5.01675300	-2.52714000	-1.92209500
H	-4.81270300	-2.43918100	2.35778600
H	-5.76359100	-3.38687600	0.27722900
C	3.04891400	-0.54303500	0.13276800
C	3.44493200	-1.05071800	1.38511900
C	3.66678600	-0.97695600	-1.05505200
C	4.44780000	-2.02281500	1.42515500
C	4.66658200	-1.94965300	-0.96787900
C	5.05428800	-2.47682000	0.25896900

H	4.75582800	-2.42392400	2.38650200
H	5.14349800	-2.29674400	-1.88011600
H	5.82823900	-3.23632000	0.30663200
C	2.83298400	-0.52832200	2.66153500
H	3.15478300	0.49808800	2.86902700
H	1.74227300	-0.50675700	2.60936900
H	3.12533000	-1.14290000	3.51541000
C	3.27665200	-0.39717700	-2.39210900
H	2.19741200	-0.25669400	-2.46721100
H	3.73950200	0.58358800	-2.55154200
H	3.60460800	-1.04511600	-3.20782200
C	-2.98094700	-0.46193000	2.62743000
H	-1.90170500	-0.30234700	2.59424100
H	-3.43418300	0.51684500	2.82151800
H	-3.20800700	-1.10048900	3.48363500
C	-3.19599800	-0.58436600	-2.44546100
H	-3.65848300	0.38746200	-2.65349500
H	-2.11578900	-0.43486600	-2.49348100
H	-3.49529700	-1.26350700	-3.24665500
C	0.04749300	-1.98420700	0.72646400
H	1.04068800	-2.22726700	1.08919700
H	-0.73664500	-1.94450000	1.47659400
C	-0.26777800	-2.16576800	-0.59781600
H	0.00246100	-0.06158100	-1.58140700
H	-1.31586100	-2.18461300	-0.87267900
C	0.65116100	-2.78500600	-1.61419800
H	1.69941800	-2.71961900	-1.32306000
H	0.40521500	-3.85039600	-1.71748200
H	0.53461800	-2.32973000	-2.60016400
Fe	-0.01842000	0.00909100	-0.07118400

$^{1/2}$Fe(0)-10

C	-1.19400700	2.40081300	0.06691000
C	-1.19496400	3.79911800	0.06931300
C	0.01259400	4.48737000	-0.04114600
C	1.22700900	3.78303600	-0.14191500
C	1.19397600	2.39696500	-0.12709400
N	0.00419400	1.74026900	-0.03352800
H	0.01676900	5.57142800	-0.04483100
H	-2.12377400	4.35162900	0.15190800
H	2.16549000	4.31942800	-0.22067500
C	-2.30304500	1.48351800	0.13747500
C	2.31921700	1.46932700	-0.16772600
N	1.98951200	0.19794800	-0.07800800

N	-1.96248700	0.19514400	0.06922900
C	3.72785300	1.98056700	-0.28523500
H	3.81303000	2.68897700	-1.11344500
H	4.02750100	2.51278700	0.62353300
H	4.43558300	1.17051300	-0.45023300
C	-3.72697100	1.95110800	0.24901900
H	-4.24868000	1.88272600	-0.71186100
H	-4.28911100	1.33504300	0.95354300
H	-3.78404900	2.98720000	0.58323300
C	2.99145400	-0.82467000	-0.04376200
C	3.62286500	-1.13561600	1.17291900
C	3.26731000	-1.54488600	-1.21871500
C	4.56396000	-2.16789400	1.18460800
C	4.21913100	-2.56445500	-1.16238000
C	4.86884800	-2.87540400	0.02734300
H	5.05550200	-2.42220100	2.11918900
H	4.44301500	-3.12674700	-2.06416600
H	5.60173900	-3.67542900	0.05505900
C	-2.97924900	-0.81018100	0.06272900
C	-3.57151900	-1.18877000	-1.15525700
C	-3.32599400	-1.44386300	1.26920000
C	-4.54416500	-2.19107300	-1.13854000
C	-4.30531300	-2.43887600	1.24141300
C	-4.91800600	-2.80968400	0.04935100
H	-5.00566300	-2.49418500	-2.07409100
H	-4.58147800	-2.93359100	2.16822000
H	-5.67505000	-3.58756200	0.04421500
C	-3.13686800	-0.56284200	-2.45699900
H	-3.35450100	0.50892200	-2.50233800
H	-2.05740800	-0.66892300	-2.59913100
H	-3.63957800	-1.03624600	-3.30271600
C	-2.62960300	-1.08015300	2.55498500
H	-1.55414600	-1.26984200	2.47498900
H	-2.74566000	-0.02179500	2.80806500
H	-3.01739600	-1.66772800	3.38961800
C	2.52897400	-1.24295700	-2.49654800
H	1.45337200	-1.40236600	-2.36362100
H	2.66093500	-0.20558100	-2.81900700
H	2.86891900	-1.89034200	-3.30714700
C	3.27485000	-0.39934000	2.44288900
H	3.62172700	0.63941300	2.43102700
H	2.19324100	-0.37083300	2.59994500
H	3.73059100	-0.88368400	3.30845800

H	-0.00781700	-1.75509100	0.02271900
Fe	-0.00583300	-0.16601500	-0.01620500

$^{3/2}$Fe(0)

$^{3/2}$Fe(0)-1

C	-1.18882700	2.46786100	0.00001100
C	-1.20111200	3.85871700	0.00001900
C	0.01540900	4.55588100	0.00001300
C	1.22939000	3.86289700	0.00000300
C	1.21099900	2.46745400	-0.00000400
N	0.01402600	1.81080000	-0.00000700
H	0.01287900	5.64001300	0.00001900
H	-2.13398400	4.40960100	0.00003000
H	2.16409000	4.41043200	0.00000300
C	-2.31038600	1.55250400	0.00001800
C	2.32184400	1.54714300	-0.00000500
N	1.97039500	0.26350200	-0.00000100
N	-1.98869400	0.25968600	0.00001300
C	3.75475800	2.00129300	-0.00001300
H	4.29142600	1.62510500	-0.87565500
H	3.83308100	3.08755700	0.00001200
H	4.29145000	1.62506200	0.87559500
C	-3.73554900	2.02890800	0.00001300
H	-3.80255400	3.11571700	0.00017100
H	-4.27600100	1.65690500	-0.87531200
H	-4.27609500	1.65664100	0.87516400
C	2.99674700	-0.73636200	-0.00000300
C	3.47153400	-1.23534900	1.22542900
C	3.47152800	-1.23535200	-1.22543500
C	4.45474000	-2.22730200	1.20236700
C	4.45473300	-2.22730500	-1.20237700
C	4.94956400	-2.71978300	-0.00000600
H	4.82900500	-2.62135300	2.14278400
H	4.82899200	-2.62135800	-2.14279500
H	5.71113700	-3.49309400	-0.00000700
C	-3.02464000	-0.72437600	0.00000300
C	-3.50255600	-1.22398800	-1.22490200
C	-3.50254400	-1.22402400	1.22489800
C	-4.49731000	-2.20427300	-1.20237500
C	-4.49729800	-2.20430800	1.20235200
C	-5.00007000	-2.68921400	-0.00001600
H	-4.87368000	-2.59626300	-2.14292600
H	-4.87366000	-2.59632500	2.14289600
H	-5.77146200	-3.45280000	-0.00002300

C	-2.92955500	-0.73847500	-2.53249900
H	-3.07223600	0.33662600	-2.67943000
H	-1.85115800	-0.91942100	-2.57558300
H	-3.39354500	-1.25274100	-3.37640700
C	-2.92953400	-0.73854100	2.53250200
H	-1.85113200	-0.91945800	2.57556200
H	-3.07224500	0.33655000	2.67947200
H	-3.39349700	-1.25285000	3.37640000
C	2.92030700	-0.72950600	-2.53530700
H	1.83862500	-0.88104300	-2.59267700
H	3.09344300	0.34218400	-2.67476100
H	3.37901300	-1.25102200	-3.37752500
C	2.92032200	-0.72950000	2.53530200
H	3.09345700	0.34219100	2.67475100
H	1.83863900	-0.88103800	2.59267900
H	3.37903200	-1.25101300	3.37751900
Fe	0.00987500	-0.12066000	-0.00000200
C	0.06699600	-2.12214400	0.00001300
H	0.61496400	-2.49440800	0.87787800
H	-0.91675100	-2.60387600	0.00000100
H	0.61498900	-2.49441800	-0.87783200

$^{3/2}$Fe(0)-2

C	1.18457800	2.37942500	-0.15159700
C	1.19938400	3.76926900	-0.21074700
C	0.00004600	4.48307700	-0.23287500
C	-1.19936400	3.76927200	-0.21058900
C	-1.18454300	2.37948200	-0.15141300
N	-0.00001400	1.67527300	-0.11531200
H	0.00005300	5.56619400	-0.27064700
H	2.14340000	4.29995600	-0.23892000
H	-2.14336700	4.29998200	-0.23868200
C	2.39629600	1.57131200	-0.15115000
C	-2.39635800	1.57137000	-0.15082800
N	-2.23387800	0.28754200	0.01444600
N	2.23375800	0.28741100	0.01411200
C	-3.73675300	2.23523500	-0.36804700
H	-3.95925400	2.94782000	0.43206500
H	-3.75764800	2.79180300	-1.30911800
H	-4.53907500	1.50028500	-0.39158600
C	3.73670800	2.23509000	-0.36853300
H	3.75760400	2.79144700	-1.30973400
H	3.95929200	2.94784500	0.43140400

H	4.53901200	1.50011500	-0.39195100
C	-3.33333900	-0.61503600	-0.07669200
C	-3.64856100	-1.17927200	-1.33042900
C	-4.05448900	-0.98174600	1.07642000
C	-4.66661200	-2.13188800	-1.40017900
C	-5.06954700	-1.93527600	0.95800300
C	-5.37299900	-2.51753500	-0.26644000
H	-4.90719900	-2.57368500	-2.36282200
H	-5.62960500	-2.21919100	1.84456600
H	-6.16044000	-3.26093000	-0.33848000
C	3.33323900	-0.61515300	-0.07697500
C	4.05477900	-0.98135400	1.07606800
C	3.64815200	-1.17987900	-1.33057800
C	5.06984300	-1.93489600	0.95773800
C	4.66623100	-2.13246500	-1.40024400
C	5.37296400	-2.51763400	-0.26655300
H	5.63017900	-2.21841800	1.84425300
H	4.90657000	-2.57462500	-2.36278200
H	6.16041900	-3.26102200	-0.33852600
C	3.76489400	-0.36262500	2.42211700
H	3.65943400	0.72361400	2.36583000
H	2.83939500	-0.74997500	2.85721500
H	4.56898100	-0.58143500	3.12768900
C	2.91832400	-0.75135100	-2.57869700
H	1.83716600	-0.83669700	-2.45733800
H	3.13064700	0.29277200	-2.83366800
H	3.21574800	-1.36396100	-3.43199400
C	-3.76407700	-0.36362800	2.42263000
H	-2.83882500	-0.75182900	2.85752100
H	-3.65779900	0.72254900	2.36669800
H	-4.56826300	-0.58209400	3.12819100
C	-2.91906800	-0.75023200	-2.57856700
H	-3.13157300	0.29395200	-2.83314600
H	-1.83787000	-0.83547600	-2.45746400
H	-3.21660800	-1.36258300	-3.43200800
C	-0.00103200	-2.25081200	-0.85604000
H	-0.00051900	-2.24727600	-1.95330700
H	0.88071900	-2.82838000	-0.54944500
H	-0.88392100	-2.82706300	-0.55024600
C	0.00107500	-1.44631800	2.38979500
H	0.92058400	-2.01085900	2.28091700
H	-0.91781500	-2.01221900	2.28266700
C	0.00036900	-0.14219200	2.69218300

H	-0.91982200	0.41254600	2.82842200
H	0.91994400	0.41402600	2.82652600
Fe	0.00002100	-0.37631600	0.00609600

$^{3/2}$Fe(0)-TS2/3

C	1.19138900	2.48219600	0.02395700
C	1.20800600	3.87295100	0.05394700
C	0.00767100	4.58660900	0.05448000
C	-1.19469200	3.87607900	0.03664800
C	-1.18134000	2.48541800	0.00783200
N	0.00414700	1.78424600	-0.00722700
H	0.00897800	5.67027900	0.07384200
H	2.15243800	4.40371000	0.07854400
H	-2.13785000	4.40949700	0.04779000
C	2.38593500	1.65826900	0.04866300
C	-2.37874900	1.66464700	0.02095700
N	-2.18426600	0.37205600	-0.03628100
N	2.18835800	0.36623800	-0.01650900
C	-3.73895000	2.31225000	0.12328000
H	-3.83464600	2.89260100	1.04585800
H	-3.91328800	3.00018000	-0.70914200
H	-4.53184600	1.56629500	0.11259600
C	3.74678500	2.30114100	0.16923300
H	3.94126900	2.97682900	-0.66890700
H	3.82677400	2.89345200	1.08555100
H	4.53604300	1.55143900	0.18448400
C	-3.26616600	-0.54848800	0.04363100
C	-3.88178800	-1.01222300	-1.13648900
C	-3.66459800	-1.03805200	1.30452600
C	-4.86232400	-2.00196300	-1.03547900
C	-4.64813400	-2.02889500	1.35758000
C	-5.23978700	-2.51928300	0.19900000
H	-5.33697000	-2.36672100	-1.94206300
H	-4.95266100	-2.41682600	2.32555500
H	-5.99682000	-3.29479400	0.25802600
C	3.26742100	-0.55844700	0.05630600
C	3.64174200	-1.08430200	1.31010700
C	3.90521300	-0.98857100	-1.12465000
C	4.62015600	-2.08042000	1.35293500
C	4.87879800	-1.98639900	-1.03399200
C	5.23025300	-2.54128800	0.19153600
H	4.90629000	-2.49612100	2.31496800
H	5.36883600	-2.32709200	-1.94178900
H	5.98214200	-3.32239000	0.24217800

C	3.04342500	-0.54781500	2.58773000
H	3.46935800	0.42911600	2.84385600
H	1.96436900	-0.40816200	2.50783400
H	3.24387700	-1.21854800	3.42587300
C	3.59428100	-0.34767200	-2.45489400
H	2.52489100	-0.19588000	-2.59985600
H	4.06714700	0.63779200	-2.53900100
H	3.96889200	-0.95716700	-3.28005800
C	-3.08441800	-0.47200700	2.57784600
H	-2.00617600	-0.32212000	2.50573000
H	-3.52311200	0.50462500	2.81280500
H	-3.28581700	-1.12965700	3.42605900
C	-3.53489200	-0.41650700	-2.47844100
H	-3.94742800	0.59348800	-2.58357600
H	-2.45815500	-0.33159700	-2.62439500
H	-3.94416200	-1.01997200	-3.29141100
C	-0.08299600	-2.64357200	-0.28860100
H	0.78021600	-3.16233500	-0.68527700
H	-1.03071200	-3.03014400	-0.64085500
C	-0.01952100	-2.10413400	1.01590600
H	-0.92439400	-2.10816200	1.61296400
H	0.91396400	-2.19253400	1.56029700
Fe	0.00451400	-0.24718300	-0.10839300
C	0.03233500	-1.39620600	-2.05362100
H	-0.80319800	-1.89244100	-2.54236600
H	-0.02608000	-0.32463000	-2.31737200
H	0.97248300	-1.78293100	-2.44002900

$^{3/2}$Fe(0)-3

C	-1.18494000	2.67144900	-0.10532600
C	-1.20427800	4.06261200	-0.08658400
C	0.00015300	4.77168500	-0.10776500
C	1.20454800	4.06254900	-0.08657900
C	1.18513700	2.67138800	-0.10532200
N	0.00008200	1.98586600	-0.20352800
H	0.00018100	5.85546800	-0.09168200
H	-2.14605200	4.59630200	-0.03423100
H	2.14635000	4.59619000	-0.03422100
C	-2.35770000	1.82230100	0.02571900
C	2.35785500	1.82217800	0.02571800
N	2.10968100	0.54051500	0.14163600
N	-2.10959400	0.54062400	0.14164300
C	3.73745000	2.43146200	0.05077900
H	3.96696400	2.93882900	-0.89126200

H	3.81989000	3.17797300	0.84579900
H	4.50062000	1.67480900	0.22359900
C	-3.73726300	2.43165600	0.05077800
H	-3.81966200	3.17818100	0.84579100
H	-3.96675500	2.93902500	-0.89126800
H	-4.50047200	1.67504500	0.22360900
C	3.14747700	-0.42512500	0.25737300
C	3.35085100	-1.03398200	1.51209400
C	3.88553100	-0.83223800	-0.87186600
C	4.31933500	-2.03215800	1.62455500
C	4.83851900	-1.84235100	-0.71453000
C	5.06240900	-2.43824200	0.52085800
H	4.48635800	-2.49956300	2.59073100
H	5.40730500	-2.16733200	-1.58102400
H	5.80589600	-3.22237500	0.62181500
C	-3.14744300	-0.42495800	0.25739400
C	-3.88552400	-0.83204200	-0.87183800
C	-3.35084700	-1.03379100	1.51212100
C	-4.83856700	-1.84210100	-0.71448800
C	-4.31938600	-2.03191100	1.62459700
C	-5.06248600	-2.43796600	0.52090700
H	-5.40737400	-2.16705900	-1.58097700
H	-4.48643200	-2.49929700	2.59077800
H	-5.80601700	-3.22205600	0.62187400
C	-3.65813500	-0.20852200	-2.22705700
H	-4.11587100	0.78377800	-2.30446300
H	-2.59435300	-0.08909800	-2.44162400
H	-4.09385500	-0.82654800	-3.01445600
C	-2.53940900	-0.60996300	2.71062800
H	-1.46824500	-0.76530700	2.54500600
H	-2.66593300	0.45254600	2.93835600
H	-2.82552500	-1.17932200	3.59712900
C	3.65817200	-0.20869100	-2.22707700
H	2.59439500	-0.08921700	-2.44164500
H	4.11595200	0.78359000	-2.30447100
H	4.09386500	-0.82672700	-3.01448300
C	2.53944400	-0.61011900	2.71060900
H	2.66603900	0.45237800	2.93835200
H	1.46826800	-0.76538800	2.54498600
H	2.82552400	-1.17951000	3.59710100
C	0.00000200	-1.78721400	-1.44262600
H	-0.87454200	-1.80263600	-2.10944500
H	0.87493300	-1.80295700	-2.10892900

C	-0.00048100	-3.06958500	-0.58906900
H	-0.87643200	-3.07927400	0.07304300
H	0.87510700	-3.07960700	0.07352200
C	-0.00050000	-4.36808800	-1.40956500
H	-0.88282600	-4.42180400	-2.05589000
H	0.88215900	-4.42213800	-2.05540700
H	-0.00084400	-5.25859300	-0.76993500
Fe	0.00002600	-0.04910500	-0.33734500

$^{3/2}$Fe(0)-4

C	1.12095200	2.58900300	-0.40559200
C	1.10623700	3.95541000	-0.67357300
C	-0.10353800	4.61866000	-0.87363100
C	-1.28657600	3.87623100	-0.81431900
C	-1.24280900	2.51522000	-0.53724700
N	-0.04927500	1.86202900	-0.31996300
H	-0.12618100	5.68255300	-1.07884000
H	2.03820200	4.50434600	-0.73205100
H	-2.23855000	4.36484000	-0.98218300
C	2.34774800	1.82654800	-0.24478100
C	-2.43987300	1.68374000	-0.47263500
N	-2.26620800	0.45089500	-0.09197100
N	2.21007500	0.56448100	0.06628500
C	-3.77461300	2.26656500	-0.87738900
H	-4.07232100	3.07932100	-0.20809100
H	-3.73507200	2.68066900	-1.88842800
H	-4.55608900	1.50939800	-0.85207800
C	3.68134800	2.50135500	-0.47055000
H	3.76343200	2.89898900	-1.48629500
H	3.81536800	3.34312700	0.21521700
H	4.50490000	1.80783900	-0.31230400
C	-3.34829100	-0.47361500	-0.04649300
C	-3.53426500	-1.35284000	-1.13292500
C	-4.17702300	-0.55213300	1.08998200
C	-4.53447200	-2.32256200	-1.04811300
C	-5.16264700	-1.54227000	1.13400700
C	-5.34140200	-2.42906800	0.07948900
H	-4.67774500	-3.00406800	-1.88164400
H	-5.79937100	-1.61103600	2.01151800
H	-6.10750200	-3.19586700	0.13353900
C	3.33277700	-0.31224400	0.08097200
C	3.97306200	-0.62381500	1.29516100
C	3.75322100	-0.90702000	-1.12625200
C	5.02481100	-1.54256800	1.28463800

C	4.80633600	-1.82375500	-1.09034700
C	5.44107800	-2.14628800	0.10364500
H	5.52211100	-1.78427000	2.21970000
H	5.12873700	-2.29067000	-2.01660100
H	6.25548500	-2.86353100	0.11366400
C	3.55157400	0.03576400	2.58339800
H	3.64459100	1.12539700	2.53449100
H	2.50752200	-0.18084600	2.81771800
H	4.16240200	-0.31168700	3.41886700
C	3.09163900	-0.55799300	-2.43644700
H	2.00332300	-0.61940100	-2.36749800
H	3.33227700	0.46167400	-2.75661700
H	3.41908500	-1.23415200	-3.22841300
C	-4.04834800	0.42965600	2.22882700
H	-3.01151300	0.57924000	2.53053100
H	-4.44226600	1.41600500	1.95879800
H	-4.60701700	0.08799500	3.10246500
C	-2.69052300	-1.22909900	-2.37579700
H	-2.87837100	-0.28574900	-2.90026000
H	-1.62552700	-1.25210000	-2.13761700
H	-2.90157200	-2.04183300	-3.07333700
C	0.01883600	-2.21576100	0.16885000
H	0.59041500	-2.52070500	1.06146400
H	-1.01632700	-2.53025300	0.37679000
C	0.55233200	-3.02681300	-1.02313500
H	1.60797000	-2.78679000	-1.19147100
H	0.03310600	-2.74102000	-1.94768900
C	0.42304500	-4.54782200	-0.85278100
H	0.97077500	-4.88966500	0.03180600
H	-0.62384100	-4.84113300	-0.72073900
H	0.81617800	-5.09447900	-1.71845600
C	-0.35828600	-0.41677800	2.98013900
H	0.46844900	-1.08097000	3.20618400
H	-1.32585400	-0.89197900	2.86428100
C	-0.19458900	0.90372500	2.88128400
H	-1.02232100	1.57270100	2.67515100
H	0.77349300	1.37253000	3.01793900
Fe	0.00850100	-0.14049400	0.19845000

$^{3/2}$Fe(0)-TS4/5

C	1.20013800	2.58096200	-0.21928000
C	1.21921200	3.95985400	-0.42556300
C	0.02490900	4.66577900	-0.55008900
C	-1.18085900	3.95764500	-0.49044700

C	-1.17037500	2.58495000	-0.27818000
N	0.00799300	1.89686100	-0.10742200
H	0.02908600	5.73750800	-0.71128200
H	2.16498800	4.48320300	-0.50127600
H	-2.12026400	4.48193100	-0.61740100
C	2.39100600	1.76291300	-0.14852000
C	-2.37661400	1.77023900	-0.24652500
N	-2.21431000	0.49825600	0.00267000
N	2.20785200	0.47848200	0.06330300
C	-3.71746300	2.41506500	-0.51410900
H	-3.93707100	3.18653600	0.22989100
H	-3.73879400	2.89896400	-1.49448700
H	-4.52137100	1.68241000	-0.48269100
C	3.74877500	2.40201200	-0.33129100
H	3.83296600	2.89638500	-1.30338600
H	3.92981400	3.16376400	0.43308300
H	4.54605900	1.66483100	-0.26033600
C	-3.31887000	-0.39995200	-0.06274800
C	-3.62216300	-1.01212300	-1.29687200
C	-4.05492100	-0.71955100	1.09501200
C	-4.64449800	-1.96199800	-1.34402600
C	-5.07312100	-1.67215100	1.00025500
C	-5.36652900	-2.29919500	-0.20473800
H	-4.87682300	-2.43859200	-2.29211200
H	-5.64399800	-1.92029600	1.89055100
H	-6.15741400	-3.04051600	-0.25725700
C	3.30652200	-0.42664000	-0.03088300
C	3.99162600	-0.86227700	1.12054500
C	3.67104800	-0.91840100	-1.30477100
C	4.99974200	-1.82149400	0.98131000
C	4.67933800	-1.87931500	-1.39542500
C	5.33866800	-2.34074300	-0.26131700
H	5.53038800	-2.15595200	1.86848100
H	4.95214900	-2.26504900	-2.37363900
H	6.12041800	-3.08860200	-0.34806000
C	3.68837200	-0.30396600	2.48961700
H	4.56011900	-0.39440800	3.14173500
H	3.40461900	0.74878300	2.45159800
H	2.86702100	-0.83795900	2.97549500
C	3.00844400	-0.40118200	-2.55803000
H	1.92157100	-0.37797500	-2.46590300
H	3.32453700	0.62209100	-2.78848000
H	3.26648100	-1.02189000	-3.41848100

C	-3.76852600	-0.05273700	2.41734300
H	-2.81938400	-0.38992300	2.84063600
H	-3.70248200	1.03448200	2.32707900
H	-4.55226700	-0.28046100	3.14265000
C	-2.87146000	-0.63891400	-2.55104900
H	-3.07429400	0.39364300	-2.85438300
H	-1.79075100	-0.71550300	-2.41453500
H	-3.15637500	-1.28622200	-3.38269500
C	-0.38424800	-2.32484000	0.45819900
H	-0.15555300	-3.24969900	0.99002600
H	-1.46964800	-2.27670400	0.34496700
C	0.33041800	-2.37402900	-0.89684200
H	1.41227600	-2.42662500	-0.74888400
H	0.14994200	-1.46313800	-1.48426700
C	-0.11476400	-3.57847400	-1.74635200
H	0.09422900	-4.51769800	-1.22532300
H	-1.18902500	-3.54580300	-1.94847800
H	0.41018000	-3.60580200	-2.70782300
C	0.00840600	-1.48060500	2.42636100
H	0.91911500	-2.06129800	2.52075400
H	-0.88125500	-2.03994100	2.69370300
C	0.05643900	-0.09359800	2.71721800
H	-0.82963800	0.39998800	3.10149700
H	0.99740500	0.36178700	2.99955800
Fe	0.00693800	0.01173600	0.58949200

$^{3/2}$Fe(0)-5

C	1.18589700	-3.07220600	-0.14402400
C	1.20569700	-4.46301100	-0.11812700
C	0.00098400	-5.17251400	-0.13326900
C	-1.20398800	-4.46346400	-0.11806900
C	-1.18470800	-3.07265000	-0.14395900
N	0.00046700	-2.38976200	-0.24249700
H	0.00118600	-6.25609700	-0.11066800
H	2.14757100	-4.99664400	-0.06642000
H	-2.14566800	-4.99744200	-0.06633500
C	2.35792300	-2.22123900	-0.02049400
C	-2.35703000	-2.22212100	-0.02033500
N	-2.11101200	-0.94012300	0.10584400
N	2.11144800	-0.93933000	0.10570500
C	-3.73822400	-2.82744000	-0.01530400
H	-3.95548900	-3.33139900	-0.96201400
H	-3.83342000	-3.57562900	0.77657500
H	-4.50116900	-2.06879200	0.14889400

C	3.73935100	-2.82601300	-0.01565500
H	3.83480000	-3.57461600	0.77579400
H	3.95689300	-3.32933500	-0.96264600
H	4.50196800	-2.06713600	0.14901000
C	-3.15079300	0.02409500	0.23121400
C	-3.38373200	0.58926700	1.50041100
C	-3.86176500	0.46702800	-0.90144300
C	-4.35646000	1.58269600	1.62217800
C	-4.82192300	1.46827800	-0.73347500
C	-5.07519300	2.02277700	0.51564800
H	-4.54573100	2.01916600	2.59861700
H	-5.37170900	1.82021000	-1.60163900
H	-5.82295800	2.80172500	0.62513200
C	3.15089500	0.02524900	0.23112400
C	3.86160400	0.46859000	-0.90153100
C	3.38375900	0.59030900	1.50038800
C	4.82142900	1.47015300	-0.73351200
C	4.35616000	1.58405000	1.62220600
C	5.07462800	2.02455000	0.51566800
H	5.37100500	1.82240400	-1.60168000
H	4.54536700	2.02045300	2.59868900
H	5.82213300	2.80374100	0.62520000
C	3.59557500	-0.10744900	-2.27053100
H	3.99503600	-1.12199900	-2.37621800
H	2.52548700	-0.16214700	-2.48283300
H	4.06151400	0.50540600	-3.04445000
C	2.59863000	0.12756300	2.70182700
H	1.52229100	0.24458700	2.54325700
H	2.76652800	-0.93207800	2.91817600
H	2.87400900	0.69755200	3.59132100
C	-3.59564600	-0.10908000	-2.27039600
H	-2.52555800	-0.16331100	-2.48282000
H	-3.99464700	-1.12382800	-2.37590900
H	-4.06196200	0.50345800	-3.04433800
C	-2.59827800	0.12702900	2.70183500
H	-2.76500900	-0.93285400	2.91785000
H	-1.52204100	0.24532000	2.54345900
H	-2.87440600	0.69647000	3.59144900
C	-0.00046900	1.52313800	-1.21356500
H	0.87296800	1.61662400	-1.87546800
H	-0.87410500	1.61612400	-1.87527600
C	-0.00070500	2.69942100	-0.21919300
H	0.87501500	2.63444200	0.44119200

H	-0.87626500	2.63392600	0.44135400
C	-0.00116100	4.08615700	-0.88366600
H	0.87504300	4.16568000	-1.54135300
H	-0.87760300	4.16523100	-1.54108300
C	-0.00128900	5.25612500	0.10620200
H	-0.87685700	5.17446800	0.76302600
H	0.87447000	5.17480500	0.76281800
C	-0.00163000	6.62898000	-0.57146600
H	-0.00174100	7.44265500	0.16049500
H	0.88013300	6.75864300	-1.20749200
H	-0.88354600	6.75828300	-1.20735400
Fe	0.00011300	-0.34819800	-0.35591600

$^{3/2}$Fe(0)-6

C	1.05655900	2.62949200	0.29517900
C	1.02509900	4.01107400	0.46458300
C	-0.19499800	4.68028600	0.55102500
C	-1.37006000	3.92891500	0.48051500
C	-1.30979000	2.55009200	0.31092600
N	-0.10434000	1.88862400	0.21001300
H	-0.23091500	5.75636700	0.67462400
H	1.95155000	4.56846700	0.52896100
H	-2.33051300	4.42359200	0.55754300
C	2.29666000	1.87235800	0.22602800
C	-2.50012000	1.71036100	0.25679500
N	-2.30912500	0.45007000	-0.01383100
N	2.18734700	0.59773300	-0.03716800
C	-3.85429200	2.32063700	0.54016800
H	-3.87913100	2.79645900	1.52438200
H	-4.10173200	3.09144600	-0.19595000
H	-4.63861800	1.56693400	0.50870900
C	3.61133500	2.57286900	0.48533700
H	3.78587500	3.36749600	-0.24625300
H	3.62745900	3.03831600	1.47490300
H	4.44578000	1.87701800	0.42598400
C	-3.38871400	-0.47979000	0.01939000
C	-4.10763800	-0.78013700	-1.15418000
C	-3.68716800	-1.13559700	1.23201600
C	-5.10124900	-1.76144200	-1.09983800
C	-4.68456800	-2.11265000	1.23793000
C	-5.38665500	-2.43431500	0.08195800
H	-5.65922400	-1.99482700	-2.00225400
H	-4.91183400	-2.62511600	2.16823100
H	-6.15692500	-3.19851700	0.10406200

C	3.33059900	-0.25358200	-0.00410800
C	3.69999900	-0.85552600	1.21672600
C	4.04523000	-0.53142800	-1.18557500
C	4.76586700	-1.75742000	1.22425800
C	5.10740600	-1.43764000	-1.13030500
C	5.46532400	-2.05735100	0.06087500
H	5.04789300	-2.22968600	2.16084700
H	5.66189100	-1.65381800	-2.03913200
H	6.28900800	-2.76359200	0.08412200
C	2.97331300	-0.52547900	2.49657700
H	3.14985300	0.50980200	2.80831400
H	1.89388300	-0.64409900	2.38669000
H	3.30663100	-1.17283200	3.30998300
C	3.70125700	0.14288700	-2.49106000
H	2.74787200	-0.20852800	-2.89381400
H	3.61977300	1.22820300	-2.38587300
H	4.46596400	-0.05981100	-3.24345400
C	-2.96421700	-0.77833700	2.50652900
H	-1.88116900	-0.82725800	2.38177900
H	-3.20264400	0.23880500	2.83639700
H	-3.24380200	-1.45788300	3.31387000
C	-3.84235800	-0.05377100	-2.45044700
H	-3.82790000	1.03173100	-2.32039200
H	-2.88003700	-0.33332900	-2.88676800
H	-4.61271600	-0.28774800	-3.18789100
C	-0.06111800	-2.08313400	0.66049900
H	0.13922300	-2.02588700	1.74288900
H	-1.10491800	-2.42324700	0.58554800
C	0.84984600	-3.16459900	0.05688600
H	1.89713100	-2.84264700	0.08454900
H	0.61253100	-3.30158100	-1.00675500
C	0.74209300	-4.53128500	0.74976600
H	1.01945800	-4.45688900	1.80677400
H	-0.28344300	-4.91362800	0.70969300
H	1.39656600	-5.27972300	0.28727100
C	-0.05768600	-0.88913300	-2.60037000
H	0.87385600	-1.44394100	-2.59575400
H	-0.96292800	-1.48461500	-2.55268700
C	-0.08801500	0.44342200	-2.72354000
H	-1.02008700	0.99381800	-2.76317200
H	0.81937400	1.02971700	-2.80301300
Fe	-0.02584000	-0.14933200	-0.09012700

$^{3/2}$Fe(0)-TS6/7

C	1.04611100	2.71242300	0.15053500
C	1.02706900	4.09998600	0.25716700
C	-0.18675500	4.78508600	0.31112200
C	-1.36756000	4.04337200	0.25222600
C	-1.31887200	2.65795100	0.14634000
N	-0.11940200	1.97671800	0.09973100
H	-0.21219400	5.86538300	0.39384500
H	1.95825300	4.65132100	0.29774500
H	-2.32474900	4.54914200	0.28846600
C	2.28460200	1.95168200	0.08487900
C	-2.51538500	1.83271700	0.07708600
N	-2.31653400	0.55002600	-0.02528900
N	2.16963200	0.65703200	-0.01856100
C	-3.88140600	2.47654000	0.12585600
H	-4.02456600	3.03386500	1.05618100
H	-4.01675100	3.18349400	-0.69774200
H	-4.66834900	1.72738800	0.05818000
C	3.60912400	2.68009500	0.13762400
H	4.44311100	1.98418800	0.07036000
H	3.70089900	3.39620900	-0.68393200
H	3.71494600	3.24359500	1.06910600
C	-3.39337000	-0.37387600	-0.09568800
C	-3.87915000	-0.77819900	-1.35540000
C	-3.91250900	-0.92978200	1.09073300
C	-4.85882400	-1.77240900	-1.40659300
C	-4.89158600	-1.92124100	0.99168100
C	-5.35941700	-2.35082100	-0.24526400
H	-5.23305600	-2.09317200	-2.37475600
H	-5.29106600	-2.35907700	1.90219400
H	-6.11432000	-3.12848200	-0.30380400
C	3.32025400	-0.17635300	-0.08774100
C	3.88105200	-0.69376600	1.09733500
C	3.85615500	-0.52045000	-1.34547400
C	4.94964900	-1.58864600	0.99908800
C	4.92580100	-1.41730900	-1.39672500
C	5.46740200	-1.96006200	-0.23654300
H	5.38124000	-1.99470200	1.90968100
H	5.33880100	-1.68881300	-2.36413100
H	6.29398100	-2.66097600	-0.29486200
C	3.37624000	-0.25721500	2.45038700
H	3.70612300	0.76012000	2.69009000
H	2.28670300	-0.25089300	2.49776100

H	3.75051900	-0.91340300	3.23880300
C	3.31885800	0.09792100	-2.61224000
H	3.73884100	-0.38985300	-3.49410600
H	2.23139100	0.03079900	-2.67061300
H	3.56939900	1.16254400	-2.67657700
C	-3.46069600	-0.43524600	2.44304400
H	-3.91502800	0.53278300	2.68441600
H	-3.74908100	-1.13370400	3.23135300
H	-2.37983000	-0.29605600	2.48819500
C	-3.39104300	-0.11917100	-2.62198800
H	-3.82326200	0.88105800	-2.74195900
H	-2.30725900	0.00432400	-2.62756600
H	-3.67353400	-0.70250700	-3.50077300
C	-0.07611700	-1.71552300	1.43866300
H	0.28885700	-1.04464600	2.22258000
H	-1.12323800	-1.97709900	1.58874000
C	0.78363200	-2.83550300	1.15271200
H	1.82239400	-2.72585900	1.46848200
H	0.98702000	-2.80600100	-0.16800300
C	0.25456700	-4.25141400	1.29713900
H	0.14886900	-4.51276600	2.35606400
H	-0.73438200	-4.34911800	0.83927500
H	0.91812500	-4.99034200	0.83697800
C	0.79929400	-2.67800000	-1.48629200
H	1.83523400	-2.58468800	-1.80769000
H	0.40393200	-3.68402000	-1.63592500
C	-0.07511100	-1.56362300	-1.68751100
H	-1.12084900	-1.80834100	-1.85454300
H	0.28995500	-0.79213900	-2.37044700
Fe	-0.08557700	-0.09234500	-0.03343100

$^{3/2}$Fe(0)-7

C	-1.10914400	2.76080000	0.09209300
C	-1.09542100	4.15354100	0.02593800
C	0.12429400	4.83098700	0.00490300
C	1.31558100	4.09303200	-0.00136400
C	1.26141200	2.70614300	0.06977800
N	0.06375600	2.05783300	0.19211200
H	0.15021200	5.91329100	-0.04932500
H	-2.02452900	4.70911700	-0.03221000
H	2.26779400	4.60419100	-0.08339100
C	-2.29278500	1.92962700	-0.01803800
C	2.41257700	1.81840100	-0.05467100
N	2.15030400	0.53679700	-0.05161900

N	-2.08231000	0.63138500	-0.01878100
C	3.79473300	2.40395000	-0.21698100
H	3.86840700	2.99851300	-1.13254700
H	4.03930200	3.06724800	0.61756200
H	4.55224300	1.62390900	-0.26385800
C	-3.65337900	2.56771400	-0.16101600
H	-3.85608800	3.25195100	0.66799500
H	-3.72572200	3.15100600	-1.08429900
H	-4.44230000	1.81778600	-0.17945000
C	3.16837700	-0.41935200	-0.33697900
C	3.92807100	-1.00362300	0.69537400
C	3.35025500	-0.81611400	-1.67814800
C	4.84991400	-2.00018000	0.36331800
C	4.28213800	-1.81646900	-1.96323600
C	5.02744100	-2.41291400	-0.95234500
H	5.43783900	-2.45505000	1.15534900
H	4.42187300	-2.12801800	-2.99448600
H	5.74524600	-3.19184200	-1.18887200
C	-3.13463600	-0.28104800	-0.31622000
C	-3.36232600	-0.62535100	-1.66510900
C	-3.88486700	-0.88242100	0.71440100
C	-4.32292100	-1.59589500	-1.95959100
C	-4.83853700	-1.84492600	0.37333100
C	-5.05648100	-2.20997900	-0.95103100
H	-4.49495900	-1.86939100	-2.99680600
H	-5.41947800	-2.31117800	1.16397200
H	-5.79731700	-2.96461100	-1.19530600
C	-2.60753400	0.05735700	-2.77987200
H	-2.99955200	1.06231500	-2.97349200
H	-1.54894300	0.18174200	-2.54283200
H	-2.68893600	-0.50753700	-3.71068800
C	-3.68498000	-0.48447100	2.15443600
H	-3.87973700	0.58131800	2.31096100
H	-4.35725300	-1.04304200	2.80877200
H	-2.66108400	-0.66366800	2.48483100
C	2.56578300	-0.16491400	-2.79038300
H	1.49518900	-0.14550600	-2.57389600
H	2.86862700	0.87612100	-2.94605800
H	2.71464700	-0.69355200	-3.73395000
C	3.76938600	-0.56068900	2.12747400
H	3.97508300	0.50744900	2.24955700
H	2.75359200	-0.72490300	2.48922700
H	4.45457800	-1.10545400	2.77992100

C	0.03947800	-2.37790600	-0.93536000
H	-0.38381900	-1.54898300	-1.49440500
H	1.11540900	-2.51049300	-0.99111700
C	-0.74757400	-3.23737300	-0.28594300
H	-1.82166100	-3.06093300	-0.28272900
H	-0.86692300	-2.34839800	2.86989000
C	-0.27358200	-4.46181000	0.43555000
H	-0.70927400	-5.36381300	-0.00957300
H	0.81407200	-4.55735400	0.40377000
H	-0.58546300	-4.44917400	1.48440300
C	0.03949000	-1.82800100	3.19761600
H	0.08899600	-1.94231200	4.29032800
H	0.88340800	-2.39047100	2.78366500
C	0.04734500	-0.36094500	2.74720200
H	0.93173300	0.14709300	3.15678200
H	-0.80223100	0.16878700	3.20092600
Fe	0.00354300	0.11956600	0.73379400

$^{3/2}$Fe(0)-8

C	1.19777200	2.55559300	-0.00029000
C	1.21179600	3.94130200	-0.13607300
C	-0.00002600	4.63847100	-0.18918400
C	-1.21182900	3.94128600	-0.13606400
C	-1.19778800	2.55556900	-0.00028300
N	0.00000100	1.89489400	0.10903200
H	-0.00003600	5.71645600	-0.30313100
H	2.14667700	4.48218900	-0.22187000
H	-2.14671300	4.48217000	-0.22183700
C	2.31514900	1.64731300	0.00054800
C	-2.31511600	1.64724600	0.00055500
N	-1.97910700	0.35874400	0.02487000
N	1.97918700	0.35880800	0.02484800
C	-3.74358700	2.11439900	-0.02751900
H	-3.81441100	3.20051800	-0.06055200
H	-4.27749400	1.71405400	-0.89377400
H	-4.28888400	1.76965300	0.85591300
C	3.74356000	2.11467800	-0.02764600
H	4.27730500	1.71487900	-0.89425600
H	3.81416700	3.20083200	-0.06015900
H	4.28916700	1.76963000	0.85546700
C	-3.01381100	-0.62898400	0.00813200
C	-3.46464700	-1.12474900	-1.22897600
C	-3.53006400	-1.12027100	1.22132100
C	-4.45422900	-2.11086300	-1.23077200

C	-4.51810300	-2.10648000	1.17305100
C	-4.98219000	-2.59985400	-0.04131800
H	-4.80752900	-2.50238500	-2.18036500
H	-4.92242900	-2.49426900	2.10360800
H	-5.74745900	-3.36929800	-0.06013800
C	3.01382200	-0.62898500	0.00812700
C	3.53001100	-1.12026700	1.22134900
C	3.46464500	-1.12483500	-1.22895000
C	4.51795000	-2.10657600	1.17314400
C	4.45412000	-2.11105900	-1.23067900
C	4.98200400	-2.60005800	-0.04119600
H	4.92222600	-2.49435800	2.10372500
H	4.80740100	-2.50265200	-2.18025000
H	5.74718900	-3.36958600	-0.05996900
C	3.02435500	-0.60646200	2.54652800
H	3.18715700	0.46915300	2.66595700
H	1.94845800	-0.77388200	2.65258800
H	3.52535400	-1.11047900	3.37528400
C	2.89463700	-0.60660100	-2.52629200
H	1.80222300	-0.62901100	-2.51988300
H	3.18290300	0.43241200	-2.71870900
H	3.24310400	-1.20484200	-3.37040400
C	-3.02435500	-0.60661000	2.54653600
H	-1.94849000	-0.77421300	2.65261300
H	-3.18697500	0.46902700	2.66601300
H	-3.52545700	-1.11057900	3.37525800
C	-2.89446400	-0.60658200	-2.52626700
H	-3.18206300	0.43265900	-2.71844200
H	-1.80206000	-0.62968300	-2.51995900
H	-3.24337200	-1.20443600	-3.37047200
C	0.00004900	-2.03071100	0.51255300
H	0.87766000	-2.31320100	1.11171800
H	-0.87755500	-2.31324000	1.11171000
C	0.00007300	-2.85757700	-0.78201200
H	0.88278100	-2.65505800	-1.39766400
H	-0.88269200	-2.65517400	-1.39762000
H	0.00014700	-3.93949700	-0.58821800
Fe	0.00002800	-0.03249600	0.25948600

$^{3/2}$Fe(0)-TS3/9

C	-1.12235600	2.56572800	0.07201000
C	-1.12254500	3.95415500	0.11202400
C	0.08964000	4.65275900	0.15015200
C	1.28057000	3.92797100	0.14744300

C	1.25098500	2.53601800	0.10433300
N	0.05431900	1.85347500	0.06545500
H	0.10146100	5.73595200	0.18203800
H	-2.05954000	4.49833100	0.11488800
H	2.23067000	4.44880300	0.17792000
C	-2.32796700	1.75570000	0.03503400
C	2.42479000	1.69359100	0.08835500
N	2.19413200	0.40135300	0.03967200
N	-2.14969100	0.46042300	0.01611400
C	3.80426000	2.30461100	0.12878800
H	3.93736100	2.92006100	1.02328800
H	4.57529500	1.53612800	0.13381600
H	3.97931000	2.95147000	-0.73611900
C	-3.68410800	2.41856400	0.02167900
H	-3.79887100	3.06690000	-0.85167300
H	-4.48391600	1.68066300	0.00129100
H	-3.82452300	3.04368300	0.90803500
C	3.25739700	-0.54228500	-0.01758300
C	3.71558400	-1.14365300	1.17215600
C	3.78607100	-0.91768600	-1.26871300
C	4.69928100	-2.13137500	1.08422600
C	4.76564000	-1.91317800	-1.30897900
C	5.22074500	-2.52181600	-0.14487000
H	5.05804400	-2.59969100	1.99636600
H	5.17409600	-2.21184400	-2.27027100
H	5.97893700	-3.29688700	-0.19459700
C	-3.24682300	-0.44488200	-0.04289900
C	-3.74451000	-0.84844200	-1.29746400
C	-3.76517300	-0.98152700	1.15223200
C	-4.76177700	-1.80547100	-1.33415400
C	-4.78499000	-1.93210700	1.06702000
C	-5.28095400	-2.34842500	-0.16413900
H	-5.14886800	-2.12601500	-2.29719300
H	-5.19086400	-2.35210200	1.98287300
H	-6.06868800	-3.09359800	-0.21112700
C	-3.20862000	-0.24669300	-2.57289900
H	-3.55797500	0.78279000	-2.71101400
H	-2.11711000	-0.21093200	-2.57313800
H	-3.53581200	-0.82014100	-3.44257200
C	-3.23855100	-0.53316900	2.49250400
H	-2.14989800	-0.61581300	2.54168500
H	-3.48344800	0.51537300	2.69364400
H	-3.66735300	-1.13121600	3.29910600

C	3.32827500	-0.24300600	-2.53879000
H	2.24224100	-0.13582300	-2.57433600
H	3.74512800	0.76636200	-2.63041300
H	3.64796300	-0.80710000	-3.41735100
C	3.17103800	-0.71720600	2.51289600
H	3.46136200	0.31040300	2.75750700
H	2.07894900	-0.74597600	2.53009700
H	3.54696100	-1.36300500	3.30918900
C	0.00960700	-1.92970000	-1.17075900
H	-0.95087200	-2.11072700	-1.64333400
H	0.85293000	-1.81727700	-1.84286200
C	0.23273600	-2.41809000	0.13922800
H	0.02248400	-1.25454800	1.33805900
H	1.26904500	-2.59637700	0.41262000
C	-0.74648400	-3.37519100	0.79019200
H	-1.78111800	-3.07416600	0.61808300
H	-0.61395000	-4.36962500	0.34781400
H	-0.58871400	-3.45609400	1.86807500
Fe	0.01605400	-0.15253500	0.07141500

$^{3/2}$Fe(0)-9

C	1.14035000	2.58346600	0.05731700
C	1.15358500	4.00993400	0.11342500
C	-0.06363100	4.68111900	0.09344700
C	-1.27115100	3.98943400	0.05467900
C	-1.22990400	2.56528200	0.00107100
N	-0.03769400	1.93003800	-0.06618600
H	-0.07332500	5.76661600	0.12808100
H	2.08927300	4.55009200	0.17114700
H	-2.21733000	4.51387200	0.07185200
C	2.25484700	1.69591800	0.16266300
C	-2.33502900	1.65788900	0.06157000
N	-2.01438600	0.35901800	0.13649400
N	1.95845000	0.38681000	0.19149400
C	-3.73889100	2.19133800	0.09418300
H	-3.85477700	2.91388600	0.90912000
H	-3.98308800	2.72282000	-0.83252400
H	-4.47399500	1.40142600	0.23761900
C	3.64166000	2.25817500	0.30006800
H	3.68183300	2.97308500	1.12889600
H	4.38188000	1.48259200	0.48797300
H	3.94222300	2.80633700	-0.59996900
C	-3.03577700	-0.63195600	0.17942600
C	-3.72724900	-1.01676900	-0.98860500

C	-3.30829100	-1.25854600	1.41451200
C	-4.66876000	-2.04710200	-0.89959800
C	-4.25951000	-2.27943500	1.45762800
C	-4.93436300	-2.67958100	0.30876900
H	-5.19881200	-2.35416700	-1.79689100
H	-4.47416900	-2.76283400	2.40637800
H	-5.66615400	-3.47977000	0.35650000
C	3.00635700	-0.57523000	0.23795700
C	3.22815500	-1.26990400	1.44635300
C	3.78060300	-0.86273500	-0.90620300
C	4.21281300	-2.25895700	1.48615500
C	4.75404000	-1.86322600	-0.82197600
C	4.97126200	-2.56168200	0.35980000
H	4.38759200	-2.79420200	2.41509300
H	5.34718100	-2.09514100	-1.70221500
H	5.72957500	-3.33699500	0.40425200
C	2.43801300	-0.92670400	2.68453500
H	2.59796200	0.11218800	2.98797700
H	1.36189600	-1.03624100	2.52440500
H	2.72413600	-1.56809600	3.52073300
C	3.58789600	-0.10964100	-2.20047800
H	2.53983300	0.13323900	-2.38017200
H	4.14044300	0.83643800	-2.19804900
H	3.95731300	-0.69280000	-3.04695600
C	-2.61886600	-0.80237800	2.67702400
H	-1.53036200	-0.80622600	2.57731100
H	-2.89630900	0.22436800	2.93570700
H	-2.88633200	-1.44181300	3.52076200
C	-3.49208500	-0.32731000	-2.31154800
H	-4.10305300	0.57810600	-2.40068100
H	-2.45274700	-0.02141600	-2.43884200
H	-3.76603100	-0.97986900	-3.14366900
C	0.01283800	-2.09758100	0.09549900
H	0.99681600	-2.38312800	0.45081900
H	-0.80441700	-2.17732500	0.80328500
C	-0.23820100	-2.00551100	-1.24574800
H	-0.02124000	0.33155400	-1.84796100
H	-1.27254000	-1.93245000	-1.56552000
C	0.74129200	-2.37929800	-2.32242000
H	1.77144600	-2.35349200	-1.96691600
H	0.53136800	-3.40597100	-2.64933900
H	0.65340100	-1.73280200	-3.19674500
Fe	-0.01985000	0.04627000	-0.29388900

$^{3/2}$Fe(0)-10

C	-1.18586700	2.34958400	-0.02325400
C	-1.20672900	3.72261500	-0.24610300
C	-0.00008900	4.42497900	-0.33302500
C	1.20660800	3.72261500	-0.24682200
C	1.18588500	2.34960200	-0.02390600
N	0.00006000	1.69367700	0.16701000
H	-0.00013900	5.49414800	-0.51078100
H	-2.14858800	4.24361900	-0.37388200
H	2.14839200	4.24361400	-0.37518400
C	-2.34818400	1.47547600	-0.03284800
C	2.34821500	1.47551200	-0.03383700
N	2.08234000	0.19115100	0.00686900
N	-2.08231100	0.19109900	0.00741900
C	3.73783800	2.05424600	-0.11047900
H	3.87801800	2.61582900	-1.03920000
H	3.92373500	2.74662000	0.71559700
H	4.49367600	1.27187700	-0.07683500
C	-3.73784800	2.05423800	-0.10872300
H	-3.87863000	2.61562900	-1.03746900
H	-4.49369600	1.27191000	-0.07442300
H	-3.92316400	2.74678100	0.71734000
C	3.11255400	-0.79439400	-0.03714600
C	3.72729500	-1.23060700	1.15169200
C	3.43612700	-1.37105800	-1.27969600
C	4.68771700	-2.24165400	1.06753500
C	4.40325200	-2.37745200	-1.31638200
C	5.02943500	-2.81237900	-0.15347000
H	5.16770700	-2.58745600	1.97836700
H	4.66099200	-2.82727200	-2.27089200
H	5.77540000	-3.59952600	-0.19739500
C	-3.11257000	-0.79438000	-0.03690400
C	-3.43672400	-1.37005700	-1.27976800
C	-3.72679400	-1.23149900	1.15186000
C	-4.40388300	-2.37640200	-1.31680100
C	-4.68728300	-2.24245900	1.06734800
C	-5.02955900	-2.81222200	-0.15394700
H	-4.66205200	-2.82549100	-2.27154000
H	-5.16688900	-2.58893500	1.97812600
H	-5.77556800	-3.59931200	-0.19816200
C	-2.75039200	-0.91221800	-2.54256500
H	-2.97626100	0.13289200	-2.77824500
H	-1.66232600	-0.98162900	-2.45243700

H	-3.06005700	-1.51784800	-3.39646700
C	-3.35056900	-0.63692800	2.48558900
H	-2.27830700	-0.74150400	2.67278700
H	-3.58483700	0.43127100	2.54243600
H	-3.88633000	-1.13439500	3.29633600
C	2.74922200	-0.91419500	-2.54253400
H	1.66121500	-0.98421700	-2.45210200
H	2.97441100	0.13093700	-2.77874200
H	3.05901400	-1.52004700	-3.39623200
C	3.35160000	-0.63509000	2.48515100
H	3.58596800	0.43312600	2.54120200
H	2.27939900	-0.73947700	2.67280200
H	3.88761300	-1.13205100	3.29604100
H	0.00059600	-1.57186100	1.62716200
Fe	0.00017400	-0.30053700	0.57026600

(^{Ar}PDI)Co^{+} (Singlet)1

^{0}Co(+)^{B}

C	1.18510600	2.45417000	0.00014600
C	1.21200400	3.84735300	0.00025100
C	-0.00002600	4.54114600	0.00030900
C	-1.21206000	3.84735700	0.00026100
C	-1.18516600	2.45417500	0.00017600
N	-0.00003100	1.80712400	0.00013600
H	-0.00002500	5.62460700	0.00042200
H	2.15353400	4.38255300	0.00026800
H	-2.15358800	4.38256100	0.00027400
C	2.30554400	1.49208500	0.00005900
C	-2.30560500	1.49208900	0.00016300
N	-1.91081300	0.25097500	0.00017300
N	1.91075300	0.25097000	0.00005500
C	-3.72355800	1.96354000	0.00009900
H	-3.92056400	2.58591400	0.87873000
H	-3.92105900	2.58409300	-0.87972400
H	-4.42533200	1.13221200	0.00112500
C	3.72349600	1.96353500	0.00004700
H	3.92076400	2.58492800	-0.87922700
H	3.92073600	2.58506800	0.87922800
H	4.42527100	1.13220600	0.00012700
C	-2.83247600	-0.85592100	0.00003100
C	-3.23231600	-1.40252900	-1.23207500

C	-3.23167900	-1.40331200	1.23196700
C	-4.06872100	-2.52062000	-1.20497500
C	-4.06812300	-2.52139600	1.20459800
C	-4.48576000	-3.07608300	-0.00025100
H	-4.39336700	-2.95923500	-2.14297200
H	-4.39228400	-2.96058400	2.14249400
H	-5.13320200	-3.94609200	-0.00038100
C	2.83244300	-0.85590900	-0.00009600
C	3.23195100	-1.40309600	1.23183800
C	3.23205900	-1.40266800	-1.23220300
C	4.06849900	-2.52109400	1.20444600
C	4.06859200	-2.52067300	-1.20512500
C	4.48595200	-3.07590700	-0.00041600
H	4.39288900	-2.96013300	2.14233300
H	4.39306200	-2.95939400	-2.14313300
H	5.13347900	-3.94585300	-0.00054600
C	2.79122900	-0.80027000	2.54344800
H	3.27456700	0.16436900	2.73185700
H	1.71187600	-0.62384500	2.57373300
H	3.04585600	-1.45602300	3.37655100
C	2.79134700	-0.79946700	-2.54364600
H	1.71189200	-0.62369700	-2.57412600
H	3.27414500	0.16554800	-2.73149200
H	3.04658900	-1.45468600	-3.37697900
C	-2.79075800	-0.80059400	2.54355800
H	-1.71133900	-0.62453600	2.57383500
H	-3.27374900	0.16422300	2.73193200
H	-3.04560100	-1.45623400	3.37668200
C	-2.79179800	-0.79915800	-2.54350200
H	-3.27370100	0.16643000	-2.73066100
H	-1.71217100	-0.62448000	-2.57451400
H	-3.04816000	-1.45375700	-3.37697700
Co	-0.00003500	0.01666000	0.00014600

^{0}Co(+)^{B}-1B

Atom	x	y	z
C	-1.17381700	2.51243100	0.01705200
C	-1.20890000	3.90623500	0.02644000
C	0.00001700	4.60245400	0.02992900
C	1.20892200	3.90620700	0.02545900
C	1.17379900	2.51240800	0.01620700
N	-0.00001800	1.85912200	0.01074300
H	0.00003000	5.68613100	0.03688900
H	-2.15142400	4.43904500	0.03121200

H	2.15145900	4.43900000	0.02941000
C	-2.31690400	1.57367800	0.01409600
C	2.31687100	1.57363600	0.01331400
N	1.97261200	0.32134900	0.00263700
N	-1.97261700	0.32139900	0.00285700
C	3.71469900	2.10776700	0.02543900
H	3.88890100	2.74007600	-0.85091700
H	3.87455200	2.73635400	0.90714100
H	4.45521600	1.31196300	0.02979400
C	-3.71472800	2.10781900	0.02653300
H	-3.87460500	2.73576900	0.90869300
H	-3.88888300	2.74076800	-0.84936500
H	-4.45526900	1.31203300	0.03028700
C	2.99321900	-0.69842500	0.00176400
C	3.42848500	-1.21888300	1.23280100
C	3.48828800	-1.16709600	-1.22710900
C	4.37304400	-2.24798400	1.20804700
C	4.43081000	-2.19863400	-1.19848300
C	4.86873700	-2.73881100	0.00519700
H	4.72177400	-2.66610000	2.14687500
H	4.82420700	-2.57873600	-2.13584600
H	5.59773600	-3.54167700	0.00610200
C	-2.99320100	-0.69840700	0.00146300
C	-3.48756600	-1.16707400	-1.22768100
C	-3.42911200	-1.21888700	1.23225400
C	-4.43011100	-2.19861000	-1.19958200
C	-4.37369100	-2.24795500	1.20698600
C	-4.86872900	-2.73876900	0.00385400
H	-4.82300600	-2.57868700	-2.13716600
H	-4.72296500	-2.66604900	2.14562000
H	-5.59774600	-3.54161900	0.00435800
C	-3.05721900	-0.55936300	-2.54139800
H	-3.56493800	0.39364300	-2.72796600
H	-1.98391600	-0.35849000	-2.57722200
H	-3.30468800	-1.21923600	-3.37391900
C	-2.93151400	-0.66409900	2.54523600
H	-1.84934800	-0.50994100	2.54809800
H	-3.38975500	0.30517400	2.77102400
H	-3.17915300	-1.33415600	3.36940300
C	3.05861400	-0.55946900	-2.54108500
H	1.98535200	-0.35847700	-2.57743100
H	3.56653100	0.39344900	-2.72755200
H	3.30638100	-1.21947400	-3.37341300

C	2.93044500	-0.66395100	2.54556400
H	3.38931900	0.30494100	2.77172000
H	1.84841400	-0.50896100	2.54785400
H	3.17713000	-1.33429400	3.36978800
Co	-0.00002700	-0.01639000	-0.00207200
C	-0.00093600	-2.07488000	0.56966100
H	-0.92255200	-2.24061300	1.11557100
H	0.91980800	-2.23983900	1.11731900
C	0.00049100	-1.99476700	-0.79480400
H	0.92107700	-2.09570600	-1.35749400
H	-0.91883200	-2.09627600	-1.35949700

$^{0}Co(+)^{B}$-2B

Atom	x	y	z
C	-1.19448200	0.74604700	2.22531600
C	-1.20697000	1.57230900	3.34557400
C	0.00034300	1.97799500	3.91861400
C	1.20741200	1.57134800	3.34573800
C	1.19440600	0.74511700	2.22547700
N	-0.00017800	0.31163600	1.70092000
H	0.00054200	2.62118300	4.79084500
H	-2.14870800	1.90046700	3.77002100
H	2.14937300	1.89875000	3.77028200
C	-2.31092000	0.22696500	1.48811300
C	2.31053300	0.22519000	1.48842500
N	1.95884800	-0.47100100	0.41534000
N	-1.95963900	-0.46952300	0.41509200
C	3.72763100	0.43246000	1.94844500
H	3.87532600	1.45372800	2.30610200
H	3.98063600	-0.23978300	2.77581300
H	4.44255400	0.24953200	1.14792100
C	-3.72793500	0.43518900	1.94794700
H	-3.98209300	-0.23815800	2.77406900
H	-3.87454600	1.45601700	2.30725100
H	-4.44278500	0.25443400	1.14685600
C	2.97321400	-1.20128600	-0.29115300
C	3.32538500	-2.48152200	0.18421800
C	3.59075100	-0.65866700	-1.43458100
C	4.27436000	-3.22126900	-0.52607000
C	4.53956200	-1.43340300	-2.10798200
C	4.87619000	-2.70821000	-1.66833700
H	4.54236900	-4.21249200	-0.17197200
H	5.02343800	-1.02170100	-2.98866900
H	5.61045400	-3.29592700	-2.20990300

C	-2.97453900	-1.19896800	-0.29150100
C	-3.59160400	-0.65576000	-1.43491400
C	-3.32779700	-2.47894400	0.18375600
C	-4.54103600	-1.42965500	-2.10840500
C	-4.27738200	-3.21783800	-0.52660100
C	-4.87875400	-2.70420300	-1.66885200
H	-5.02452500	-1.01748100	-2.98908300
H	-4.54622600	-4.20886100	-0.17257800
H	-5.61348300	-3.29127800	-2.21048300
C	-3.28580700	0.74097300	-1.91415100
H	-3.39834400	1.47907800	-1.11569300
H	-2.26200500	0.83560600	-2.27867300
H	-3.95800000	1.02499900	-2.72584900
C	-2.72072800	-3.04653900	1.44437800
H	-1.65813800	-2.81175600	1.52596300
H	-3.20448500	-2.64020700	2.33955800
H	-2.84128200	-4.13123100	1.47842400
C	3.28605700	0.73824300	-1.91404100
H	2.26296400	0.83307700	-2.28056600
H	3.39717400	1.47616300	-1.11524200
H	3.95980000	1.02231300	-2.72444000
C	2.71783300	-3.04848300	1.44488900
H	3.20191700	-2.64244200	2.34002600
H	1.65543700	-2.81281400	1.52644400
H	2.83749500	-4.13327000	1.47905500
Co	-0.00033400	-0.44591200	0.03977500
C	-0.00101900	-2.34434600	-0.96221500
H	-0.91824500	-2.85830200	-0.70801800
H	0.91575400	-2.85898200	-0.70775200
C	-0.00048800	-1.32245000	-1.88709600
H	0.91590600	-1.02610300	-2.38235000
H	-0.91655800	-1.02530300	-2.38247700
Al	0.00302600	4.14627400	-1.36807400
C	-1.69350800	4.61714000	-0.45284800
H	-2.57615600	4.13853500	-0.89194500
H	-1.68612700	4.36997000	0.61490600
H	-1.87330100	5.69967500	-0.51240000
C	1.69887700	4.61480200	-0.45037900
H	1.69028100	4.36552700	0.61688400
H	2.58189200	4.13686700	-0.88945800
H	1.87896500	5.69741900	-0.50752600
C	0.00049100	1.40182100	-0.82343000
H	0.90259000	1.88649800	-0.44516700

H	-0.90128100	1.88735000	-0.44549600
H	0.00067500	1.37066300	-1.91226400
C	0.00402900	3.96005700	-3.34105900
H	0.00405100	4.94981300	-3.81893200
H	0.88612600	3.43714000	-3.72743200
H	-0.87761700	3.43688400	-3.72812300

^{0}Co(+)^{B}-TS2B/3B

Atom	x	y	z
C	3.61831600	1.23949300	-0.33137400
C	5.00210100	1.28744500	-0.47608900
C	5.72227000	0.09366000	-0.55478500
C	5.04608300	-1.12532500	-0.47346600
C	3.66138600	-1.12720800	-0.32904700
N	2.96329600	0.04390000	-0.27937800
H	6.79981700	0.11321400	-0.66793900
H	5.51408700	2.24138900	-0.52408500
H	5.59204600	-2.06033400	-0.51911800
C	2.68909800	2.34794300	-0.19928700
C	2.77310500	-2.26851000	-0.19593000
N	1.51818800	-1.93812100	-0.00272300
N	1.44715000	1.97260900	-0.00452700
C	3.30501700	-3.66955600	-0.27861800
H	3.81431200	-3.83276200	-1.23338900
H	4.04096100	-3.85192400	0.51094000
H	2.51329700	-4.40920300	-0.18222200
C	3.16970400	3.76724200	-0.28474800
H	3.91033300	3.97337300	0.49439300
H	3.65872200	3.95103600	-1.24643400
H	2.35375800	4.47809300	-0.17471600
C	0.52435900	-2.96680800	0.13412900
C	0.23978500	-3.48158300	1.41114800
C	-0.17496100	-3.39524700	-1.00780200
C	-0.78290100	-4.42628400	1.52709600
C	-1.19056700	-4.34041700	-0.84282900
C	-1.49927400	-4.84995600	0.41331100
H	-1.02312400	-4.82544400	2.50781100
H	-1.74987500	-4.67140000	-1.71233800
H	-2.30101100	-5.57220800	0.52433300
C	0.41750600	2.96506100	0.13588600
C	-0.30075200	3.36916500	-1.00314400
C	0.11833400	3.46732400	1.41465100
C	-1.35026700	4.27569300	-0.83335700
C	-0.93795200	4.37362400	1.53529600

C	-1.67349400	4.77167600	0.42451200
H	-1.92506200	4.58640800	-1.70023600
H	-1.18941900	4.76236800	2.51736900
H	-2.50167200	5.46281000	0.53917500
C	0.06332200	2.86544100	-2.37894600
H	0.96738000	3.35500200	-2.75865200
H	0.26364600	1.79149200	-2.38321400
H	-0.73847600	3.06641300	-3.09132900
C	0.92704500	3.06341600	2.62300600
H	1.09814700	1.98520300	2.65695300
H	1.91357000	3.54065700	2.62427700
H	0.42302900	3.35914000	3.54465200
C	0.17384700	-2.87556700	-2.38162700
H	0.32732300	-1.79393100	-2.38453800
H	1.10022900	-3.32486000	-2.75725600
H	-0.61501900	-3.11075200	-3.09798500
C	1.02970800	-3.05014600	2.62234500
H	2.03116600	-3.49518700	2.62812600
H	1.16555600	-1.96694600	2.65526400
H	0.53182300	-3.36096900	3.54235300
Co	1.17199000	0.01143400	0.07977300
C	-0.63410100	-0.01987900	1.07537800
H	-0.74120800	0.88888300	1.66038300
H	-0.71197600	-0.93047100	1.66230500
C	-1.21518100	-0.03073800	-0.20304100
H	-1.26794600	-0.94731300	-0.77270500
H	-1.29487200	0.88132900	-0.77674600
Al	-5.81010200	-0.05583200	-0.23110500
C	-6.24878100	-1.70730100	-1.28914900
H	-5.86709200	-1.67322100	-2.31850100
H	-5.85091700	-2.62515600	-0.83600600
H	-7.33467500	-1.85561100	-1.37273700
C	-6.31392600	-0.13288700	1.71082900
H	-5.95950900	-1.04425500	2.21039500
H	-5.92542900	0.71466100	2.29090000
H	-7.40508800	-0.11764200	1.84309200
C	-3.57715700	-0.05883000	-0.20734300
H	-3.42463300	-0.99249500	0.31668900
H	-3.45423500	-0.04850400	-1.28328300
H	-3.43537600	0.86663800	0.33371700
C	-6.23456900	1.67903000	-1.15325800
H	-7.31868400	1.83067200	-1.25169500
H	-5.85270200	2.55508300	-0.61203900

H	-5.82665500	1.73528000	-2.17157700

^{0}Co(+)^{B}-3B

Atom	x	y	z
C	-1.19022100	2.69903200	0.09065500
C	-1.20735300	4.08769000	0.00535300
C	0.00000000	4.79119800	-0.02662900
C	1.20735400	4.08769000	0.00535100
C	1.19022200	2.69903200	0.09065400
N	0.00000000	2.01600700	0.16461300
H	0.00000000	5.87291900	-0.09399800
H	-2.15153800	4.61892900	-0.04276000
H	2.15153900	4.61892800	-0.04276300
C	-2.30446000	1.78299600	0.08871100
C	2.30446000	1.78299600	0.08871000
N	1.94226600	0.51438700	0.05862700
N	-1.94226700	0.51438800	0.05862800
C	3.72183800	2.28156300	0.12352900
H	3.96964000	2.82413600	-0.79484800
H	3.86562700	2.97785800	0.95474200
H	4.43392700	1.46611300	0.23464300
C	-3.72183800	2.28156400	0.12353100
H	-3.86562600	2.97785800	0.95474500
H	-3.96963900	2.82413900	-0.79484500
H	-4.43392700	1.46611500	0.23464300
C	2.93470200	-0.51700000	0.06980300
C	3.20928900	-1.17556200	1.28220100
C	3.57632800	-0.88764200	-1.12540900
C	4.14833000	-2.20879500	1.27967500
C	4.50493000	-1.93131000	-1.08214900
C	4.79362400	-2.58913000	0.10766500
H	4.36988500	-2.72251000	2.21060900
H	5.00217300	-2.23128900	-2.00003600
H	5.51507200	-3.39987800	0.12111200
C	-2.93470300	-0.51699900	0.06980300
C	-3.57632800	-0.88764100	-1.12540900
C	-3.20928900	-1.17556300	1.28220100
C	-4.50492900	-1.93131000	-1.08215000
C	-4.14833000	-2.20879700	1.27967400
C	-4.79362300	-2.58913100	0.10766300
H	-5.00217200	-2.23128800	-2.00003700
H	-4.36988400	-2.72251200	2.21060800
H	-5.51507100	-3.39987900	0.12111000
C	-3.28783500	-0.17559600	-2.42416800

H	-3.78451900	0.80004800	-2.47138300
H	-2.21902700	0.00185900	-2.55616400
H	-3.64496800	-0.76086800	-3.27382200
C	-2.51468600	-0.76865000	2.55763000
H	-1.42689000	-0.81983900	2.45470800
H	-2.75036600	0.26212600	2.84046600
H	-2.80881900	-1.41710400	3.38517900
C	3.28783400	-0.17559800	-2.42416800
H	2.21902600	0.00185800	-2.55616400
H	3.78451900	0.80004600	-2.47138500
H	3.64496600	-0.76087100	-3.27382300
C	2.51468600	-0.76864800	2.55763000
H	2.75036500	0.26212800	2.84046400
H	1.42689000	-0.81983800	2.45470800
H	2.80882000	-1.41710100	3.38518000
C	-0.00000100	-1.52365300	-0.97712000
H	-0.87897400	-1.60105400	-1.62855400
H	0.87897200	-1.60105400	-1.62855500
C	0.00000000	-2.72839400	-0.01594600
H	-0.87712800	-2.69397500	0.64142400
H	0.87712800	-2.69397500	0.64142400
C	0.00000000	-4.08374500	-0.74323900
H	-0.88312800	-4.18430000	-1.38210000
H	0.88312900	-4.18429900	-1.38210000
H	0.00000100	-4.92387500	-0.03852200
Co	0.00000000	0.20716300	-0.01227000

^{0}Co(+)^{B}-1C

C	-1.03156700	3.20945500	0.05767100
C	-0.99338300	4.60093800	0.10180400
C	0.24332900	5.24880000	0.12674000
C	1.41743100	4.49326700	0.10596100
C	1.33178900	3.10384800	0.06163100
N	0.11985900	2.47835700	0.03862600
H	0.29169800	6.33096000	0.16139000
H	-1.91375900	5.17308800	0.11680500
H	2.38484300	4.98169500	0.12456700
C	-2.19247800	2.33764100	0.02110700
C	2.41026900	2.13182800	0.02859000
N	1.99762600	0.88649200	-0.00624100
N	-1.89151500	1.06094200	-0.01341900
C	3.84310300	2.58095500	0.03023400
H	4.03509600	3.25686400	-0.80878500

H	4.07134400	3.13634600	0.94571100
H	4.53267300	1.74301000	-0.04060000
C	-3.58006400	2.91116300	0.01812600
H	-3.75459100	3.50256400	0.92267700
H	-3.71688200	3.58408500	-0.83414300
H	-4.33992200	2.13483800	-0.03380300
C	2.96935300	-0.16994600	-0.05346200
C	3.46499500	-0.70116200	1.14814800
C	3.37667400	-0.66364900	-1.30386800
C	4.40695400	-1.72943300	1.07433700
C	4.32061600	-1.69309100	-1.32956800
C	4.83835000	-2.22112600	-0.15220800
H	4.79422100	-2.15692800	1.99410300
H	4.64385300	-2.08808500	-2.28805800
H	5.56247600	-3.02819400	-0.18992500
C	-2.95049300	0.09225800	-0.06140300
C	-3.37893100	-0.38365200	-1.31187500
C	-3.49906500	-0.38620400	1.13931900
C	-4.39444700	-1.34216600	-1.33910500
C	-4.51404100	-1.34304700	1.06416700
C	-4.96411600	-1.81718400	-0.16279500
H	-4.73321100	-1.72409400	-2.29737900
H	-4.94277000	-1.72955300	1.98361000
H	-5.74604600	-2.56844000	-0.20168800
C	-2.75530000	0.12217100	-2.58805700
H	-2.98552800	1.17808300	-2.76710100
H	-1.66551300	0.03878800	-2.55484700
H	-3.11547800	-0.44436100	-3.44841100
C	-3.00411100	0.11137600	2.47443000
H	-1.91292900	0.08395800	2.52940400
H	-3.30553100	1.14759200	2.66441700
H	-3.40113700	-0.49939100	3.28684100
C	2.81336000	-0.09750100	-2.58323100
H	1.72036800	-0.07889000	-2.56104000
H	3.14260300	0.93280800	-2.75712700
H	3.12794500	-0.69192100	-3.44284100
C	2.99740500	-0.17617000	2.48284500
H	3.37988900	0.83055700	2.68466600
H	1.90718300	-0.11443700	2.52762200
H	3.33613700	-0.82285700	3.29408700
Co	0.04025400	0.65305800	-0.00031300
Al	-0.24771600	-3.91962400	0.14614500
C	-0.77778800	-4.25881400	-1.74172100

H	-1.74561900	-3.81596200	-2.00518100
H	-0.04539600	-3.88285500	-2.46653300
H	-0.87062100	-5.33651900	-1.93525200
C	1.59326200	-4.44059000	0.68302200
H	2.36670600	-4.13938200	-0.03143500
H	1.88873200	-4.03564600	1.65818100
H	1.66399400	-5.53409100	0.77332700
C	-0.03876400	-1.35060300	0.01007100
H	0.77785800	-1.75649800	-0.59300800
H	-1.01807200	-1.68072400	-0.34391000
H	0.10476400	-1.60595900	1.06937400
C	-1.64588800	-4.09196600	1.55005400
H	-1.88220100	-5.15093700	1.72640300
H	-1.33353200	-3.68721300	2.52075400
H	-2.59069900	-3.60467400	1.28714900

^{1}Co(+)^{B}

Atom	x	y	z
C	1.17456000	2.41075600	-0.07718100
C	1.21197800	3.80692300	-0.08130600
C	-0.00000300	4.49725600	-0.00001700
C	-1.21198300	3.80692200	0.08128500
C	-1.17456100	2.41075500	0.07719400
N	0.00000100	1.78262600	0.00002000
H	-0.00000400	5.58114700	-0.00003100
H	2.14731200	4.34928000	-0.14229800
H	-2.14731800	4.34927800	0.14225600
C	2.32828200	1.45960400	-0.14324300
C	-2.32828100	1.45960200	0.14325500
N	-2.02224500	0.19992800	0.08650200
N	2.02224600	0.19992900	-0.08652300
C	-3.71258900	2.01467900	0.28200600
H	-3.76892000	2.67732900	1.15086300
H	-3.97812500	2.61573400	-0.59341700
H	-4.45494000	1.22839400	0.39779900
C	3.71259200	2.01468600	-0.28196000
H	3.76893800	2.67734300	-1.15081100
H	3.97811000	2.61573400	0.59347300
H	4.45494600	1.22840400	-0.39774800
C	-3.02828400	-0.82693400	0.10611500
C	-3.76703800	-1.11070800	-1.05594700
C	-3.16358100	-1.58861900	1.28094000
C	-4.67776200	-2.16968100	-1.00430900

C	-4.09418000	-2.62814500	1.28563200
C	-4.84935700	-2.91813700	0.15405400
H	-5.25539600	-2.40933000	-1.89131700
H	-4.22209200	-3.21867500	2.18708500
H	-5.56371900	-3.73376400	0.17234700
C	3.02828500	-0.82693300	-0.10611900
C	3.76702900	-1.11069900	1.05595100
C	3.16359000	-1.58862800	-1.28093700
C	4.67775100	-2.16967500	1.00432900
C	4.09418800	-2.62815500	-1.28561300
C	4.84935500	-2.91814000	-0.15402600
H	5.25537600	-2.40931900	1.89134500
H	4.22210700	-3.21869300	-2.18706100
H	5.56371500	-3.73376800	-0.17230600
C	3.58348000	-0.32602200	2.33270700
H	4.06987700	0.65425800	2.29053700
H	2.52823200	-0.15250300	2.56105200
H	4.02017900	-0.85945900	3.17761700
C	2.33063900	-1.28985400	-2.50213300
H	1.25567400	-1.36738600	-2.28928800
H	2.50373600	-0.28120700	-2.88901500
H	2.54941100	-1.99276200	-3.30643000
C	-2.33061700	-1.28983600	2.50212600
H	-1.25565400	-1.36737400	2.28927100
H	-2.50370700	-0.28118600	2.88900200
H	-2.54938300	-1.99273800	3.30643100
C	-3.58349600	-0.32603900	-2.33270900
H	-4.06984900	0.65426200	-2.29052500
H	-2.52824700	-0.15256500	-2.56108300
H	-4.02024200	-0.85945800	-3.17760500
Co	-0.00000100	-0.18030400	-0.00002600

^{1}Co(+)^{B}-1B

Atom	x	y	z
C	1.16360000	2.43085300	-0.08676600
C	1.19967200	3.82539000	-0.15475400
C	-0.00000800	4.52783300	-0.18076800
C	-1.19968200	3.82538500	-0.15456400
C	-1.16360300	2.43084800	-0.08662300
N	0.00000500	1.76412200	-0.03729600
H	-0.00001600	5.61064600	-0.22925200
H	2.14248600	4.35504000	-0.18811000
H	-2.14250200	4.35503600	-0.18774200
C	2.38581500	1.57450300	-0.08843700

C	-2.38583100	1.57448000	-0.08829100
N	-2.18006100	0.30888100	-0.03236800
N	2.18001400	0.30889700	-0.03242200
C	-3.72905400	2.24205300	-0.18332700
H	-3.89510300	2.90692600	0.66943100
H	-3.79011500	2.85671700	-1.08615600
H	-4.53475900	1.51268300	-0.21182700
C	3.72905300	2.24203400	-0.18363000
H	3.79014300	2.85644300	-1.08663200
H	3.89510200	2.90713700	0.66894400
H	4.53473700	1.51263600	-0.21192500
C	-3.27717600	-0.61506300	-0.03976400
C	-3.60043100	-1.25527000	-1.24901500
C	-3.93725600	-0.92105400	1.16290600
C	-4.62071600	-2.20865400	-1.23501800
C	-4.94644200	-1.88720600	1.12743800
C	-5.29050000	-2.52603600	-0.05822200
H	-4.88889700	-2.70770300	-2.16078800
H	-5.46597200	-2.13929200	2.04646100
H	-6.07666000	-3.27290500	-0.06472900
C	3.27712500	-0.61507100	-0.03976100
C	3.93713900	-0.92098100	1.16297700
C	3.60044300	-1.25534400	-1.24894500
C	4.94627400	-1.88718600	1.12764400
C	4.62068800	-2.20877600	-1.23481400
C	5.29037200	-2.52611800	-0.05795400
H	5.46575200	-2.13921900	2.04671000
H	4.88890700	-2.70789900	-2.16053300
H	6.07650100	-3.27302100	-0.06436300
C	3.58019000	-0.23339900	2.45864600
H	3.93275900	0.80325400	2.48485900
H	2.49958800	-0.20446000	2.62687800
H	4.03471500	-0.74542200	3.30750200
C	2.87865800	-0.91422000	-2.52906100
H	1.79250700	-1.01056300	-2.42377200
H	3.07233700	0.11446300	-2.85006500
H	3.19164800	-1.57181400	-3.34072400
C	-3.58037400	-0.23361300	2.45867400
H	-2.49974300	-0.20377800	2.62650000
H	-3.93387200	0.80271400	2.48537800
H	-4.03412600	-0.74631700	3.30753800
C	-2.87845600	-0.91417400	-2.52903200
H	-3.07107800	0.11487900	-2.84946000

H	-1.79238600	-1.01171800	-2.42390700
H	-3.19219600	-1.57101400	-3.34101200
Co	0.00009500	-0.30915300	0.17041700
C	0.68508400	-2.28105900	0.63572000
H	1.24678800	-2.20441800	1.56140900
H	1.25331400	-2.62761800	-0.22081200
C	-0.68496300	-2.28106800	0.63542600
H	-1.25279400	-2.62757100	-0.22140700
H	-1.24708400	-2.20453600	1.56086000

^{1}Co(+)^{B}-2B

Atom	x	y	z
C	1.12467500	0.63400200	-2.18520400
C	1.20650000	1.40812500	-3.34423600
C	0.03486200	1.88880600	-3.91871700
C	-1.18855600	1.57010100	-3.33791900
C	-1.20358800	0.80041400	-2.17323800
N	-0.06055700	0.37408500	-1.60475200
H	0.07456300	2.50134500	-4.81207800
H	2.16558900	1.63947700	-3.78850500
H	-2.11102500	1.92040100	-3.78302300
C	2.29998300	0.00054200	-1.53449500
C	-2.44665200	0.35891200	-1.49269800
N	-2.28367500	-0.36590000	-0.44063300
N	2.04699300	-0.72172200	-0.49875500
C	-3.77703900	0.75422000	-2.07786200
H	-3.88336600	1.84302000	-2.09335300
H	-3.87214800	0.40507900	-3.11012800
H	-4.59991100	0.33883600	-1.49997500
C	3.66456800	0.21667900	-2.13348600
H	3.69499000	-0.11208500	-3.17631100
H	3.92257900	1.27994800	-2.11988200
H	4.42737000	-0.32813400	-1.58131800
C	-3.39129500	-0.94748300	0.24837700
C	-3.77705000	-2.25396400	-0.10920400
C	-4.01628500	-0.26067700	1.30629500
C	-4.79989400	-2.86653000	0.61794400
C	-5.03476000	-0.91627200	2.00333100
C	-5.42582400	-2.20805400	1.67001900
H	-5.10437500	-3.87432500	0.35151500
H	-5.52522700	-0.39827400	2.82193200
H	-6.21527300	-2.69959600	2.22903100
C	3.06086700	-1.49879300	0.14119100
C	3.82584000	-0.96846900	1.19707300

C	3.20636400	-2.83940800	-0.26866600
C	4.73839000	-1.81395400	1.83524400
C	4.12942300	-3.64388400	0.40218100
C	4.89113300	-3.14061000	1.45047800
H	5.33654400	-1.41581300	2.64920000
H	4.24822800	-4.67845900	0.09398100
H	5.60238000	-3.77901800	1.96418500
C	3.68245100	0.46396100	1.64795700
H	3.72777600	1.17447400	0.81907600
H	2.73143000	0.64038400	2.15632400
H	4.47632600	0.72917700	2.34758900
C	2.39994300	-3.39222800	-1.41841500
H	1.33562900	-3.16749300	-1.31238300
H	2.71591100	-2.96820400	-2.37810800
H	2.51558500	-4.47527800	-1.48833100
C	-3.62060400	1.14686400	1.67688700
H	-2.55499400	1.23117300	1.89690300
H	-3.82796800	1.85922500	0.87190400
H	-4.17099000	1.48495200	2.55607600
C	-3.12239600	-2.96968700	-1.26560900
H	-3.42358100	-2.54351800	-2.22928900
H	-2.03275200	-2.90296700	-1.22056100
H	-3.40045000	-4.02507500	-1.27776200
Co	-0.10789000	-0.37805700	0.33282900
C	-0.23155700	-2.27198200	1.29470200
H	0.64669300	-2.84195000	1.01233700
H	-1.18942600	-2.71730100	1.04867500
C	-0.14479200	-1.27881800	2.24951600
H	-1.03126900	-0.91783100	2.76152100
H	0.79912800	-1.04575900	2.73189300
Al	0.69442500	3.91423100	1.27478500
C	1.60729000	4.27721000	-0.49577000
H	2.53187400	3.69440800	-0.62822500
H	0.97168500	4.05908100	-1.36640100
H	1.90315700	5.33038500	-0.59754800
C	-1.05066200	4.90057000	1.47944300
H	-1.73283200	4.74825200	0.63012500
H	-1.60660500	4.60547900	2.38028500
H	-0.90675400	5.98709800	1.55763200
C	0.15740800	1.84302800	1.16607900
H	-0.67333500	1.90005600	0.46611300
H	1.09333900	1.44282900	0.77498000
H	-0.10019800	1.51932600	2.17000600

C	1.93675200	4.08695300	2.84905600
H	2.27620900	5.12262900	2.98995100
H	1.46906200	3.79150200	3.79839600
H	2.84967300	3.48238500	2.75243100

^{1}Co(+)^{B}-TS2B/3B

Atom	x	y	z
C	-1.09017700	-0.82058000	2.45619800
C	-1.10467500	-0.85065700	3.84637600
C	0.09060000	-0.73108000	4.55901100
C	1.28734000	-0.61523500	3.84854100
C	1.27238500	-0.59531900	2.45762100
N	0.08730000	-0.67011200	1.76157200
H	0.09073400	-0.74146300	5.64262300
H	-2.04150200	-0.96573400	4.37824200
H	2.22736900	-0.54688700	4.38292800
C	-2.27752600	-0.97527700	1.62739300
C	2.47266100	-0.56277900	1.63291200
N	2.28563500	-0.52323000	0.34134500
N	-2.10042600	-0.85847200	0.33868800
C	3.83115000	-0.62784600	2.28987600
H	3.97456300	0.20968400	2.97858200
H	3.94816400	-1.54692600	2.87142900
H	4.62815800	-0.59419600	1.54943800
C	-3.60634100	-1.28472500	2.27358800
H	-3.54116900	-2.16870500	2.91338200
H	-3.93795100	-0.45329600	2.90311500
H	-4.37525700	-1.46396100	1.52442200
C	3.37131800	-0.64010100	-0.57167400
C	3.74074800	-1.92204500	-1.02826200
C	4.01362800	0.51313300	-1.06249800
C	4.74381800	-2.02418800	-1.99485600
C	5.01231500	0.36308600	-2.02797200
C	5.37600700	-0.89328200	-2.49943900
H	5.02949900	-3.00863200	-2.35435300
H	5.51050500	1.24914100	-2.41094400
H	6.14965700	-0.99064900	-3.25432800
C	-3.16156400	-1.07745100	-0.58631300
C	-4.02726300	-0.02797900	-0.94803100
C	-3.28306300	-2.35099700	-1.18392700
C	-4.97744700	-0.25851000	-1.94792800
C	-4.24976500	-2.53621400	-2.17317700
C	-5.08735100	-1.49703900	-2.56640500
H	-5.64166500	0.55114600	-2.23727500

H	-4.34498900	-3.51256400	-2.63960300
H	-5.82610800	-1.65575900	-3.34544700
C	-3.99437400	1.30676700	-0.24451000
H	-4.68862200	1.32001200	0.60412300
H	-3.00847700	1.54434900	0.15229000
H	-4.29618000	2.11377300	-0.91565700
C	-2.42284600	-3.50538100	-0.73198300
H	-1.36664300	-3.23345700	-0.68850900
H	-2.70290400	-3.84329500	0.27223000
H	-2.53074000	-4.35825200	-1.40508400
C	3.65971900	1.88128900	-0.53686800
H	2.58552100	2.06580900	-0.57041200
H	3.96594400	2.00605100	0.50766200
H	4.15387600	2.66381800	-1.11547500
C	3.08629600	-3.16138800	-0.46972400
H	3.38627800	-3.34399300	0.56819200
H	1.99750700	-3.07606600	-0.47139700
H	3.36433300	-4.04387200	-1.04937900
Co	0.06960500	-0.49764800	-0.18862000
C	0.20278900	-1.21747300	-2.13692400
H	-0.68423400	-1.79121200	-2.38824900
H	1.14578700	-1.73048400	-2.29484000
C	0.17161000	0.17777600	-2.44405600
H	1.10322000	0.62553100	-2.76986900
H	-0.69481900	0.57452400	-2.96269800
Al	-0.59009100	4.46041300	-0.05611300
C	-1.19393700	3.95159200	1.75906400
H	-1.36838100	4.85162700	2.36545500
H	-2.13500900	3.39165700	1.76867300
H	-0.45761000	3.35574100	2.30930400
C	1.27436200	5.07739200	-0.30263200
H	1.99215400	4.58814500	0.36418700
H	1.64522200	4.95620200	-1.32636000
H	1.34252400	6.15275000	-0.08507300
C	-0.13897800	1.64754400	-1.01631000
H	0.32309600	1.76078200	-0.02669200
H	-1.21326800	1.80561400	-0.96705300
H	0.33156600	2.34762100	-1.70179300
C	-1.91878400	4.88449500	-1.45944500
H	-2.84404400	4.30479600	-1.37668600
H	-2.21420300	5.94128100	-1.39939000
H	-1.53353500	4.73800700	-2.47462100

^{1}Co(+)^{B}-3B

Atom	x	y	z
C	1.18583200	2.67571500	0.10616600
C	1.20677500	4.06507000	0.03196000
C	0.00009800	4.77249000	0.03276400
C	-1.20661600	4.06512200	0.03195700
C	-1.18572700	2.67577300	0.10617000
N	0.00002700	2.00769300	0.25831300
H	0.00011800	5.85468700	-0.02788900
H	2.14657300	4.59810200	-0.05356500
H	-2.14638800	4.59819900	-0.05356500
C	2.33869100	1.79857900	-0.03424000
C	-2.33863600	1.79868500	-0.03424700
N	-2.05967300	0.52199100	-0.15754700
N	2.05967500	0.52188100	-0.15758000
C	-3.73055200	2.37676500	-0.05949200
H	-3.99218600	2.82686700	0.90323900
H	-3.80972000	3.16383000	-0.81412600
H	-4.47265300	1.61497600	-0.29141600
C	3.73064800	2.37654900	-0.05941500
H	3.80990700	3.16361100	-0.81404500
H	3.99229200	2.82661600	0.90332500
H	4.47268900	1.61470000	-0.29133600
C	-3.07620400	-0.46536400	-0.29120600
C	-3.21970600	-1.09301600	-1.54538200
C	-3.84885400	-0.87263800	0.81430800
C	-4.16372200	-2.11081300	-1.68210500
C	-4.77505500	-1.90403300	0.63291200
C	-4.94028100	-2.51858300	-0.60207400
H	-4.28437700	-2.59294100	-2.64792300
H	-5.36918100	-2.23072500	1.48160900
H	-5.66318700	-3.31932700	-0.72086900
C	3.07621000	-0.46549600	-0.29117000
C	3.84876300	-0.87277300	0.81441300
C	3.21984800	-1.09310100	-1.54534300
C	4.77497400	-1.90417000	0.63309100
C	4.16387300	-2.11091000	-1.68199300
C	4.94030600	-2.51871300	-0.60188900
H	5.36900600	-2.23089500	1.48184100
H	4.28462400	-2.59301500	-2.64781000
H	5.66321100	-3.31946800	-0.72062100
C	3.69351600	-0.23103100	2.17159700
H	4.24269300	0.71447700	2.24066500

H	2.64878200	-0.01641300	2.40142300
H	4.08234800	-0.88584500	2.95384600
C	2.37357200	-0.66452000	-2.71722000
H	1.30655000	-0.74220500	-2.48831900
H	2.55477500	0.37878400	-2.99361100
H	2.57777100	-1.28294500	-3.59348300
C	-3.69364100	-0.23092400	2.17150900
H	-2.64886800	-0.01661600	2.40146900
H	-4.24253300	0.71474800	2.24053400
H	-4.08276300	-0.88562700	2.95370300
C	-2.37327200	-0.66448400	-2.71716200
H	-2.55424100	0.37887400	-2.99347000
H	-1.30628000	-0.74241400	-2.48817900
H	-2.57751000	-1.28280800	-3.59348800
C	-0.00008100	-1.59217100	1.58988000
H	0.87493800	-1.59032100	2.25564500
H	-0.87489800	-1.59010100	2.25590000
C	-0.00039300	-2.89071600	0.76399600
H	0.87524500	-2.91651000	0.10201300
H	-0.87623800	-2.91625300	0.10227700
C	-0.00041100	-4.17018800	1.61519300
H	0.88218500	-4.20890700	2.26221300
H	-0.88284900	-4.20870900	2.26244000
H	-0.00058800	-5.07527900	0.99641500
Co	0.00003100	0.05375100	0.42648100

^{1}Co(+)^{B}-1C

C	-1.16670100	3.00936200	-0.70197100
C	-1.18002300	4.35652600	-1.04931900
C	0.03006600	5.02138500	-1.27144700
C	1.23277400	4.33780400	-1.06733700
C	1.20366100	2.99123500	-0.71834200
N	0.01357300	2.31927600	-0.64818900
H	0.03623500	6.07073900	-1.54223500
H	-2.11673300	4.89607600	-1.12455500
H	2.17644500	4.86287000	-1.15672000
C	-2.32569300	2.22073400	-0.30155700
C	2.35482600	2.18718200	-0.32609900
N	2.06954900	1.01220800	0.17886400
N	-2.05355200	1.03938900	0.19516400
C	3.74844100	2.73860700	-0.47807300
H	4.00502400	2.88214200	-1.53214800
H	3.83417600	3.71334700	0.00953500

H	4.48831200	2.07550600	-0.03403700
C	-3.71194900	2.79462300	-0.43801400
H	-3.78018800	3.76223500	0.06650600
H	-3.97163600	2.95994500	-1.48804100
H	-4.45931000	2.13547300	-0.00083900
C	3.08180100	0.10351700	0.60514100
C	3.23220800	-0.10712100	1.99041500
C	3.83865400	-0.63058900	-0.32829700
C	4.17189200	-1.04132000	2.42635500
C	4.76010400	-1.56468800	0.15501200
C	4.93432300	-1.76882100	1.51802400
H	4.29898800	-1.20451100	3.49252300
H	5.34006400	-2.14510900	-0.55620100
H	5.65218000	-2.50158700	1.87189200
C	-3.07586000	0.13839900	0.61255700
C	-3.84761000	-0.56978400	-0.32921500
C	-3.22097600	-0.09461200	1.99465200
C	-4.78004800	-1.49832800	0.14361000
C	-4.17180700	-1.02229100	2.42007300
C	-4.95024200	-1.72261400	1.50400400
H	-5.37249300	-2.05822100	-0.57384200
H	-4.29486800	-1.20232600	3.48397100
H	-5.67713200	-2.45040600	1.84956300
C	-3.68453500	-0.35966800	-1.81522700
H	-4.22887100	0.52444800	-2.16541000
H	-2.63860100	-0.22639600	-2.09739700
H	-4.07178700	-1.21617900	-2.36950800
C	-2.36765400	0.64725300	2.99226800
H	-1.30200700	0.46837600	2.81735900
H	-2.51354500	1.73016300	2.93440300
H	-2.59743400	0.33300200	4.01205000
C	3.67315300	-0.44058000	-1.81647900
H	2.63044200	-0.27804900	-2.09413300
H	4.24332800	0.42005700	-2.18386900
H	4.02910900	-1.31850700	-2.35799700
C	2.39765500	0.66603600	2.98030800
H	2.56494900	1.74488400	2.90576100
H	1.32784200	0.50652800	2.81275100
H	2.62596200	0.36264000	4.00371000
Co	0.00571800	0.41938800	-0.19728400
Al	-0.03503000	-4.12657200	-1.14575300
C	-1.60657400	-4.21877100	-2.36178600
H	-2.54781100	-3.94424500	-1.87081500

H	-1.50630800	-3.58047900	-3.24808500
H	-1.74657600	-5.24110700	-2.73949700
C	1.76549400	-4.31522500	-1.96939800
H	1.86177800	-3.79020600	-2.92764600
H	2.57192100	-3.95453400	-1.31998600
H	1.99022500	-5.37052000	-2.17740800
C	-0.01746200	-1.55323500	-0.69124000
H	0.78693700	-1.75722800	-1.40144200
H	-0.99924000	-1.80242900	-1.09895800
H	0.15917700	-2.05622200	0.26654000
C	-0.27279700	-4.77730100	0.71635500
H	-0.37922900	-5.87083700	0.73523500
H	0.57581600	-4.54320100	1.37019600
H	-1.17184000	-4.37656700	1.19950200