

Supporting Information

How reliable is DFT for predicting the redox potentials in polypyridine-based hydrogen evolution catalysts?

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Table S1A. Relative energetics (ΔG in kcal/mol) of different spin states calculated for each of the Co^{II} complexes **1-8** using the methodologies M1-M20. The energy values of the high spin quartet and low spin doublet states are represented in black and red, respectively.

	1	2	3	4	5	6	7	8
M1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4.86	5.77	9.89	3.76	6.50	6.43	-4.95	9.24
M2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	7.23	6.09	10.76	5.56	6.59	6.76	-3.47	11.09
M3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	1.98	6.05	6.71	6.32	3.85	3.50	-5.25	32.60
M4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	7.87	8.67	11.49	7.72	20.52	8.61	0.83	11.53
M5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3.28	4.22	7.33	3.85	5.52	5.35	-4.08	8.07
M6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	5.39	5.19	9.63	4.97	5.52	5.83	-2.98	9.41
M7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	5.07	6.13	10.90	4.93	7.44	7.11	-3.37	9.83
M8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	9.72	4.54	14.08	8.81	10.45	10.08	0.47	13.41
M9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	9.08	9.17	13.25	7.93	10.55	10.54	-0.77	34.66
M10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	11.96	11.28	14.69	11.93	12.08	11.95	3.06	15.40
M11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	-11.71	-9.83	-7.65	-9.64	-2.84	-2.77	-17.34	-6.78
M12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	-7.40	-6.09	-4.31	-5.59	-5.61	-5.68	-12.93	-2.45
M13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	-8.69	-7.18	-5.21	-8.50	0.22	-7.21	-15.63	-5.08
M14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	0.45	-0.66	2.63	-1.23	-0.13	-0.08	-8.39	-1.81
M15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	6.55	3.84	11.63	4.80	7.86	7.74	-3.78	10.06
M16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	8.93	8.12	12.35	8.47	8.27	8.11	-1.12	11.43
M17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	-12.95	-11.44	-9.32	-12.51	-4.18	-4.77	-18.54	-8.32
M18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	-8.05	-7.80	-5.60	-7.49	-7.44	-7.56	-14.26	-4.21
M19	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	-1.20	-1.05	2.50	2.89	-1.75	-1.59	-11.08	3.28
M20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2.99	85	5.98	1.78	1.30	1.73	-7.05	5.22

Table S1B. Relative energetics (ΔG in kcal/mol) of different spin states for each of the Fe^{III} complexes **9-11** using the methodologies M1-M20. The energy values of the high spin hextet, intermediate spin quartet, and low spin doublet states are represented in black, blue, and red, respectively.

	9	10	11
M1	0.00	0.00	0.00
	16.30	17.31	16.56
	17.57	18.39	16.48
M2	0.00	0.00	0.00
	6.72	12.32	12.33
	13.60	13.64	12.22
M3	0.00	0.00	0.00
	27.58	27.25	27.28
	38.74	39.41	38.03
M4	0.00	0.00	0.00
	15.80	24.82	24.04
	40.48	39.84	37.70
M5	0.00	0.00	0.00
	15.90	15.55	15.93
	17.98	19.55	17.33
M6	0.00	0.00	0.00
	7.69	12.59	12.75
	13.83	18.19	12.61
M7	0.00	0.00	0.00
	16.36	18.12	16.64
	17.83	19.35	16.99
M8	0.00	0.00	0.00
	2.65	16.17	16.10
	15.96	16.83	15.08
M9	0.00	0.00	0.00
	19.63	19.08	19.45
	23.42	24.77	22.78
M10	0.00	0.00	0.00
	7.46	16.19	16.45
	20.98	21.32	19.92
M11	0.00	0.00	0.00
	8.41	7.63	8.26
	3.44	4.70	2.40
M12	0.00	0.00	0.00
	7.27	6.46	7.19
	3.20	3.65	2.07
M13	0.00	0.00	0.00
	6.90	6.50	8.86
	-1.01	0.28	-2.02
M14	0.00	0.00	0.00
	8.30	7.88	8.23
	3.92	4.28	2.57
M15	0.00	0.00	0.00
	12.70	17.60	16.25
	17.58	18.64	16.87

M16	0.00	0.00	0.00
	2.06	13.21	14.64
	13.57	13.99	12.62
M17	0.00	0.00	0.00
	6.46	5.77	6.45
	0.25	1.74	-0.69
M18	0.00	0.00	0.00
	5.32	4.38	5.10
	-0.56	-0.23	-1.70
M19	0.00	0.00	0.00
	23.13	26.01	23.83
	27.31	28.30	26.62
M20	0.00	0.00	0.00
	16.61	19.55	16.82
	18.42	19.55	16.46

Table S1C. Relative energetics (ΔG in kcal/mol) of different spin states calculated for each of the Ni^{II} complexes **12**, **13** using the methodologies M1-M20. The energy values of the high spin triplet and low spin singlet states are represented in black and red, respectively.

	12	13
M1	0.00	0.00
	14.28	9.22
M2	0.00	0.00
	16.82	13.19
M3	0.00	0.00
	15.34	10.98
M4	0.00	0.00
	15.37	11.52
M5	0.00	0.00
	17.80	13.33
M6	0.00	0.00
	21.01	17.39
M7	0.00	0.00
	21.89	15.16
M8	0.00	0.00
	26.82	23.03
M9	0.00	0.00
	19.96	15.16
M10	0.00	0.00
	23.79	20.47
M11	0.00	0.00
	-1.25	-5.64
M12	0.00	0.00
	5.09	1.31
M13	0.00	0.00
	5.98	1.25
M14	0.00	0.00
	10.90	7.67
M15	0.00	0.00
	17.96	13.43
M16	0.00	0.00
	20.70	17.53
M17	0.00	0.00
	-0.44	-4.71
M18	0.00	0.00
	5.04	1.63
M19	0.00	0.00
	20.99	16.51
M20	0.00	0.00
	21.64	17.22

Table S2. Calculated Mulliken Spin Density (MSD) values on Co^{II} metal atom in complex **7**.

	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20
MSD value on Co ^{II} metal	0.90	0.84	0.89	2.71	0.89	0.82	0.89	2.66	0.91	2.73	0.82	0.78	0.84	0.84	0.91	0.87	0.81	0.77	0.92	0.84

We have performed a detailed electronic structure analysis of compound **7** to figure out the underlying reason(s) why most of the functionals fail to predict the correct spin ground state for **7**. We have performed Mulliken Spin Density (MSD) analysis and have calculated the MSD value on the Co metal atom. Analysis of the MSD values across our methodology set M1–M20 reveals an interesting feature. The calculated MSD values are consistent across the functionals M4, M8, and M10. The MSD values are 2.71, 2.66, and 2.73 for M4, M8, and M10, respectively, whereas the MSD values are much smaller, ranging from 0.77 to 0.92, for all the other functionals. These results indicate that the electronic states obtained with M4, M8, and M10 are significantly different than the electronic states obtained with the other functionals. The MSD values of 2.66 to 2.73, predicted by M4, M8, and M10, support the presence of three unpaired electrons on Co leading to the electronic state **A** (Fig S1). The lower MSD values, 0.77 to 0.92, support electronic state **B** for complex **7** with one unpaired electron on Co.

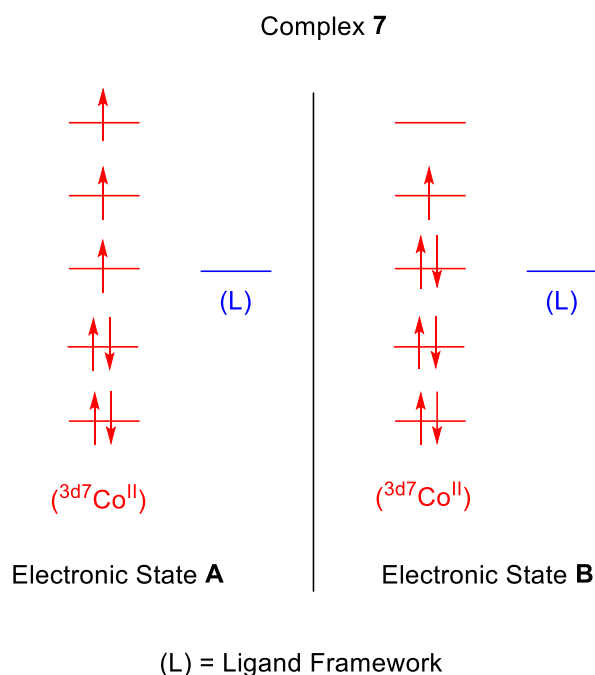
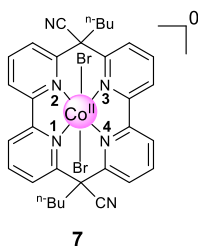
**Fig S1.** Different electronic states, **A** and **B**, obtained with the use of different functionals for the ground state of complex **7**.

Table S3. Calculated Co^{II}–N bond distances (Å) for complex **7** bearing macrocyclic polypyridine unit.

	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10
Co ^{II} –N1	1.95	1.94	1.94	2.01	1.95	1.95	1.95	2.02	1.93	2.02
Co ^{II} –N2	1.95	1.95	1.93	2.02	1.94	1.95	1.94	2.03	1.93	2.01
Co ^{II} –N3	1.95	1.94	1.94	2.01	1.95	1.95	1.95	2.02	1.93	2.02
Co ^{II} –N4	1.95	1.95	1.93	2.02	1.94	1.95	1.94	2.03	1.93	2.01
Average	1.95	1.95	1.94	2.02	1.95	1.95	1.95	2.03	1.93	2.02

	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20
Co ^{II} –N1	1.92	1.92	1.92	1.92	1.94	1.94	1.92	1.92	1.93	1.93
Co ^{II} –N2	1.92	1.92	1.92	1.92	1.94	1.94	1.92	1.92	1.93	1.93
Co ^{II} –N3	1.92	1.92	1.92	1.92	1.94	1.94	1.92	1.92	1.93	1.93
Co ^{II} –N4	1.92	1.92	1.92	1.92	1.94	1.94	1.92	1.92	1.93	1.93
Average	1.92	1.92	1.92	1.92	1.94	1.94	1.92	1.92	1.93	1.93

All the bond distances are in Å

As the part of further investigation, we calculated the bond distances of Co^{II}–N bonds within the core of the polypyridine macrocycle in complex **7**. As reported in Table S3, methodologies M4, M8, and M10 predict elongated Co–N bond distances, resulting in an expanded macrocyclic core. This expanded core weakens the ligand field strength, thereby favoring electronic state **A** with a high spin quartet Co^{II} center in the ground state (Fig. S1). In contrast, all other functionals predict shorter Co–N bond distances which leads to a more constrained coordination environment around the metal atom. The failure of all other functionals to predict the correct ground spin state of **7** can be attributed to the size of their computed macrocyclic core which is too small and as a result, pairing of the 3d electrons on Co^{II} is artificially enforced, leading to electronic state **B** (Fig. S1) and low-spin doublet ground state.

Table S4A. Relative energetics (ΔG in kcal/mol) of different spin states calculated for each of the Co^I complexes **1a-8a** using the methodologies M1-M20. The energy values of the high spin triplet and low spin singlet states are represented in black and red, respectively.

	1a	2a	3a	4a	5a	6a	7a	8a
M1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	4.61	25.91	15.78	10.79	10.80	17.43	6.46	21.29
M2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	20.19	29.45	19.95	14.36	18.41	13.34	7.58	24.49
M3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3.25	24.01	14.76	10.10	10.22	14.96	6.45	19.18
M4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	15.83	23.69	16.84	-7.32	14.67	7.78	6.36	17.57
M5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	5.21	25.02	14.73	9.19	10.52	13.13	5.52	20.14
M6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	6.65	27.18	18.43	13.10	16.63	12.95	7.38	28.50
M7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	16.64	26.50	20.12	14.41	23.83	19.44	11.93	26.36
M8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	22.91	32.62	22.95	11.03	26.38	28.04	13.74	23.86
M9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	8.77	28.84	21.36	17.83	14.87	15.09	12.94	27.65
M10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	23.23	33.64	26.09	21.59	26.84	17.04	12.24	31.36
M11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	-2.31	9.52	-4.05	-5.94	-9.91	-4.95	-9.09	-1.26
M12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2.99	15.41	2.28	-3.15	-2.62	-1.75	-5.01	5.18
M13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	-0.82	11.61	-2.21	-9.40	-7.06	-2.94	-7.52	0.26
M14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	6.73	18.12	5.70	-0.89	0.80	-0.13	-2.45	8.87
M15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	17.35	27.23	21.29	16.13	7.18	7.39	12.74	27.45
M16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	20.54	31.18	16.58	17.96	24.50	27.18	10.78	30.05
M17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	-4.17	7.93	-4.97	-6.52	-11.00	-5.46	-9.93	-2.61
M18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	2.07	13.27	0.34	-3.84	-4.59	-2.47	-5.75	3.41
M19	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	11.19	23.54	9.51	3.57	3.81	3.43	0.49	11.35
M20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	12.42	21.93	10.54	5.86	3.66	3.58	1.95	12.26

Table S4B. Relative energetics (ΔG in kcal/mol) of different spin states for each of the Fe^{II} complexes **9-11** using the methodologies M1-M20. The energy values of the high spin quintet, intermediate spin triplet, and low spin singlet states are represented in black, blue, and red, respectively.

M1	0.00 (9a')	0.00 (10a')	0.00 (11a')
	20.85 (9a')	15.85 (10a')	20.14 (11a')
	29.59 (9a')	25.76 (10a')	27.52 (11a')
	-0.03 (9a'')	-5.38 (10a'')	-0.35 (11a'')
	18.29 (9a'')	14.86 (10a'')	18.11 (11a'')
	28.21 (9a'')	26.30 (10a'')	26.91 (11a'')
M2	0.00 (9a')	0.00 (10a')	0.00 (11a')
	17.95 (9a')	20.70 (10a')	17.85 (11a')
	27.80 (9a')	29.22 (10a')	24.95 (11a')
	0.03 (9a'')	-0.48 (10a'')	-1.13 (11a'')
	18.05 (9a'')	20.84 (10a'')	15.51 (11a'')
	27.12 (9a'')	30.67 (10a'')	24.23 (11a'')
M3	0.00 (9a')	0.00 (10a')	0.00 (11a')
	30.65 (9a')	24.15 (10a')	29.94 (11a')
	40.48 (9a')	36.85 (10a')	39.05 (11a')
	-0.24 (9a'')	-6.25 (10a'')	-0.05 (11a'')
	30.59 (9a'')	25.71 (10a'')	27.80 (11a'')
	39.33 (9a'')	37.83 (10a'')	38.55 (11a'')
M4	0.00 (9a')	0.00 (10a')	0.00 (11a')
	29.44 (9a')	34.06 (10a')	31.78 (11a')
	46.14 (9a')	48.03 (10a')	46.49 (11a')
	-5.05 (9a'')	-0.13 (10a'')	0.01 (11a'')
	29.56 (9a'')	31.64 (10a'')	31.06 (11a'')
	48.72 (9a'')	47.44 (10a'')	46.39 (11a'')
M5	0.00 (9a')	0.00 (10a')	0.00 (11a')
	16.24 (9a')	15.27 (10a')	15.68 (11a')
	23.30 (9a')	23.74 (10a')	21.07 (11a')
	-4.08 (9a'')	-3.91 (10a'')	-4.90 (11a'')
	13.48 (9a'')	14.77 (10a'')	13.04 (11a'')
	23.39 (9a'')	23.76 (10a'')	21.16 (11a'')
M6	0.00 (9a')	0.00 (10a')	0.00 (11a')
	17.12 (9a')	15.98 (10a')	18.86 (11a')
	25.72 (9a')	23.52 (10a')	23.98 (11a')
	0.11 (9a'')	-2.82 (10a'')	-0.26 (11a'')
	15.89 (9a'')	16.64 (10a'')	17.17 (11a'')
	24.70 (9a'')	24.54 (10a'')	24.46 (11a'')
M7	0.00 (9a')	0.00 (10a')	0.00 (11a')
	21.91 (9a')	17.23 (10a')	18.36 (11a')
	29.68 (9a')	25.57 (10a')	25.22 (11a')
	-0.43 (9a'')	-6.47 (10a'')	-3.66 (11a'')
	19.22 (9a'')	14.77 (10a'')	16.01 (11a'')
	28.55 (9a'')	26.39 (10a'')	24.84 (11a'')

M8	0.00 (9a')	0.00 (10a')	0.00 (11a')
	20.54 (9a')	19.36 (10a')	19.45 (11a')
	29.00 (9a')	26.73 (10a')	25.57 (11a')
	-0.14 (9a'')	-4.50 (10a'')	-2.49 (11a'')
	20.44 (9a'')	19.36 (10a'')	18.60 (11a'')
	27.86 (9a'')	27.91 (10a'')	25.18 (11a'')
M9	0.00 (9a')	0.00 (10a')	0.00 (11a')
	21.52 (9a')	20.37 (10a')	20.51 (11a')
	32.84 (9a')	32.49 (10a')	30.58 (11a')
	-3.62 (9a'')	-5.44 (10a'')	-4.61 (11a'')
	18.62 (9a'')	17.94 (10a'')	17.68 (11a'')
	31.72 (9a'')	33.70 (10a'')	29.88 (11a'')
M10	0.00 (9a')	0.00 (10a')	0.00 (11a')
	22.71 (9a')	21.91 (10a')	21.88 (11a')
	38.10 (9a')	35.87 (10a')	33.81 (11a')
	0.01 (9a'')	-3.75 (10a'')	-3.31 (11a'')
	22.56 (9a'')	24.66 (10a'')	19.92 (11a'')
	37.25 (9a'')	38.21 (10a'')	33.85 (11a'')
M11	0.00 (9a')	0.00 (10a')	0.00 (11a')
	6.54 (9a')	3.58 (10a')	6.79 (11a')
	9.28 (9a')	7.51 (10a')	7.78 (11a')
	-0.15 (9a'')	-5.34 (10a'')	0.15 (11a'')
	6.06 (9a'')	3.85 (10a'')	6.78 (11a'')
	8.62 (9a'')	8.41 (10a'')	8.44 (11a'')
M12	0.00 (9a')	0.00 (10a')	0.00 (11a')
	8.27 (9a')	9.60 (10a')	8.36 (11a')
	12.16 (9a')	14.45 (10a')	9.52 (11a')
	-0.14 (9a'')	0.15 (10a'')	-0.45 (11a'')
	8.22 (9a'')	9.99 (10a'')	8.05 (11a'')
	12.15 (9a'')	16.70 (10a'')	10.66 (11a'')
M13	0.00 (9a')	0.00 (10a')	0.00 (11a')
	6.99 (9a')	2.79 (10a')	4.15 (11a')
	7.94 (9a')	4.59 (10a')	5.89 (11a')
	0.66 (9a'')	-6.47 (10a'')	-0.40 (11a'')
	4.36 (9a'')	1.03 (10a'')	6.01 (11a'')
	7.44 (9a'')	5.40 (10a'')	5.37 (11a'')
M14	0.00 (9a')	0.00 (10a')	0.00 (11a')
	9.07 (9a')	10.99 (10a')	10.22 (11a')
	16.06 (9a')	17.22 (10a')	13.27 (11a')
	0.40 (9a'')	-0.38 (10a'')	-0.41 (11a'')
	8.96 (9a'')	14.85 (10a'')	8.88 (11a'')
	16.02 (9a'')	20.35 (10a'')	14.47 (11a'')

M15	0.00 (9a')	0.00 (10a')	0.00 (11a')
	22.45 (9a')	17.44 (10a')	22.49 (11a')
	31.81 (9a')	27.29 (10a')	30.12 (11a')
	0.02 (9a'')	-5.42 (10a'')	-0.27 (11a'')
	19.29 (9a'')	15.58 (10a'')	19.23 (11a'')
	30.23 (9a'')	28.18 (10a'')	29.02 (11a'')
M16	0.00 (9a')	0.00 (10a')	0.00 (11a')
	18.81 (9a')	18.84 (10a')	16.58 (11a')
	29.75 (9a')	27.65 (10a')	25.86 (11a')
	-0.84 (9a'')	-4.80 (10a'')	-3.09 (11a'')
	18.59 (9a'')	17.18 (10a'')	16.54 (11a'')
	28.44 (9a'')	29.46 (10a'')	25.51 (11a'')
M17	0.00 (9a')	0.00 (10a')	0.00 (11a')
	6.37 (9a')	0.11 (10a')	5.87 (11a')
	6.74 (9a')	3.61 (10a')	5.31 (11a')
	-0.14 (9a'')	-6.99 (10a'')	-0.23 (11a'')
	4.23 (9a'')	1.00 (10a'')	4.98 (11a'')
	5.43 (9a'')	3.97 (10a'')	5.68 (11a'')
M18	0.00 (9a')	0.00 (10a')	0.00 (11a')
	5.99 (9a')	8.99 (10a')	5.94 (11a')
	8.97 (9a')	12.45 (10a')	6.29 (11a')
	0.12 (9a'')	1.92 (10a'')	-0.45 (11a'')
	6.17 (9a'')	9.73 (10a'')	6.26 (11a'')
	8.68 (9a'')	13.97 (10a'')	7.30 (11a'')
M19	0.00 (9a')	0.00 (10a')	0.00 (11a')
	22.61 (9a')	18.30 (10a')	22.49 (11a')
	25.29 (9a')	21.84 (10a')	23.89 (11a')
	-0.01 (9a'')	-7.27 (10a'')	0.29 (11a'')
	21.34 (9a'')	19.65 (10a'')	20.68 (11a'')
	24.90 (9a'')	22.08 (10a'')	23.88 (11a'')
M20	0.00 (9a')	0.00 (10a')	0.00 (11a')
	16.24 (9a')	18.17 (10a')	15.40 (11a')
	21.80 (9a')	20.36 (10a')	18.04 (11a')
	-0.09 (9a'')	-3.34 (10a'')	-2.73 (11a'')
	16.01 (9a'')	13.35 (10a'')	12.91 (11a'')
	21.70 (9a'')	21.03 (10a'')	18.64 (11a'')

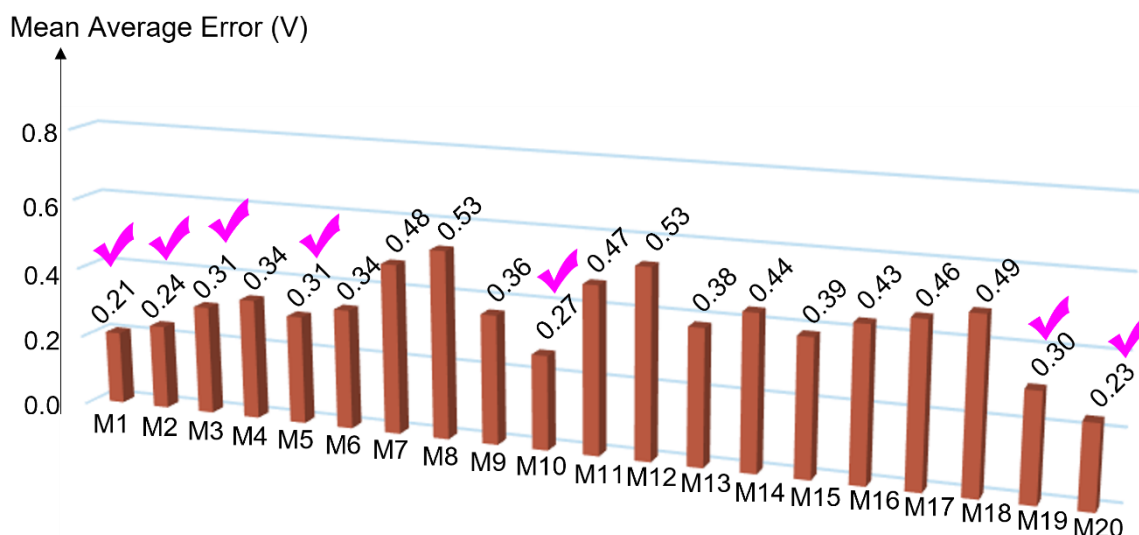


Fig S2. The mean average error (MAE in V) in calculating potentials for all the catalysts **1-6,8-15** with methodologies M1-M20. The methods with $0 < \text{MAE} < \sim 0.30\text{V}$ are M1 (B3LYP/Def2TZVP), M2 (B3LYP/LANL2DZ(f)/6-311++G**), M3 (M06/Def2TZVP), M5 (B3LYP-D3/Def2TZVP), M10 (PBE1PBE/LANL2DZ(f)/6-311++G**), M19 (M06-L/Def2TZVP), and M20 (M06-L/LANL2DZ(f)/6-311++G**).

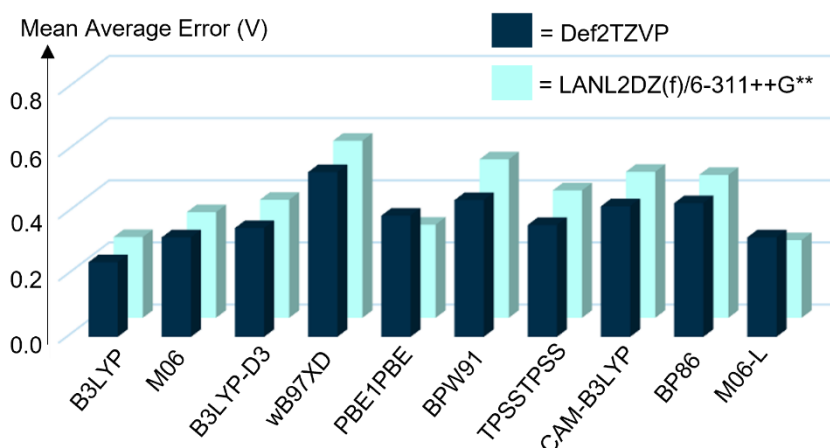
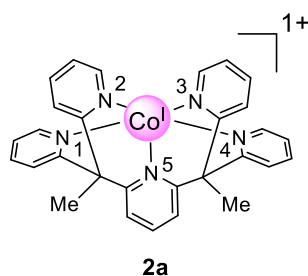


Fig S3. Comparison of performance of all-electron Def2TZVP vs. ECP-corrected LANL2DZ(f)/6-311++G** basis sets in calculating reduction potentials in presence of 10 GGA functionals.

Fig. S3 shows performance comparison between all-electron Def2TZVP and ECP-corrected LANL2DZ(f)/6-311++G** basis sets in calculating the reduction potentials across all the functionals for the catalyst series **1-15**. As expected, the all-electron basis depicts superior results compared to the ECP-corrected basis in case of a majority of functionals. The Def2TZVP-calculated MAEs are 0.24 (M1), 0.32 (M3), 0.35 (M5), 0.53 (M7), 0.44 (M11), 0.36 (M13), 0.42 (M15), and 0.43 V (M17). The corresponding ECP basis set-calculated MAE values are found higher: 0.26 (M2), 0.34 (M4), 0.38 (M6), 0.57 (M8), 0.51 (M12), 0.41 (M14), 0.47 (M16), and 0.46 V (M18).

Table S5. Comparison of the structural parameters between DFT (M1)-calculated geometry and crystal structure geometry for **2a**.



2a	Co–N1	Co–N2	Co–N3	Co–N4	Co–N5	∠N1–Co–N2	∠N2–Co–N3	∠N3–Co–N4	∠N4–Co–N1	∠N5–Co–N1	∠N5–Co–N2	∠N5–Co–N3	∠N5–Co–N4
DFT (M1)-struc.	2.07	2.16	2.07	2.18	1.99	81.6	99.1	81.6	98.1	94.2	88.2	94.3	87.8
Crystal struc.	2.12	2.01	2.11	2.02	1.96	82.3	99.4	84.1	94.9	87.6	94.7	86.9	94.9
Deviation	0.05	0.15	0.04	0.16	0.03	0.7	0.3	2.5	3.2	6.6	6.5	7.4	7.1

The bond lengths are in Å and the bond angles are in °

There is a general consensus that the reaction pathway for hydrogen generation does involve formation of a stable five-coordinate complex.^{a-e} The existence of this catalytically active complex has been proven unambiguously by experimental studies. Chang *et al.* have in fact isolated a stable crystal structure of a five-coordinate species which resulted from loss of a ligand from metal.^a This species is complex **2a** in our present study. We have compared the structural parameters between the crystal geometry and our DFT-optimized (M1 methodology) geometry for this catalytically active species. The results are reported in Table S5. Analysis of the DFT-calculated and crystal structures reveals that the DFT-calculated structural parameters, crucial metal-ligand bond distances and bond angles, are in well agreement with those obtained from a stable crystal geometry.

a) A. E. King, Y. Surendranath, N. A. Piro, J. P. Bigi, J. R. Long and C.J. Chang, *Chem. Sci.*, 2013, **4**, 1578.

b) D. Basu, S. Mazumder, X. Shi, R. J. Staples, H. B. Schlegel and C. N. Verani, *Angew. Chem. Int. Ed.*, 2015, **54**, 7139.

c) D. Basu, S. Mazumder, X. Shi, H. Baydoun, J. Niklas, O. Poluektov, H. B. Schlegel and C. N. Verani, *Angew. Chem. Int. Ed.*, 2015, **54**, 2105.

d) W. K. C. Lo, C. E. Castillo, R. Gueret, J. Fortage, M. Rebarz, M. Sliwa, F. Thomas, C. J. McAdam, G. B. Jameson, D. A. McMorran, J. D. Crowley, M.-N. Collomb and A. G. Blackman, *Inorg. Chem.*, 2016, **55**, 4564.

e) C. Li, Y. Li, Y. Luo, K. Michaliszyn, I. B. Losada, M. K. Hossain, F. Elantabli, M. Guo, L. Hizbullah, D. A. Tocher, M. Haukka, P. Persson, J. L. Fillol, B. D. Ivansic and E. Nordlander, *Chem. Eur. J.*, 2025, **31**, e202404499

Table S6: Metal–ligand bond distances of catalytically active species **1a–13a** calculated using DFT (M1)-methodology.

Complex	BD1	BD2	BD3	BD4	BD5
1a	Co–Npy 1.90	Co–Npy 1.97	Co–Npy 1.99	Co–N(ACN) 1.93	Co–Npy 2.21
2a	Co–Npy 2.07	Co–Npy 2.16	Co–Npy 2.07	Co–Npy 2.18	Co–Npy 1.99
3a	Co–Npy 2.14	Co–Npy 2.17	Co–Npy 2.09	Co–Npy 2.01	Co–Npy 2.09
4a	Co–Npy 2.20	Co–Npy 2.02	Co–Npy 2.20	Co–Npy 2.02	Co–O 2.12
5a	Co–Npy 1.95	Co–Npy 1.95	Co–Npy 1.92	Co–Npy 2.00	Co–Cl 2.49
6a	Co–Npy 2.17	Co–Npy 2.07	Co–Npy 2.07	Co–Npy 2.14	Co–Cl 2.32
7a	Co–Npy 2.13	Co–Npy 2.09	Co–Npy 2.04	Co–Npy 2.01	Co–Br 2.49
8a	Co–Npy 2.11	Co–Npy 2.07	Co–Npy 2.12	Co–Npy 2.00	Co– N(amine) 2.32
9a	Fe–Npy 2.17	Fe– N(amine) 2.36	Fe–O 1.97	Fe–Cl 2.38	Fe–Npy 2.21
10a	Fe–Npy 2.16	Fe– N(amine) 2.42	Fe–S 1.95	Fe–Cl 2.39	Fe–Npy 2.21
11a	Fe–Npy 2.16	Fe– N(amine) 2.34	Fe–O 2.01	Fe–Cl 2.37	Fe–Npy 2.19

12a	Ni–Npy 2.09	Ni–Npy 1.96	Ni– N(amine) 2.24	Ni–Npy 2.10	Ni– N(amine) 2.23
13a	Ni–S 2.58	Ni–py 2.09	Ni–N (ACN) 1.94	Ni–Npy 2.09	Ni–S 2.58

The bond lengths are in Å. BD= Bond Distance

The DFT (M1)-calculated metal–ligand bond distances for complexes **1a–13a** are summarized in Table S6. The calculated Co–Npy bond lengths span 1.90–2.21Å, in good agreement with reported values (1.86–2.18Å)^{f,k} for stable Co–polypyridine complexes. Similarly, the computed Fe–Npy distances range from 2.16 to 2.21Å, closely matching the bond lengths (2.17–2.19Å)^l observed in well-defined Fe–polypyridine species. The calculated Ni–Npy bond lengths fall within 1.96–2.10Å, which also compares favorably with literature values (2.05–2.11Å)^{m,n} reported for stable Ni–polypyridine compounds. These findings further support structural stability of our calculated structures.

- f) J.P. Bigi, T.E. Hanna, W.H. Harman, A. Chang and C. J. Chang, *Chem. Commun.*, 2010, **46**, 958.
- g) A.E. King, Y. Surendranath, N.A. Piro, J.P. Bigi, J.R. Long and C.J. Chang, *Chem. Sci.*, 2013, **4**, 1578.
- h) M. Nippe, R.S. Khayzer, J.A. Panetier, D.Z. Zee, B.S. Olaiya, M. Head-Gordon, C. J. Chang, F.N. Castellano and J.R. Long, *Chem. Sci.*, 2013, **4**, 3934.
- i) L. Tong, R. Zong and R.P. Thummel, *J. Am. Chem. Soc.*, 2014, **136**, 4881.
- j) E. Joliat, S. Schnidrig, B. Probst, C. Bachmann, B. Spingler, K.K. Baldrige, F. von Rohr, A. Schilling and R. Alberto, *Dalton Trans.*, 2016, **45**, 1737.
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- m) P.H. Kankanamalage, S. Mazumder, V. Tiwari, K.K. Kpogo, H. Bernhard Schlegel and C.N. Verani, *Chem. Commun.*, 2016, **52**, 13357.
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Table S7. DFT-optimized XYZ coordinates calculated with M1 [B3LYP/Def2TZVP].

1 high spin

C	-2.869224000	1.077152000	-5.635147000
C	0.693486000	-1.229266000	-5.444315000
C	-0.121631000	-0.103585000	-5.327843000
C	-0.157139000	3.961873000	-4.573057000
C	0.760620000	4.981766000	-4.310826000
C	1.257105000	-1.782767000	-4.295152000
C	-0.368435000	0.436638000	-4.059435000
C	-1.228590000	1.718236000	-3.913855000
C	-0.228347000	2.882815000	-3.690164000
C	1.575658000	4.892929000	-3.182054000
C	1.008988000	-1.156386000	-3.078459000
C	-3.549157000	2.136049000	-2.870986000
C	-2.208530000	1.763040000	-2.706342000
C	1.442601000	3.778761000	-2.355345000
C	-4.345483000	2.308594000	-1.738812000
C	3.559013000	0.796606000	-0.750746000
C	-3.784339000	2.181910000	-0.470726000
C	4.989248000	0.632365000	-0.593037000
C	-2.427355000	1.858111000	-0.376277000
C	-0.050478000	-1.807032000	0.496283000
C	-1.667967000	1.876517000	0.900396000
C	-0.248276000	-3.020841000	1.265631000
C	0.451689000	1.854429000	1.859249000
C	-2.267256000	2.036877000	2.156279000
C	-0.069006000	2.035078000	3.140389000
C	-1.454891000	2.116694000	3.287688000
H	-3.821058000	1.607716000	-5.791294000
H	0.889190000	-1.662042000	-6.428322000
H	-0.542335000	0.357272000	-6.217071000
H	-2.526363000	0.705415000	-6.612873000
H	-0.811550000	3.992540000	-5.441998000
H	0.834501000	5.838096000	-4.985615000
H	-3.044744000	0.216679000	-4.973248000
H	1.897842000	-2.665354000	-4.335797000

H	-3.969229000	2.317689000	-3.855170000
H	2.304188000	5.668565000	-2.939512000
H	1.462585000	-1.526057000	-2.157285000
H	-5.396847000	2.583128000	-1.848993000
H	2.060569000	3.665165000	-1.460829000
H	5.386572000	0.047818000	-1.437070000
H	5.473641000	1.620646000	-0.574943000
H	-4.380128000	2.375055000	0.420865000
H	5.199780000	0.103688000	0.349259000
H	-0.012213000	-3.897583000	0.643402000
H	-1.295614000	-3.082972000	1.598253000
H	1.528733000	1.762022000	1.697014000
H	-3.351113000	2.097042000	2.253200000
H	0.412207000	-3.012301000	2.146214000
H	0.602255000	2.099684000	3.998559000
H	-1.903614000	2.242535000	4.275699000
N	0.225593000	-0.070047000	-2.967733000
N	0.562433000	2.797905000	-2.605944000
N	-1.695088000	1.608790000	-1.480957000
N	2.417158000	0.924139000	-0.878247000
N	0.111321000	-0.839409000	-0.116037000
N	-0.327916000	1.778111000	0.775065000
Co	0.340040000	1.134013000	-1.178542000
O	-1.909881000	2.000360000	-5.107240000

1 low spin

C	-2.783944000	0.977409000	-5.611558000
C	0.869595000	-1.194737000	-5.355665000
C	0.026419000	-0.088168000	-5.273544000
C	-0.221703000	4.010617000	-4.529003000
C	0.632834000	5.076743000	-4.236021000
C	1.426043000	-1.708155000	-4.184339000
C	-0.246069000	0.476725000	-4.022963000
C	-1.175598000	1.700686000	-3.898410000
C	-0.255615000	2.928414000	-3.647663000
C	1.417361000	5.026385000	-3.083075000
C	1.156939000	-1.059098000	-2.985523000
C	-3.498464000	1.991999000	-2.815552000

C	-2.146289000	1.652107000	-2.691771000	N	0.357061000	0.022276000	-2.911178000
C	1.318209000	3.903219000	-2.261277000	N	0.501797000	2.880290000	-2.541548000
C	-4.276879000	2.112201000	-1.664128000	N	-1.608052000	1.467126000	-1.479325000
C	3.303818000	0.780592000	-0.766055000	N	2.160523000	0.870755000	-0.904769000
C	-3.679245000	2.002054000	-0.409779000	N	-0.183186000	-0.976331000	-0.143155000
C	4.736644000	0.663610000	-0.589123000	N	-0.139801000	1.799234000	0.604066000
C	-2.313325000	1.722922000	-0.350448000	Co	0.254564000	1.063482000	-1.208915000
C	-0.473774000	-1.945230000	0.419092000	O	-1.865647000	1.946000000	-5.089676000
C	-1.474728000	1.839893000	0.856958000	1a high spin			
C	-0.839995000	-3.161066000	1.123031000	C	-2.754222000	1.031170000	-5.649506000
C	0.724911000	2.005842000	1.605931000	C	0.815772000	-1.248368000	-5.293006000
C	-1.966764000	2.066095000	2.144782000	C	0.014717000	-0.107708000	-5.255847000
C	0.304673000	2.253364000	2.912917000	C	-0.214386000	4.070500000	-4.575586000
C	-1.062720000	2.271196000	3.187817000	C	0.626096000	5.148949000	-4.290825000
H	-3.763628000	1.459349000	-5.752208000	C	1.353085000	-1.739533000	-4.102640000
H	1.086893000	-1.647993000	-6.325625000	C	-0.236209000	0.516398000	-4.028560000
H	-0.405398000	0.341769000	-6.173275000	C	-1.148077000	1.758836000	-3.929458000
H	-2.432800000	0.629699000	-6.595110000	C	-0.228331000	2.984936000	-3.695904000
H	-0.851029000	4.009800000	-5.417167000	C	1.420769000	5.110510000	-3.143637000
H	0.681302000	5.939151000	-4.905445000	C	1.116524000	-1.028973000	-2.931669000
H	-2.905596000	0.106249000	-4.951605000	C	-3.469532000	2.019160000	-2.850252000
H	2.078022000	-2.583252000	-4.192217000	C	-2.121853000	1.714755000	-2.721885000
H	-3.937041000	2.189860000	-3.789269000	C	1.345347000	3.985625000	-2.323193000
H	2.095057000	5.840012000	-2.817731000	C	-4.272963000	2.062706000	-1.674435000
H	1.599530000	-1.404723000	-2.051726000	C	3.328565000	0.868073000	-0.798910000
H	-5.339561000	2.349832000	-1.746577000	C	-3.689571000	1.927364000	-0.434712000
H	1.912233000	3.819848000	-1.346993000	C	4.759373000	0.729746000	-0.616565000
H	5.164711000	0.090424000	-1.425818000	C	-2.285675000	1.726709000	-0.344676000
H	5.189169000	1.666789000	-0.565671000	C	-1.479252000	1.838186000	0.823539000
H	-4.252897000	2.180196000	0.499516000	C	0.742916000	1.969734000	1.614843000
H	4.950974000	0.143387000	0.357149000	C	-1.958428000	2.029600000	2.150118000
H	-0.600226000	-4.037669000	0.502070000	C	0.327846000	2.180464000	2.919515000
H	-1.919418000	-3.154640000	1.338303000	C	-1.067805000	2.199492000	3.188027000
H	1.786006000	1.968706000	1.357746000	H	-3.734615000	1.516045000	-5.775857000
H	-3.040834000	2.086047000	2.330217000	H	1.014473000	-1.747532000	-6.244381000
H	-0.282823000	-3.225246000	2.070057000	H	-0.402649000	0.300315000	-6.172644000
H	1.047126000	2.420801000	3.694926000	H	-2.416548000	0.687700000	-6.640117000
H	-1.426154000	2.448024000	4.202474000	H	-0.852258000	4.060542000	-5.457468000

H	0.655941000	6.012194000	-4.960417000	C	-4.251501000	2.323696000	-1.679488000
H	-2.875499000	0.156507000	-4.994837000	C	3.325305000	1.300135000	-0.859040000
H	1.966744000	-2.641667000	-4.077631000	C	-3.674799000	2.140925000	-0.431053000
H	-3.906334000	2.244561000	-3.818095000	C	4.765199000	1.190000000	-0.719408000
H	2.087910000	5.934386000	-2.882854000	C	-2.298534000	1.875812000	-0.350626000
H	1.552668000	-1.346700000	-1.983188000	C	-1.507847000	1.743735000	0.852341000
H	-5.346458000	2.247361000	-1.761124000	C	0.670140000	1.470104000	1.666045000
H	1.946992000	3.910357000	-1.413115000	C	-2.015478000	1.769464000	2.163929000
H	5.183088000	0.144877000	-1.447314000	C	0.223280000	1.488426000	2.973069000
H	5.227389000	1.726048000	-0.597757000	C	-1.153684000	1.640459000	3.241576000
H	-4.283557000	2.023263000	0.475793000	H	-3.773819000	1.503814000	-5.708083000
H	4.963693000	0.213549000	0.334137000	H	0.920616000	-1.913872000	-5.950159000
H	1.807268000	1.937405000	1.373245000	H	-0.495072000	0.133964000	-6.032572000
H	-3.034378000	2.043756000	2.333356000	H	-2.489124000	0.583427000	-6.527859000
H	1.065939000	2.319632000	3.710970000	H	-0.704171000	3.907413000	-5.691317000
H	-1.432853000	2.349303000	4.207332000	H	0.923099000	5.806003000	-5.394095000
N	0.361869000	0.085670000	-2.904572000	H	-2.933316000	0.183593000	-4.842557000
N	0.542701000	2.948913000	-2.596739000	H	1.932111000	-2.601329000	-3.735203000
N	-1.564005000	1.508947000	-1.513173000	H	-3.897793000	2.398140000	-3.813366000
N	2.186882000	0.980073000	-0.941046000	H	2.314782000	5.878451000	-3.286940000
N	-0.107444000	1.797387000	0.583572000	H	1.539865000	-1.138931000	-1.748640000
Co	0.294800000	1.210156000	-1.254479000	H	-5.314105000	2.559875000	-1.767857000
O	-1.822323000	1.987784000	-5.137415000	H	2.014933000	4.066718000	-1.593882000
1a low spin				H	5.179805000	0.628087000	-1.570548000
C	-2.802772000	1.006049000	-5.560319000	H	5.217616000	2.193460000	-0.695128000
C	0.741289000	-1.331175000	-5.043517000	H	-4.269971000	2.228486000	0.478638000
C	-0.061459000	-0.191906000	-5.090377000	H	5.009292000	0.661017000	0.214900000
C	-0.080964000	3.984423000	-4.802173000	H	1.731319000	1.353331000	1.447458000
C	0.824171000	5.031916000	-4.629099000	H	-3.089013000	1.888725000	2.320602000
C	1.310385000	-1.708537000	-3.825319000	H	0.948277000	1.384179000	3.783440000
C	-0.282896000	0.537941000	-3.916063000	H	-1.529615000	1.656049000	4.266496000
C	-1.156504000	1.819464000	-3.918596000	N	0.325385000	0.205646000	-2.765061000
C	-0.180124000	3.013492000	-3.801658000	N	0.564521000	3.056520000	-2.684230000
C	1.597628000	5.075088000	-3.466301000	N	-1.547257000	1.758494000	-1.488405000
C	1.087828000	-0.903102000	-2.714140000	N	2.175328000	1.386141000	-0.963185000
C	-3.458541000	2.219557000	-2.835776000	N	-0.158374000	1.592193000	0.587317000
C	-2.109495000	1.905222000	-2.708473000	Co	0.304180000	1.557008000	-1.253832000
C	1.434761000	4.067471000	-2.519519000	O	-1.840749000	1.973898000	-5.132987000

2 high spin

C	0.483021000	1.602349000	-4.088889000
C	1.220218000	0.450532000	-3.844569000
C	2.774988000	-1.840003000	-3.543127000
C	-0.035003000	2.322290000	-3.019691000
C	1.422282000	0.034345000	-2.522777000
C	2.258846000	-1.241296000	-2.222291000
C	1.156876000	-3.570451000	-2.035771000
C	4.792738000	-1.076887000	-1.748759000
C	0.188920000	1.865623000	-1.715005000
C	1.384292000	-2.296559000	-1.492165000
C	3.471244000	-0.890905000	-1.313746000
C	0.416246000	-4.510892000	-1.320318000
C	-1.113321000	3.910477000	-0.997714000
C	5.854168000	-0.819569000	-0.881383000
C	-0.377469000	2.652936000	-0.500238000
C	-0.077244000	-4.168948000	-0.063991000
C	5.579771000	-0.395636000	0.416229000
C	-2.718723000	2.119932000	0.458897000
C	-1.372320000	1.760946000	0.290947000
C	0.774951000	3.080131000	0.452783000
C	4.247023000	-0.217367000	0.772483000
C	0.177289000	-2.885061000	0.406573000
C	1.060770000	4.432474000	0.696539000
C	-3.562452000	1.316814000	1.225893000
C	2.051580000	4.781025000	1.614198000
C	-1.704811000	-0.127157000	1.608793000
C	-3.045435000	0.172234000	1.827653000
C	2.407577000	2.454061000	1.986321000
C	2.731317000	3.772058000	2.291308000
C	1.658068000	-1.062045000	3.603338000
C	1.835427000	-1.559817000	4.952376000
H	0.315756000	1.941450000	-5.113817000
H	1.627294000	-0.105557000	-4.683068000
H	1.945125000	-2.126068000	-4.199710000
H	3.401672000	-1.122702000	-4.085907000
H	3.377017000	-2.736492000	-3.353475000
H	-0.604370000	3.225509000	-3.215671000

H	1.554390000	-3.846083000	-3.008563000
H	5.009720000	-1.425097000	-2.754717000
H	-1.953533000	3.645290000	-1.649866000
H	0.239708000	-5.502872000	-1.743050000
H	-0.442484000	4.566218000	-1.565064000
H	6.882925000	-0.963244000	-1.220444000
H	-1.511890000	4.486383000	-0.153724000
H	-3.121118000	3.021264000	0.004979000
H	0.517855000	5.222964000	0.186137000
H	-0.647544000	-4.872137000	0.545457000
H	6.371762000	-0.202392000	1.141820000
H	-4.610805000	1.595693000	1.356563000
H	3.989931000	0.104866000	1.781174000
H	-0.186790000	-2.583695000	1.389101000
H	2.274538000	5.834047000	1.802328000
H	-1.257912000	-1.007045000	2.072452000
H	-3.657408000	-0.479565000	2.453556000
H	2.909640000	1.635862000	2.502292000
H	3.497851000	3.989437000	3.037138000
H	2.060142000	-2.636911000	4.922992000
H	2.669253000	-1.026334000	5.433977000
H	0.914026000	-1.392607000	5.530983000
N	0.898903000	0.738460000	-1.496944000
N	3.224781000	-0.437218000	-0.069548000
N	0.871340000	-1.970127000	-0.290249000
N	-0.898038000	0.631829000	0.849401000
N	1.476670000	2.115783000	1.080019000
N	1.516683000	-0.663823000	2.526930000
Co	1.162773000	0.024820000	0.514030000

2 low spin

C	0.546480000	1.685370000	-4.169104000
C	1.268821000	0.519434000	-3.931959000
C	2.747166000	-1.856448000	-3.524429000
C	0.006669000	2.391351000	-3.097827000
C	1.433907000	0.089213000	-2.610067000
C	2.219660000	-1.186641000	-2.244977000
C	0.957624000	-3.415791000	-2.009046000
C	4.730684000	-1.010971000	-1.713820000

C	0.208724000	1.902703000	-1.801641000	H	-0.663797000	-4.672817000	0.705840000
C	1.298384000	-2.165772000	-1.474144000	H	6.242213000	-0.208863000	1.227428000
C	3.401426000	-0.820122000	-1.311409000	H	-4.527399000	1.284334000	1.232833000
C	0.224084000	-4.328516000	-1.253066000	H	3.866026000	0.098788000	1.815324000
C	-1.130733000	3.867880000	-0.969511000	H	-0.018426000	-2.438535000	1.530097000
C	5.776504000	-0.771341000	-0.824351000	H	2.306906000	5.713400000	1.827104000
C	-0.352639000	2.609646000	-0.551021000	H	-1.017398000	-1.021621000	2.136494000
C	-0.129295000	-3.985361000	0.048139000	H	-3.434279000	-0.651490000	2.458173000
C	5.470949000	-0.372557000	0.473019000	H	2.895298000	1.505932000	2.463600000
C	-2.655682000	1.904640000	0.351120000	H	3.485868000	3.827052000	3.050109000
C	-1.285545000	1.639951000	0.217854000	H	2.066251000	-2.568615000	4.998439000
C	0.810903000	2.996840000	0.396300000	H	2.683009000	-0.948907000	5.464576000
C	4.133465000	-0.185103000	0.801444000	H	0.928540000	-1.307450000	5.581375000
C	0.220621000	-2.721524000	0.508755000	N	0.908181000	0.779906000	-1.589578000
C	1.101031000	4.339256000	0.677371000	N	3.123542000	-0.362220000	-0.068596000
C	-3.459536000	1.076603000	1.132563000	N	0.876694000	-1.815010000	-0.236973000
C	2.081792000	4.666254000	1.611935000	N	-0.739128000	0.552578000	0.810230000
C	-1.508468000	-0.209914000	1.607217000	N	1.510322000	2.006660000	0.997756000
C	-2.867813000	0.008082000	1.798658000	N	1.509296000	-0.657330000	2.550534000
C	2.416460000	2.327762000	1.938284000	Co	1.201868000	0.077602000	0.430634000
C	2.738385000	3.636450000	2.278270000	2a high spin			
C	1.659380000	-1.026784000	3.637378000	C	0.468561000	1.660156000	-4.269906000
C	1.844991000	-1.490416000	4.999735000	C	1.248850000	0.535522000	-4.006349000
H	0.403585000	2.044246000	-5.191052000	C	2.813468000	-1.767849000	-3.623068000
H	1.689657000	-0.031776000	-4.768738000	C	-0.104785000	2.357179000	-3.207573000
H	1.923038000	-2.125664000	-4.195519000	C	1.437477000	0.126977000	-2.681606000
H	3.411143000	-1.180255000	-4.075935000	C	2.261350000	-1.143489000	-2.329668000
H	3.308368000	-2.769831000	-3.290591000	C	1.087315000	-3.442152000	-2.150330000
H	-0.557654000	3.301218000	-3.284267000	C	4.781293000	-1.056319000	-1.738270000
H	1.269381000	-3.692182000	-3.012352000	C	0.120654000	1.918142000	-1.898276000
H	4.961425000	-1.356044000	-2.717806000	C	1.336156000	-2.169003000	-1.610757000
H	-1.961495000	3.611631000	-1.637382000	C	3.445830000	-0.821206000	-1.372782000
H	-0.041377000	-5.301212000	-1.673640000	C	0.280020000	-4.346859000	-1.460517000
H	-0.482426000	4.569216000	-1.508137000	C	-1.314332000	3.858583000	-1.161378000
H	6.811406000	-0.918513000	-1.141866000	C	5.804203000	-0.877092000	-0.805557000
H	-1.543149000	4.386736000	-0.095006000	C	-0.456980000	2.678301000	-0.671577000
H	-3.105001000	2.761212000	-0.143340000	C	-0.261210000	-3.965384000	-0.233391000
H	0.559822000	5.139192000	0.179973000	C	5.472096000	-0.488661000	0.492592000

C	-2.692497000	2.005028000	0.449546000	N	3.149557000	-0.368459000	-0.134416000
C	-1.328165000	1.754842000	0.229893000	N	0.786856000	-1.804835000	-0.431986000
C	0.718947000	3.213541000	0.196838000	N	-0.714358000	0.731851000	0.864433000
C	4.132849000	-0.245896000	0.776862000	N	1.568113000	2.310198000	0.733882000
C	0.023377000	-2.686285000	0.234927000	Co	1.199228000	0.235900000	0.219450000
C	0.891387000	4.586546000	0.439068000	2a low spin			
C	-3.405801000	1.234289000	1.369222000	C	0.440953000	1.681383000	-4.341256000
C	1.935788000	5.026506000	1.252492000	C	1.163134000	0.515232000	-4.089916000
C	-1.391213000	0.025034000	1.787946000	C	2.671502000	-1.850350000	-3.611028000
C	-2.734662000	0.237698000	2.078054000	C	-0.070512000	2.425462000	-3.278623000
C	2.563080000	2.739774000	1.528335000	C	1.360181000	0.126054000	-2.759015000
C	2.790569000	4.081318000	1.818702000	C	2.165687000	-1.134534000	-2.348345000
H	0.307468000	1.991241000	-5.298454000	C	0.944817000	-3.370018000	-1.964146000
H	1.695608000	-0.006047000	-4.835942000	C	4.682755000	-0.904413000	-1.860249000
H	2.003491000	-2.046038000	-4.307896000	C	0.155942000	1.969487000	-1.973903000
H	3.470151000	-1.065337000	-4.151055000	C	1.286209000	-2.087883000	-1.506609000
H	3.393986000	-2.673181000	-3.407018000	C	3.353392000	-0.718037000	-1.450064000
H	-0.715103000	3.232007000	-3.416054000	C	0.264455000	-4.257958000	-1.133991000
H	1.517898000	-3.742837000	-3.102183000	C	-1.167290000	3.944772000	-1.139226000
H	5.038378000	-1.388367000	-2.741069000	C	5.736748000	-0.612416000	-0.998122000
H	-2.145690000	3.509076000	-1.786063000	C	-0.379255000	2.696076000	-0.711650000
H	0.086473000	-5.337905000	-1.878407000	C	-0.026016000	-3.855487000	0.171815000
H	-0.720765000	4.560135000	-1.759732000	C	5.434244000	-0.167629000	0.290706000
H	6.843257000	-1.060200000	-1.089956000	C	-2.652589000	1.988913000	0.263933000
H	-1.739134000	4.415658000	-0.317297000	C	-1.282871000	1.734285000	0.093025000
H	-3.209022000	2.802106000	-0.079448000	C	0.790761000	3.091212000	0.218047000
H	0.218193000	5.321799000	0.005488000	C	4.100177000	0.000944000	0.633327000
H	-0.889930000	-4.637571000	0.354169000	C	0.327449000	-2.570571000	0.558864000
H	6.228574000	-0.371016000	1.271169000	C	1.089955000	4.434910000	0.492207000
H	-4.467319000	1.429196000	1.540366000	C	-3.432510000	1.158354000	1.064578000
H	3.826650000	0.051075000	1.782378000	C	2.071208000	4.764192000	1.424204000
H	-0.380706000	-2.355756000	1.192517000	C	-1.452625000	-0.108302000	1.503580000
H	2.070012000	6.094144000	1.443268000	C	-2.809025000	0.092246000	1.716463000
H	-0.824316000	-0.739828000	2.323420000	C	2.379295000	2.420218000	1.780943000
H	-3.235248000	-0.367563000	2.836530000	C	2.714862000	3.727362000	2.103754000
H	3.211061000	1.974176000	1.956617000	H	0.276042000	2.011595000	-5.369834000
H	3.617238000	4.368486000	2.471750000	H	1.557351000	-0.062718000	-4.922679000
N	0.879661000	0.821552000	-1.661045000	H	1.834504000	-2.155683000	-4.250990000

H	3.314321000	-1.190709000	-4.206807000	C	1.744408000	-1.309132000	-2.020364000
H	3.249065000	-2.748096000	-3.356405000	C	-0.518341000	3.240302000	-1.606419000
H	-0.630861000	3.335473000	-3.480136000	C	2.117010000	-0.958483000	-0.623734000
H	1.214471000	-3.686554000	-2.968765000	C	-0.647943000	3.133262000	-0.129508000
H	4.904155000	-1.283827000	-2.854788000	C	3.375643000	-1.202553000	-0.063238000
H	-2.009579000	3.675777000	-1.788243000	C	-2.585719000	-1.678234000	0.338218000
H	-0.003791000	-5.254296000	-1.492837000	C	-0.892190000	4.230079000	0.703703000
H	-0.529522000	4.637598000	-1.701972000	C	-3.194798000	-2.487968000	1.292770000
H	6.770553000	-0.754714000	-1.321225000	C	3.561033000	-0.914201000	1.286857000
H	-1.566514000	4.481486000	-0.269253000	C	1.261105000	-0.202662000	1.426337000
H	-3.119176000	2.840486000	-0.224876000	C	-0.385144000	1.699989000	1.708418000
H	0.554427000	5.233686000	-0.014942000	C	-1.160141000	-0.711074000	1.908310000
H	-0.500491000	-4.525912000	0.891023000	C	-0.903836000	4.024968000	2.080330000
H	6.211444000	0.029635000	1.031520000	C	2.496746000	-0.431055000	2.049748000
H	-4.499062000	1.356828000	1.192993000	C	0.001623000	0.279982000	2.199348000
H	3.840974000	0.292930000	1.646784000	C	-2.757130000	-2.387969000	2.610841000
H	0.167466000	-2.255817000	1.587448000	C	-0.627595000	2.758732000	2.595389000
H	2.305241000	5.810554000	1.633372000	C	-1.732582000	-1.492235000	2.921446000
H	-0.939994000	-0.899367000	2.042627000	C	0.304040000	0.318136000	3.706022000
H	-3.352042000	-0.567762000	2.395724000	H	0.109215000	3.272281000	-5.396183000
H	2.824386000	1.599835000	2.338466000	H	0.384483000	-2.327761000	-5.473727000
H	3.451384000	3.918692000	2.886546000	H	2.748736000	-2.944317000	-4.832450000
N	0.855830000	0.852955000	-1.759081000	H	-0.488419000	5.427328000	-4.216870000
N	3.071911000	-0.217521000	-0.215091000	H	0.221516000	1.177475000	-4.057292000
N	0.916189000	-1.674844000	-0.263912000	H	-0.993472000	-1.021476000	-3.826671000
N	-0.697972000	0.654432000	0.682229000	H	3.593916000	-2.298023000	-2.582768000
N	1.481150000	2.089054000	0.827017000	H	-0.881432000	5.376250000	-1.759112000
Co	1.180990000	0.236199000	0.187671000	H	-2.902762000	-1.710268000	-0.704637000
3 high spin				H	4.192031000	-1.609023000	-0.659482000
C	-0.081999000	3.299971000	-4.321878000	H	-1.061883000	5.224604000	0.292925000
C	0.803213000	-2.045887000	-4.506033000	H	-3.992576000	-3.172818000	0.999786000
C	2.107774000	-2.386691000	-4.145673000	H	4.533181000	-1.084057000	1.755172000
C	-0.409704000	4.486665000	-3.667018000	H	-1.104414000	4.857814000	2.757996000
C	-3.977539000	1.307174000	-3.855895000	H	-3.203899000	-2.999495000	3.398556000
C	-0.012548000	2.125832000	-3.570837000	H	2.641791000	-0.240294000	3.110262000
C	0.030960000	-1.323231000	-3.596199000	H	-0.601947000	2.613102000	3.672328000
C	2.585458000	-2.018932000	-2.887403000	H	-1.389478000	-1.415722000	3.949934000
C	-0.631938000	4.458559000	-2.290795000	H	1.087395000	1.054009000	3.927843000

H	0.647840000	-0.660699000	4.062748000	C	2.523030000	-0.416280000	2.102634000
H	-0.587262000	0.591341000	4.283588000	C	0.011395000	0.329491000	2.174081000
N	0.495736000	-0.956390000	-2.395023000	C	-2.551776000	-2.556181000	2.324276000
N	-0.224544000	2.093874000	-2.252185000	C	-0.766580000	2.769843000	2.524489000
N	1.121569000	-0.435228000	0.115662000	C	-1.628221000	-1.594318000	2.739344000
N	-0.447777000	1.903549000	0.384695000	C	0.235366000	0.365637000	3.690563000
N	-1.600618000	-0.816211000	0.638710000	H	0.477351000	3.122599000	-5.355457000
O	-2.324748000	0.135809000	-2.186504000	H	-0.008388000	-2.411604000	-5.189286000
O	-4.740195000	-0.452974000	-2.040519000	H	2.409492000	-3.004829000	-4.769039000
O	-3.937361000	1.796238000	-1.245960000	H	-0.544388000	5.217183000	-4.379264000
F	-3.669759000	0.379888000	-4.767902000	H	0.742130000	1.128173000	-3.890827000
F	-3.200103000	2.373984000	-4.059476000	H	-1.212173000	-1.009982000	-3.482981000
F	-5.248396000	1.672602000	-4.037444000	H	3.480758000	-2.251388000	-2.639608000
S	-3.752747000	0.633182000	-2.125535000	H	-1.191197000	5.223272000	-1.967963000
Co	-0.594183000	0.253653000	-0.970289000	H	-2.504839000	-1.772477000	-0.977210000
3 low spin				H	4.168715000	-1.731913000	-0.586673000
C	0.165264000	3.169457000	-4.310631000	H	-1.311359000	5.164055000	0.168207000
C	0.505944000	-2.090182000	-4.281956000	H	-3.596218000	-3.381538000	0.603240000
C	1.841019000	-2.418237000	-4.043858000	H	4.511891000	-1.213627000	1.836241000
C	-0.395162000	4.325497000	-3.766231000	H	-1.369397000	4.839667000	2.648045000
C	-4.030943000	1.505978000	-3.664279000	H	-3.010160000	-3.224453000	3.057369000
C	0.318074000	2.050796000	-3.491206000	H	2.642489000	-0.286325000	3.176406000
C	-0.176709000	-1.323429000	-3.336960000	H	-0.715242000	2.647278000	3.603539000
C	2.443944000	-1.994657000	-2.858290000	H	-1.371901000	-1.517349000	3.793643000
C	-0.759187000	4.330588000	-2.420313000	H	0.978432000	1.129799000	3.954878000
C	1.696373000	-1.249494000	-1.942528000	H	0.601574000	-0.601995000	4.055253000
C	-0.557989000	3.174101000	-1.658892000	H	-0.695286000	0.593293000	4.225241000
C	2.174643000	-0.866473000	-0.593925000	N	0.402948000	-0.909117000	-2.201373000
C	-0.798014000	3.093602000	-0.204134000	N	-0.037010000	2.048597000	-2.201511000
C	3.391282000	-1.230296000	-0.009573000	N	1.240561000	-0.221413000	0.128585000
C	-2.263365000	-1.765311000	0.086258000	N	-0.570800000	1.871727000	0.333760000
C	-1.108281000	4.187147000	0.606123000	N	-1.372130000	-0.847536000	0.486135000
C	-2.877208000	-2.647875000	0.972642000	O	-2.273114000	0.414645000	-2.066364000
C	3.569205000	-0.956747000	1.347794000	O	-4.682801000	-0.084655000	-1.657430000
C	1.329170000	-0.073842000	1.452922000	O	-3.760308000	2.189303000	-1.121873000
C	-0.473901000	1.703158000	1.664685000	F	-3.898025000	0.487664000	-4.522862000
C	-1.044407000	-0.747900000	1.788615000	F	-3.193468000	2.479539000	-4.040390000
C	-1.121905000	4.006748000	1.986427000	F	-5.280395000	1.970939000	-3.758030000

S	-3.669138000	0.951164000	-1.914962000
Co	-0.340366000	0.416046000	-0.922594000
3a high spin			
C	-1.005975000	3.013513000	-4.391438000
C	1.335148000	-2.096484000	-4.431966000
C	2.652422000	-2.373761000	-4.002752000
C	-1.198839000	4.239500000	-3.750894000
C	-0.686487000	1.902609000	-3.613115000
C	0.490515000	-1.420221000	-3.567483000
C	3.032700000	-2.000224000	-2.724645000
C	-1.064479000	4.304912000	-2.365520000
C	2.112795000	-1.340284000	-1.877588000
C	-0.743481000	3.141482000	-1.650799000
C	2.373287000	-1.022102000	-0.483414000
C	-0.586407000	3.113026000	-0.177152000
C	3.537578000	-1.375385000	0.228139000
C	-2.454245000	-1.471478000	-0.081873000
C	-0.638010000	4.252355000	0.635061000
C	-3.282777000	-2.193995000	0.769900000
C	3.582361000	-1.156291000	1.594941000
C	1.333423000	-0.268226000	1.509686000
C	-0.223573000	1.714131000	1.666578000
C	-1.174198000	-0.629648000	1.684704000
C	-0.476839000	4.089510000	2.008464000
C	2.446759000	-0.631919000	2.257776000
C	0.017262000	0.262820000	2.149988000
C	-3.028771000	-2.123348000	2.139612000
C	-0.266839000	2.814108000	2.536556000
C	-1.969306000	-1.339035000	2.598329000
C	0.130526000	0.235140000	3.681336000
H	-1.098310000	2.911609000	-5.474280000
H	0.980615000	-2.398817000	-5.419259000
H	3.357273000	-2.887055000	-4.661160000
H	-1.452175000	5.135895000	-4.321654000
H	-0.521384000	0.931401000	-4.081647000
H	-0.535709000	-1.188199000	-3.866985000
H	4.037376000	-2.226768000	-2.364769000
H	-1.215454000	5.250958000	-1.846136000

H	-2.602684000	-1.496018000	-1.165408000
H	4.382814000	-1.835950000	-0.285067000
H	-0.794453000	5.243629000	0.210502000
H	-4.099236000	-2.795026000	0.365225000
H	4.472955000	-1.421397000	2.169238000
H	-0.511915000	4.956346000	2.672330000
H	-3.647514000	-2.673695000	2.852654000
H	2.463557000	-0.528397000	3.340318000
H	-0.140033000	2.694195000	3.609905000
H	-1.774293000	-1.289269000	3.666835000
H	0.960322000	0.865577000	4.023441000
H	0.313863000	-0.783357000	4.045824000
H	-0.787760000	0.606767000	4.154120000
N	0.854014000	-1.015364000	-2.330767000
N	-0.558218000	1.958304000	-2.280053000
N	1.337264000	-0.394114000	0.161368000
N	-0.383336000	1.890384000	0.348634000
N	-1.437665000	-0.714570000	0.362522000
Co	-0.176762000	0.236294000	-1.008764000
3a low spin			
C	-0.669580000	2.934203000	-4.363125000
C	0.854515000	-2.116381000	-4.180090000
C	2.170219000	-2.496682000	-3.899168000
C	-0.987727000	4.180727000	-3.788989000
C	-0.387948000	1.855638000	-3.545876000
C	0.193894000	-1.271435000	-3.291582000
C	2.749271000	-2.071237000	-2.704843000
C	-0.989529000	4.270148000	-2.406989000
C	2.015409000	-1.249867000	-1.841785000
C	-0.688575000	3.138631000	-1.626321000
C	2.410333000	-0.921196000	-0.465463000
C	-0.631032000	3.140550000	-0.182279000
C	3.547238000	-1.376503000	0.207009000
C	-2.215045000	-1.366855000	-0.251111000
C	-0.921342000	4.229605000	0.654421000
C	-3.010763000	-2.203198000	0.526813000
C	3.631617000	-1.160634000	1.582780000
C	1.439049000	-0.152873000	1.532013000

C	-0.197552000	1.756342000	1.679927000	O	-2.998243000	0.530190000	0.849899000
C	-1.024950000	-0.598659000	1.603278000	O	1.048421000	0.998435000	2.114853000
C	-0.818461000	4.067215000	2.027351000	N	-0.588913000	2.166139000	-0.352450000
C	2.550311000	-0.588711000	2.262701000	N	-0.255578000	-0.405016000	-0.405476000
C	0.111039000	0.329848000	2.154913000	N	-0.813558000	-1.266609000	2.010634000
C	-2.790119000	-2.224915000	1.903860000	N	-1.308499000	2.765468000	2.099678000
C	-0.460866000	2.812729000	2.548604000	C	-0.050842000	2.542488000	-2.640509000
C	-1.790254000	-1.416090000	2.447026000	C	0.354108000	-0.539191000	-2.702011000
C	0.183748000	0.257753000	3.684584000	C	-0.270966000	3.908991000	-2.445814000
H	-0.639319000	2.798961000	-5.446434000	C	0.492523000	-1.923109000	-2.562344000
H	0.338563000	-2.464272000	-5.076914000	C	-0.221949000	1.682635000	-1.550049000
H	2.726767000	-3.138548000	-4.585576000	C	-0.028808000	0.204088000	-1.580188000
H	-1.219146000	5.048373000	-4.410070000	C	-0.650243000	4.390154000	-1.191853000
H	-0.137391000	0.899259000	-3.997598000	C	0.252394000	-2.535252000	-1.331225000
H	-0.834617000	-0.960471000	-3.481666000	C	-0.804634000	3.470209000	-0.144346000
H	3.755139000	-2.390892000	-2.429786000	C	-0.129199000	-1.727776000	-0.249658000
H	-1.216113000	5.215749000	-1.912131000	C	-1.201795000	3.814001000	1.249537000
H	-2.351138000	-1.309604000	-1.334355000	C	-0.423028000	-2.215908000	1.126842000
H	4.336275000	-1.908884000	-0.325183000	C	-1.447311000	5.122362000	1.680379000
H	-1.224774000	5.184781000	0.225297000	C	-0.304864000	-3.556425000	1.509693000
H	-3.783671000	-2.815618000	0.058389000	C	-0.595708000	-3.914447000	2.827493000
H	4.513523000	-1.488662000	2.137259000	C	-1.805228000	5.342818000	3.011772000
H	-1.029498000	4.899857000	2.701809000	C	-1.091729000	-1.612270000	3.272872000
H	-3.389288000	-2.864468000	2.556572000	C	-1.648666000	2.979297000	3.375889000
H	2.578153000	-0.503413000	3.347389000	C	-0.997118000	-2.928228000	3.728628000
H	-0.402535000	2.676035000	3.626074000	C	-1.907781000	4.255161000	3.879214000
H	-1.616783000	-1.433515000	3.520854000	H	0.540237000	-0.057257000	-3.662010000
H	0.965748000	0.926442000	4.067568000	H	-0.145573000	4.603972000	-3.278846000
H	0.417777000	-0.760393000	4.020955000	H	0.789516000	-2.528551000	-3.421394000
H	-0.768821000	0.552615000	4.142819000	H	-0.820294000	5.455681000	-1.038689000
N	0.766718000	-0.800420000	-2.168251000	H	0.359821000	-3.614297000	-1.221599000
N	-0.391645000	1.909329000	-2.183690000	H	0.014321000	-4.312948000	0.792965000
N	1.448110000	-0.227321000	0.191256000	H	-1.360178000	5.960876000	0.989377000
N	-0.245813000	1.937325000	0.337593000	H	-1.999942000	6.358091000	3.364727000
N	-1.253714000	-0.592100000	0.273643000	H	-1.400774000	-0.806545000	3.944424000
Co	0.052297000	0.525768000	-0.904084000	H	-1.715367000	2.097181000	4.018875000
4 high spin				H	-2.182623000	4.383110000	4.927673000
Co	-0.913057000	0.781981000	1.228907000	H	-1.233238000	-3.164265000	4.767694000

H	0.245668000	2.161767000	-3.618014000
H	-3.432808000	-0.313798000	1.063274000
H	-3.628226000	1.226033000	1.106506000
H	1.379612000	0.256101000	2.649357000
H	1.203372000	1.792657000	2.654895000
H	-0.506774000	-4.956245000	3.143644000

4 low spin

Co	-0.765717000	0.821285000	0.971512000
O	-2.978236000	0.586816000	0.542823000
O	1.362622000	1.104489000	1.692709000
N	-0.573026000	2.123239000	-0.389368000
N	-0.248480000	-0.339633000	-0.433537000
N	-0.821002000	-0.962005000	1.979752000
N	-1.254867000	2.493446000	2.050831000
C	-0.047373000	2.597287000	-2.660062000
C	0.388660000	-0.577925000	-2.712699000
C	-0.302015000	3.949695000	-2.403460000
C	0.506821000	-1.957033000	-2.502914000
C	-0.197224000	1.688656000	-1.611250000
C	0.000874000	0.221756000	-1.636886000
C	-0.693059000	4.372201000	-1.130330000
C	0.242363000	-2.512738000	-1.248426000
C	-0.820907000	3.411840000	-0.118009000
C	-0.142226000	-1.657382000	-0.207546000
C	-1.213034000	3.629151000	1.293785000
C	-0.471239000	-2.019577000	1.190491000
C	-1.516909000	4.879400000	1.834899000
C	-0.437959000	-3.323266000	1.687680000
C	-0.774310000	-3.549207000	3.024263000
C	-1.873976000	4.968826000	3.182245000
C	-1.143825000	-1.188494000	3.257267000
C	-1.593777000	2.589994000	3.341597000
C	-1.134703000	-2.465387000	3.822570000
C	-1.912749000	3.806231000	3.949465000
H	0.591984000	-0.134513000	-3.688271000
H	-0.194957000	4.682048000	-3.206317000
H	0.808291000	-2.605394000	-3.328185000
H	-0.893317000	5.425352000	-0.932013000

H	0.332742000	-3.587028000	-1.086165000
H	-0.151657000	-4.151387000	1.038761000
H	-1.473898000	5.772676000	1.211095000
H	-2.116391000	5.938278000	3.623014000
H	-1.422202000	-0.321031000	3.856818000
H	-1.611525000	1.664529000	3.918384000
H	-2.183694000	3.826332000	5.006291000
H	-1.407108000	-2.592949000	4.871570000
H	0.257811000	2.257145000	-3.650557000
H	-3.282309000	-0.335993000	0.500684000
H	-3.532838000	0.985517000	1.235002000
H	1.827636000	0.281217000	1.919707000
H	1.417424000	1.637510000	2.504121000
H	-0.754241000	-4.562226000	3.431880000

4a high spin

Co	-1.090084000	0.766119000	1.040136000
O	-3.194809000	0.515824000	1.148434000
N	-0.673514000	2.131165000	-0.399515000
N	-0.357668000	-0.396605000	-0.446421000
N	-0.859315000	-1.211562000	1.976039000
N	-1.357976000	2.705838000	2.049370000
C	-0.013660000	2.555099000	-2.667376000
C	0.393413000	-0.556479000	-2.720619000
C	-0.168520000	3.922107000	-2.444278000
C	0.595510000	-1.924475000	-2.546027000
C	-0.262149000	1.657681000	-1.615120000
C	-0.077209000	0.209284000	-1.640982000
C	-0.559523000	4.389735000	-1.171733000
C	0.338352000	-2.520882000	-1.293520000
C	-0.803712000	3.458853000	-0.165149000
C	-0.139379000	-1.720744000	-0.258699000
C	-1.210177000	3.776486000	1.224764000
C	-0.445454000	-2.180175000	1.116721000
C	-1.435448000	5.081083000	1.692388000
C	-0.323703000	-3.513363000	1.540598000
C	-0.627273000	-3.841991000	2.859397000
C	-1.812979000	5.276420000	3.018600000
C	-1.156169000	-1.536185000	3.242550000

C	-1.727325000	2.900765000	3.323260000
C	-1.053108000	-2.835483000	3.734132000
C	-1.963737000	4.165687000	3.856976000
H	0.610053000	-0.083237000	-3.680145000
H	0.023632000	4.633983000	-3.249795000
H	0.966187000	-2.533863000	-3.372973000
H	-0.662062000	5.459742000	-0.987867000
H	0.517776000	-3.586390000	-1.145947000
H	0.004552000	-4.285283000	0.843857000
H	-1.319153000	5.933633000	1.022484000
H	-1.990507000	6.286683000	3.395015000
H	-1.490126000	-0.718846000	3.888547000
H	-1.838315000	2.003948000	3.939946000
H	-2.258376000	4.273523000	4.902466000
H	-1.300709000	-3.049116000	4.775542000
H	0.306322000	2.186646000	-3.643776000
H	-3.535621000	-0.294102000	1.565385000
H	-3.713712000	1.245455000	1.528562000
H	-0.534383000	-4.875225000	3.202326000

4a low spin

Co	-1.018506000	0.791451000	0.817482000
O	-3.163056000	0.537174000	0.763943000
N	-0.617228000	2.082042000	-0.436248000
N	-0.304772000	-0.313281000	-0.473933000
N	-0.831865000	-0.900713000	1.915933000
N	-1.259894000	2.437393000	1.971757000
C	-0.036798000	2.600219000	-2.706427000
C	0.386473000	-0.591859000	-2.755602000
C	-0.224763000	3.957454000	-2.429243000
C	0.560005000	-1.959139000	-2.521277000
C	-0.239763000	1.667745000	-1.684901000
C	-0.049516000	0.223522000	-1.707418000
C	-0.607187000	4.365331000	-1.143028000
C	0.300061000	-2.492245000	-1.250406000
C	-0.801884000	3.396942000	-0.155921000
C	-0.139565000	-1.639625000	-0.235541000
C	-1.184332000	3.598165000	1.244741000
C	-0.457410000	-1.978194000	1.154601000

C	-1.443574000	4.848748000	1.821650000
C	-0.387642000	-3.271636000	1.689832000
C	-0.709035000	-3.477273000	3.027695000
C	-1.791826000	4.924036000	3.166642000
C	-1.155625000	-1.122750000	3.202610000
C	-1.613058000	2.529904000	3.266909000
C	-1.104012000	-2.378738000	3.799113000
C	-1.880243000	3.738137000	3.903657000
H	0.591559000	-0.157867000	-3.735936000
H	-0.068674000	4.702080000	-3.212303000
H	0.904019000	-2.612345000	-3.325634000
H	-0.747964000	5.423103000	-0.916836000
H	0.440970000	-3.556638000	-1.057650000
H	-0.083839000	-4.105254000	1.055380000
H	-1.371782000	5.751341000	1.213387000
H	-1.994471000	5.890660000	3.633198000
H	-1.464040000	-0.257079000	3.787879000
H	-1.680798000	1.597064000	3.825753000
H	-2.150737000	3.740866000	4.961053000
H	-1.368785000	-2.485730000	4.852605000
H	0.268863000	2.265404000	-3.699428000
H	-3.428291000	-0.395596000	0.841909000
H	-3.614331000	0.977010000	1.505467000
H	-0.656743000	-4.478072000	3.462089000

5 high spin

C	3.662821000	-1.098398000	-4.784184000
C	4.762467000	-1.806849000	-4.296891000
C	2.528152000	-0.972888000	-3.983213000
C	4.680846000	-2.356904000	-3.017325000
C	2.521399000	-1.566384000	-2.711080000
C	0.077360000	-1.102267000	-2.263526000
C	1.355817000	-1.491003000	-1.788052000
C	-0.983893000	-1.130199000	-1.395259000
C	5.846964000	-4.920921000	-0.294998000
C	6.888810000	-5.675996000	0.244759000
C	-0.788329000	-1.505325000	-0.041962000
C	0.546693000	-1.827963000	0.389827000
C	-1.884796000	-1.565518000	0.855199000

C	7.060986000	-5.671797000	1.630409000	C	4.861081000	-2.293685000	-2.596271000
C	5.172874000	-4.183010000	1.798741000	C	2.598626000	-1.777896000	-2.603274000
C	0.756582000	-2.136316000	1.787219000	C	0.134973000	-1.302699000	-2.278242000
C	6.189342000	-4.922663000	2.420909000	C	1.396466000	-1.669463000	-1.756598000
C	-1.676307000	-1.931939000	2.163896000	C	-0.938878000	-1.242895000	-1.427388000
C	4.173884000	-3.379395000	2.554120000	C	5.516442000	-4.764704000	-0.544843000
C	2.071294000	-2.354777000	2.469641000	C	6.610241000	-5.528358000	-0.140170000
C	-0.366273000	-2.199133000	2.612259000	C	-0.765102000	-1.516784000	-0.047524000
C	4.373650000	-2.983518000	3.880349000	C	0.551660000	-1.844766000	0.430653000
C	2.242659000	-1.873853000	3.784485000	C	-1.871667000	-1.477346000	0.838122000
C	3.400180000	-2.192411000	4.487526000	C	6.989417000	-5.497304000	1.203490000
H	3.687005000	-0.641755000	-5.776400000	C	5.148521000	-4.003068000	1.620780000
H	5.671507000	-1.928894000	-4.889102000	C	0.731952000	-2.077498000	1.841321000
H	1.668440000	-0.407801000	-4.342278000	C	6.237942000	-4.739383000	2.101072000
H	-0.069016000	-0.825895000	-3.306760000	C	-1.692135000	-1.760661000	2.171914000
H	5.524073000	-2.900510000	-2.583531000	C	4.184942000	-3.281759000	2.474047000
H	5.654741000	-4.909411000	-1.371024000	C	2.038362000	-2.332486000	2.507861000
H	-1.990619000	-0.873211000	-1.733703000	C	-0.400862000	-2.050807000	2.654863000
H	7.541939000	-6.256164000	-0.410103000	C	4.383541000	-3.022600000	3.829618000
H	-2.883757000	-1.326911000	0.482129000	C	2.212574000	-1.995471000	3.866411000
H	7.858979000	-6.255558000	2.095470000	C	3.387377000	-2.339150000	4.524759000
H	-2.509947000	-2.008323000	2.865539000	H	3.976114000	-1.020830000	-5.623201000
H	-0.235860000	-2.478694000	3.658587000	H	5.999757000	-1.883543000	-4.379668000
H	1.479391000	-1.247599000	4.245365000	H	1.794618000	-0.905461000	-4.419932000
H	3.544517000	-1.822637000	5.505322000	H	0.016436000	-1.100395000	-3.341913000
N	3.590414000	-2.243558000	-2.256739000	H	5.719273000	-2.637374000	-2.019582000
N	1.566737000	-1.832414000	-0.517732000	H	5.156646000	-4.789220000	-1.573554000
N	5.026160000	-4.188546000	0.461376000	H	-1.935066000	-0.990509000	-1.797877000
N	3.054588000	-3.051334000	1.876478000	H	7.144727000	-6.138927000	-0.870280000
Cl	2.295021000	-4.934637000	-1.055543000	H	-2.857024000	-1.231178000	0.435381000
Cl	4.846433000	-0.983501000	0.294941000	H	7.844267000	-6.078889000	1.556230000
Co	3.406901000	-2.935768000	-0.236760000	H	-2.536606000	-1.759619000	2.864505000
H	5.285438000	-3.249606000	4.414889000	H	-0.297705000	-2.277338000	3.716055000
H	6.289339000	-4.930473000	3.506567000	H	1.434997000	-1.452159000	4.400678000
5 low spin				H	3.526088000	-2.075571000	5.575506000
C	3.895783000	-1.372354000	-4.592120000	N	3.677834000	-2.292039000	-1.973600000
C	5.014529000	-1.853406000	-3.910709000	N	1.589701000	-1.929378000	-0.456158000
C	2.672727000	-1.319053000	-3.924656000	N	4.833207000	-3.990232000	0.306370000

N	3.044066000	-2.919496000	1.833339000
Cl	2.088955000	-4.956727000	-0.918165000
Cl	4.720247000	-0.699494000	0.485275000
Co	3.287479000	-2.831394000	-0.101261000
H	5.308701000	-3.317211000	4.324674000
H	6.480391000	-4.742047000	3.163904000

5a high spin

C	3.974801000	-1.275532000	-4.494004000
C	5.081435000	-1.802594000	-3.802499000
C	2.739222000	-1.242740000	-3.868425000
C	4.876917000	-2.309124000	-2.524324000
C	2.603738000	-1.754523000	-2.556222000
C	0.156248000	-1.244451000	-2.260534000
C	1.404109000	-1.672225000	-1.757567000
C	-0.932476000	-1.192403000	-1.426306000
C	5.467439000	-4.839660000	-0.539196000
C	6.589851000	-5.557138000	-0.133944000
C	-0.793903000	-1.526898000	-0.040224000
C	0.514555000	-1.924515000	0.438486000
C	-1.891671000	-1.470199000	0.834795000
C	6.997928000	-5.469964000	1.200192000
C	5.123074000	-4.017221000	1.613742000
C	0.670724000	-2.165512000	1.851741000
C	6.247157000	-4.703890000	2.090122000
C	-1.740398000	-1.782640000	2.187090000
C	4.157990000	-3.291373000	2.461090000
C	1.964187000	-2.412041000	2.505151000
C	-0.480540000	-2.109300000	2.675834000
C	4.372970000	-2.994574000	3.802653000
C	2.156387000	-2.063327000	3.865812000
C	3.351585000	-2.346534000	4.507037000
H	4.088990000	-0.877407000	-5.505361000
H	6.078917000	-1.823391000	-4.244617000
H	1.879789000	-0.801122000	-4.373667000
H	0.057018000	-0.979949000	-3.313947000
H	5.713627000	-2.722961000	-1.958758000
H	5.083286000	-4.904169000	-1.557219000
H	-1.912940000	-0.888953000	-1.800825000

H	7.126072000	-6.176696000	-0.855088000
H	-2.867205000	-1.184280000	0.432270000
H	7.876828000	-6.015639000	1.551168000
H	-2.600811000	-1.770156000	2.860502000
H	-0.383478000	-2.356663000	3.733593000
H	1.367967000	-1.542008000	4.406405000
H	3.496368000	-2.061695000	5.551543000
N	3.676152000	-2.324872000	-1.924123000
N	1.554136000	-2.023167000	-0.434107000
N	4.777845000	-4.057940000	0.305067000
N	2.991032000	-2.982785000	1.824725000
Cl	2.099953000	-5.110627000	-0.957148000
Co	3.171498000	-3.024469000	-0.117003000
H	5.316921000	-3.243475000	4.286999000
H	6.514418000	-4.662847000	3.146111000

5a low spin

C	4.004342000	-1.324852000	-4.443673000
C	5.094637000	-1.836971000	-3.711399000
C	2.760363000	-1.282701000	-3.839349000
C	4.877110000	-2.315346000	-2.430891000
C	2.610577000	-1.753243000	-2.515491000
C	0.155677000	-1.214886000	-2.244771000
C	1.402175000	-1.657269000	-1.733211000
C	-0.935573000	-1.177441000	-1.420896000
C	5.433685000	-4.844454000	-0.567007000
C	6.567331000	-5.544586000	-0.174744000
C	-0.799790000	-1.526990000	-0.041517000
C	0.498755000	-1.928037000	0.439671000
C	-1.902706000	-1.482274000	0.834916000
C	6.999832000	-5.440736000	1.155150000
C	5.116174000	-3.998207000	1.583105000
C	0.667245000	-2.167855000	1.846627000
C	6.256859000	-4.674822000	2.046176000
C	-1.744626000	-1.808086000	2.174374000
C	4.167556000	-3.268851000	2.421762000
C	1.978025000	-2.388562000	2.481789000
C	-0.477596000	-2.132849000	2.666000000
C	4.374226000	-2.982638000	3.768673000

C	2.166012000	-2.055597000	3.838511000
C	3.367064000	-2.331956000	4.482818000
H	4.139972000	-0.953419000	-5.462031000
H	6.102675000	-1.856814000	-4.130265000
H	1.901844000	-0.871474000	-4.371565000
H	0.069330000	-0.934124000	-3.294646000
H	5.708532000	-2.709178000	-1.845557000
H	5.035411000	-4.926747000	-1.578447000
H	-1.915372000	-0.872733000	-1.795844000
H	7.096674000	-6.166754000	-0.898913000
H	-2.879328000	-1.196081000	0.436236000
H	7.889644000	-5.975060000	1.495913000
H	-2.602358000	-1.804842000	2.851412000
H	-0.381457000	-2.380751000	3.723332000
H	1.366440000	-1.558662000	4.386018000
H	3.513164000	-2.054902000	5.528724000
N	3.663958000	-2.302904000	-1.831438000
N	1.551116000	-2.034423000	-0.432016000
N	4.747020000	-4.050597000	0.276853000
N	3.013327000	-2.912375000	1.760042000
Cl	2.093287000	-5.042302000	-0.961765000
Co	3.110398000	-3.090636000	-0.132867000
H	5.315634000	-3.249145000	4.249694000
H	6.540446000	-4.620518000	3.097533000

6 high spin

C	3.628824000	-1.187198000	-4.828584000
C	4.689150000	-1.970389000	-4.369675000
C	2.519545000	-0.998334000	-4.004908000
C	4.596929000	-2.525672000	-3.093208000
C	2.497837000	-1.604005000	-2.738506000
C	0.092650000	-1.008398000	-2.259240000
C	1.351234000	-1.470582000	-1.798048000
C	-0.959101000	-0.982399000	-1.380425000
C	5.920049000	-4.921154000	-0.273511000
C	7.052895000	-5.514890000	0.318545000
C	-0.771930000	-1.379743000	-0.032652000
C	0.546766000	-1.780037000	0.387323000
C	-1.868434000	-1.390678000	0.866005000

C	7.246090000	-5.378878000	1.681793000
C	5.171187000	-4.135253000	1.764215000
C	0.743815000	-2.115101000	1.784091000
C	6.291856000	-4.672097000	2.452025000
C	-1.678503000	-1.789151000	2.167596000
C	4.135923000	-3.449197000	2.505509000
C	2.040251000	-2.421499000	2.465582000
C	-0.384341000	-2.131979000	2.606648000
C	4.305227000	-3.244765000	3.896538000
C	2.188185000	-2.083689000	3.844139000
C	3.296538000	-2.499840000	4.549603000
H	3.663738000	-0.722242000	-5.816609000
H	5.576755000	-2.145558000	-4.980775000
H	1.691669000	-0.375743000	-4.343005000
H	-0.048487000	-0.719339000	-3.299612000
H	5.411956000	-3.126455000	-2.681864000
H	5.744582000	-5.006000000	-1.349807000
H	-1.953438000	-0.667569000	-1.706281000
H	7.763790000	-6.061758000	-0.304001000
H	-2.852941000	-1.091477000	0.498374000
H	8.122188000	-5.810237000	2.172926000
H	-2.513188000	-1.832662000	2.870678000
H	-0.273134000	-2.435620000	3.647613000
H	1.425764000	-1.489602000	4.345567000
H	3.402390000	-2.255939000	5.609707000
N	3.531238000	-2.349573000	-2.309871000
N	1.555627000	-1.833068000	-0.531865000
N	5.022301000	-4.242954000	0.424891000
N	3.031316000	-3.047886000	1.831595000
Cl	2.189495000	-4.985308000	-0.996215000
Cl	4.846754000	-1.051369000	0.180812000
Co	3.363929000	-2.996785000	-0.276222000
C	5.466252000	-3.767601000	4.560832000
C	6.413707000	-4.469378000	3.870012000
H	5.569319000	-3.598363000	5.635508000
H	7.287782000	-4.880581000	4.381012000

6 low spin

C	3.825269000	-1.452887000	-4.652590000
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C	4.952024000	-1.926834000	-3.979773000	N	1.571836000	-1.920934000	-0.470617000
C	2.614015000	-1.378467000	-3.966198000	N	4.880025000	-3.982953000	0.284535000
C	4.816905000	-2.340021000	-2.654761000	N	3.012527000	-2.904485000	1.798079000
C	2.557916000	-1.810130000	-2.634620000	Cl	2.088540000	-4.963897000	-0.866396000
C	0.111468000	-1.288011000	-2.288197000	Cl	4.699482000	-0.699636000	0.426469000
C	1.369134000	-1.674609000	-1.773016000	Co	3.283684000	-2.820961000	-0.132309000
C	-0.948455000	-1.180037000	-1.425822000	C	5.510518000	-3.823175000	4.408804000
C	5.670019000	-4.712162000	-0.494096000	C	6.424262000	-4.486170000	3.635126000
C	6.798530000	-5.394307000	0.003067000	H	5.653975000	-3.737023000	5.488605000
C	-0.764699000	-1.433591000	-0.043843000	H	7.305989000	-4.947530000	4.086409000
C	0.545760000	-1.799192000	0.427135000	6a high spin			
C	-1.862883000	-1.336793000	0.847722000	C	3.820679000	-1.248640000	-4.626761000
C	7.106656000	-5.317261000	1.350742000	C	4.861704000	-2.029005000	-4.093632000
C	5.123370000	-3.971156000	1.618520000	C	2.660488000	-1.070780000	-3.889457000
C	0.724338000	-2.026477000	1.842633000	C	4.674136000	-2.598139000	-2.840089000
C	6.244631000	-4.599071000	2.212501000	C	2.539231000	-1.673510000	-2.614857000
C	-1.684722000	-1.602011000	2.184703000	C	0.167018000	-0.924467000	-2.202860000
C	4.132158000	-3.340009000	2.435640000	C	1.369394000	-1.521498000	-1.757745000
C	2.014279000	-2.362069000	2.500871000	C	-0.913892000	-0.869453000	-1.356606000
C	-0.403483000	-1.938918000	2.660921000	C	5.763896000	-5.012802000	-0.371164000
C	4.326237000	-3.250924000	3.830251000	C	6.976485000	-5.483632000	0.171332000
C	2.182044000	-2.149723000	3.901942000	C	-0.805839000	-1.350692000	-0.013961000
C	3.311873000	-2.587652000	4.558517000	C	0.471265000	-1.889623000	0.407659000
H	3.890468000	-1.122754000	-5.691746000	C	-1.897158000	-1.305610000	0.872076000
H	5.929446000	-1.972469000	-4.463519000	C	7.271355000	-5.208835000	1.494879000
H	1.731131000	-0.969223000	-4.456308000	C	5.141107000	-4.066658000	1.646052000
H	-0.014630000	-1.101596000	-3.353737000	C	0.637232000	-2.234002000	1.805009000
H	5.681801000	-2.678039000	-2.085502000	C	6.340579000	-4.490681000	2.283235000
H	5.405522000	-4.774156000	-1.550592000	C	-1.754974000	-1.754692000	2.185052000
H	-1.941361000	-0.903685000	-1.787725000	C	4.114524000	-3.396776000	2.406065000
H	7.419553000	-5.968050000	-0.687414000	C	1.925247000	-2.534834000	2.447515000
H	-2.840762000	-1.060914000	0.446130000	C	-0.511972000	-2.187605000	2.635791000
H	7.988589000	-5.818332000	1.757509000	C	4.336994000	-3.146718000	3.779598000
H	-2.522147000	-1.555077000	2.884095000	C	2.105042000	-2.221410000	3.833324000
H	-0.309585000	-2.158092000	3.723493000	C	3.279919000	-2.511194000	4.484471000
H	1.412723000	-1.627891000	4.467393000	H	3.923778000	-0.779719000	-5.608567000
H	3.423766000	-2.429898000	5.633903000	H	5.794965000	-2.189611000	-4.636317000
N	3.644269000	-2.318741000	-2.012683000	H	1.852647000	-0.455516000	-4.285759000

H	0.085402000	-0.541411000	-3.220321000
H	5.458224000	-3.211053000	-2.389631000
H	5.497569000	-5.227223000	-1.409538000
H	-1.865528000	-0.449433000	-1.691469000
H	7.662938000	-6.053618000	-0.457658000
H	-2.854759000	-0.922061000	0.509848000
H	8.206435000	-5.551364000	1.945748000
H	-2.610083000	-1.757529000	2.865661000
H	-0.427599000	-2.522574000	3.670161000
H	1.308295000	-1.715382000	4.376155000
H	3.409056000	-2.254745000	5.538948000
N	3.554885000	-2.435077000	-2.117880000
N	1.482700000	-2.018675000	-0.491176000
N	4.890838000	-4.307649000	0.334964000
N	2.954729000	-3.082453000	1.764226000
Cl	2.023167000	-5.392228000	-0.982718000
Co	3.014994000	-3.407972000	-0.288650000
C	5.573850000	-3.539637000	4.387716000
C	6.540912000	-4.193388000	3.671325000
H	5.721598000	-3.319192000	5.448061000
H	7.473776000	-4.507860000	4.145389000

6a low spin

C	3.921699000	-1.419541000	-4.526563000
C	5.030166000	-1.902206000	-3.801588000
C	2.690741000	-1.363823000	-3.898082000
C	4.840637000	-2.342738000	-2.503407000
C	2.569983000	-1.792899000	-2.556436000
C	0.133826000	-1.214290000	-2.257308000
C	1.377478000	-1.673497000	-1.754862000
C	-0.940342000	-1.126698000	-1.417242000
C	5.557851000	-4.777345000	-0.531402000
C	6.721742000	-5.407788000	-0.057497000
C	-0.791021000	-1.448048000	-0.032510000
C	0.502834000	-1.882579000	0.440457000
C	-1.882107000	-1.343898000	0.851649000
C	7.092333000	-5.267297000	1.273577000
C	5.096158000	-3.945831000	1.573539000
C	0.671852000	-2.108168000	1.855013000

C	6.256113000	-4.532576000	2.141901000
C	-1.723563000	-1.645339000	2.197435000
C	4.130235000	-3.297224000	2.385820000
C	1.966432000	-2.398492000	2.480914000
C	-0.467939000	-2.010308000	2.681963000
C	4.352037000	-3.167667000	3.771393000
C	2.162107000	-2.173481000	3.875101000
C	3.327560000	-2.534995000	4.518115000
H	4.033678000	-1.080367000	-5.558976000
H	6.029860000	-1.928338000	-4.239586000
H	1.819671000	-0.975707000	-4.426909000
H	0.038220000	-0.952503000	-3.311146000
H	5.686261000	-2.711384000	-1.923075000
H	5.238553000	-4.900186000	-1.567106000
H	-1.917345000	-0.801435000	-1.781937000
H	7.322203000	-6.000127000	-0.750520000
H	-2.851109000	-1.031298000	0.454409000
H	8.001267000	-5.736763000	1.657981000
H	-2.573551000	-1.594398000	2.882288000
H	-0.377082000	-2.245030000	3.741914000
H	1.373041000	-1.692373000	4.450453000
H	3.455953000	-2.353165000	5.587507000
N	3.639838000	-2.318920000	-1.880105000
N	1.538877000	-2.029863000	-0.446771000
N	4.787063000	-4.018203000	0.248423000
N	2.990584000	-2.883917000	1.733172000
Cl	2.126171000	-5.054181000	-0.925729000
Co	3.111724000	-3.074397000	-0.160511000
C	5.568623000	-3.693264000	4.327593000
C	6.479525000	-4.359818000	3.550237000
H	5.740797000	-3.572276000	5.400147000
H	7.385615000	-4.781984000	3.991713000

7 high spin

C	1.649774000	-4.298216000	-3.145559000
C	1.845627000	-2.904440000	-2.550741000
C	2.433518000	-2.929167000	-1.134355000
C	2.596148000	-1.519439000	-0.566452000
C	4.596983000	2.212123000	0.849578000

C	4.623935000	-1.959319000	0.766098000	H	3.430494000	4.007463000	1.176767000
C	4.586109000	0.815926000	0.824241000	H	1.291618000	4.766113000	0.988199000
C	3.260084000	-1.403983000	0.867851000	H	3.878273000	-3.949455000	1.893618000
C	3.433971000	2.917238000	1.157136000	H	-0.988507000	5.552117000	1.649734000
C	3.394713000	0.136551000	1.117494000	H	2.376511000	-5.448703000	3.170142000
C	2.286681000	2.183902000	1.472887000	H	-2.490673000	4.052774000	2.925632000
C	0.618335000	4.112942000	1.544094000	H	0.096316000	-4.662985000	3.831635000
C	2.450285000	-2.308305000	1.854181000	H	-2.042558000	-3.904668000	3.643927000
C	2.891944000	-3.596154000	2.191270000	H	-4.131941000	-2.647775000	4.199230000
C	0.986036000	2.804417000	1.871921000	H	-4.107390000	-0.171496000	4.255565000
C	-0.653970000	4.546382000	1.913833000	H	-0.385170000	3.630316000	5.304689000
C	2.041747000	-4.443120000	2.905750000	H	-0.226746000	1.131694000	5.304965000
C	-1.504390000	3.699362000	2.627964000	H	-2.021503000	3.556227000	5.971693000
C	0.401399000	-2.701445000	2.947349000	H	-1.828669000	1.017204000	6.067442000
C	-1.063055000	2.411279000	2.964677000	H	0.421233000	5.009556000	7.350155000
C	0.769398000	-4.009824000	3.275487000	H	0.505622000	2.475463000	7.348086000
C	-0.899233000	-2.081012000	3.346566000	H	-1.221944000	4.950701000	8.028479000
C	-2.046213000	-2.814437000	3.663178000	H	-1.122081000	2.415701000	8.027880000
C	-2.007441000	-0.033724000	3.701715000	H	0.155757000	4.350839000	8.981563000
C	-3.237407000	2.062001000	4.051087000	N	5.686739000	-2.402548000	0.640745000
C	-1.873324000	1.506988000	3.950658000	N	2.304008000	0.835443000	1.445486000
C	-3.209175000	-2.109425000	3.971200000	N	1.241401000	-1.903053000	2.257223000
C	-3.198527000	-0.713235000	3.996035000	N	0.145787000	2.005944000	2.561664000
C	-1.210445000	1.623142000	5.385437000	N	-0.916823000	-0.732532000	3.373383000
C	-1.048431000	3.033068000	5.952995000	N	-4.300416000	2.505029000	4.175411000
C	-0.461526000	3.008823000	7.369802000	Co	0.693685000	0.051475000	2.409628000
C	-0.266131000	4.402799000	7.964297000	Br	-0.793978000	-0.052288000	0.141379000
H	1.227135000	-4.245911000	-4.162496000	Br	2.179908000	0.155575000	4.678085000
H	2.605530000	-4.846112000	-3.210630000	7 low spin			
H	2.505753000	-2.311133000	-3.209084000	C	1.738869000	-4.326511000	-3.178538000
H	0.962854000	-4.905171000	-2.531114000	C	1.916503000	-2.933344000	-2.576914000
H	0.878517000	-2.371054000	-2.528171000	C	2.480919000	-2.958259000	-1.150656000
H	3.406496000	-3.452472000	-1.153883000	C	2.622422000	-1.547460000	-0.581342000
H	3.213995000	-0.913354000	-1.248675000	C	4.533530000	2.179823000	0.734850000
H	1.770623000	-3.526499000	-0.485745000	C	4.629051000	-1.970458000	0.803911000
H	1.612578000	-1.027862000	-0.485148000	C	4.521767000	0.787773000	0.737670000
H	5.519990000	2.750380000	0.622312000	C	3.260298000	-1.418817000	0.867616000
H	5.495039000	0.274109000	0.565122000	C	3.374119000	2.865534000	1.080798000

C	3.360477000	0.100502000	1.116835000	H	2.265355000	-5.479445000	3.013290000
C	2.255471000	2.126902000	1.471363000	H	-2.398447000	4.074555000	3.065448000
C	0.661873000	4.079452000	1.616792000	H	0.023298000	-4.622910000	3.729355000
C	2.434523000	-2.279221000	1.843733000	H	-1.960906000	-3.851111000	3.750573000
C	2.822969000	-3.600257000	2.106044000	H	-4.051001000	-2.618959000	4.371088000
C	0.981362000	2.745372000	1.878575000	H	-4.024196000	-0.135081000	4.391355000
C	-0.582222000	4.553682000	2.016827000	H	-0.423692000	3.664190000	5.334434000
C	1.967420000	-4.450517000	2.801777000	H	-0.246460000	1.165846000	5.336932000
C	-1.437406000	3.703543000	2.713152000	H	-2.070662000	3.578087000	5.974718000
C	0.404066000	-2.642022000	2.940166000	H	-1.863452000	1.042071000	6.071247000
C	-1.048694000	2.382641000	2.975758000	H	0.342208000	5.042749000	7.396175000
C	0.723255000	-3.976261000	3.201548000	H	0.441663000	2.508949000	7.386151000
C	-0.869971000	-2.023451000	3.347451000	H	-1.310765000	4.971868000	8.049198000
C	-1.988746000	-2.762003000	3.737765000	H	-1.195405000	2.437483000	8.042191000
C	-1.974551000	0.003040000	3.702823000	H	0.055829000	4.376957000	9.021121000
C	-3.242774000	2.074179000	4.016500000	N	5.694641000	-2.413597000	0.706700000
C	-1.874130000	1.522333000	3.952235000	N	2.269512000	0.772018000	1.515266000
C	-3.147973000	-2.076199000	4.084156000	N	1.263198000	-1.810278000	2.301992000
C	-3.135928000	-0.684159000	4.081900000	N	0.122539000	1.913694000	2.517286000
C	-1.235684000	1.650874000	5.400917000	N	-0.883745000	-0.668529000	3.304071000
C	-1.093919000	3.061659000	5.970200000	N	-4.308192000	2.517634000	4.114146000
C	-0.528602000	3.036729000	7.396099000	Co	0.693062000	0.051759000	2.409980000
C	-0.350827000	4.429881000	7.997718000	Br	-0.779447000	-0.119337000	0.039701000
H	1.332875000	-4.273600000	-4.202205000	Br	2.165957000	0.221682000	4.779151000
H	2.698744000	-4.868671000	-3.229361000	7a high spin			
H	2.583816000	-2.334262000	-3.222631000	C	1.747924000	-4.300165000	-3.058646000
H	1.045342000	-4.939210000	-2.577390000	C	1.913312000	-2.904719000	-2.458494000
H	0.946321000	-2.405406000	-2.567621000	C	2.479276000	-2.923944000	-1.033146000
H	3.457613000	-3.474785000	-1.154547000	C	2.612775000	-1.514896000	-0.456038000
H	3.250444000	-0.938644000	-1.251423000	C	4.470887000	2.263099000	0.677280000
H	1.810231000	-3.560696000	-0.515288000	C	4.654597000	-1.920275000	0.886573000
H	1.633123000	-1.062472000	-0.517735000	C	4.514057000	0.852183000	0.768339000
H	5.436495000	2.722640000	0.447829000	C	3.287097000	-1.374314000	0.974886000
H	5.410182000	0.238735000	0.428550000	C	3.302368000	2.930509000	0.990593000
H	3.346043000	3.954629000	1.067521000	C	3.386668000	0.164439000	1.201195000
H	1.361569000	4.726006000	1.088517000	C	2.198949000	2.191076000	1.470671000
H	3.784088000	-3.971284000	1.753972000	C	0.471892000	4.030020000	1.418747000
H	-0.880365000	5.582501000	1.805080000	C	2.468095000	-2.263828000	1.946048000

C	2.854158000	-3.581525000	2.227497000	H	-4.244100000	-2.559336000	3.724887000
C	0.932969000	2.777069000	1.871283000	H	-4.168663000	-0.093123000	4.015245000
C	-0.811164000	4.435419000	1.737271000	H	-0.277809000	3.568482000	5.338689000
C	1.947466000	-4.434793000	2.861091000	H	-0.213670000	1.069978000	5.364844000
C	-1.623148000	3.593932000	2.537700000	H	-1.894568000	3.561384000	6.054009000
C	0.374751000	-2.632507000	2.919863000	H	-1.796842000	1.012864000	6.149934000
C	-1.106935000	2.398428000	3.012631000	H	0.632942000	4.934958000	7.355611000
C	0.671582000	-3.975437000	3.179469000	H	0.628221000	2.399127000	7.371221000
C	-0.929924000	-1.998974000	3.248681000	H	-0.992024000	4.938454000	8.078814000
C	-2.117520000	-2.725824000	3.379497000	H	-0.981851000	2.402004000	8.093760000
C	-2.026527000	0.025981000	3.686360000	H	0.389476000	4.296504000	8.998495000
C	-3.227239000	2.101667000	4.220857000	N	5.719500000	-2.364345000	0.782713000
C	-1.878375000	1.531825000	4.041343000	N	2.276135000	0.824066000	1.601562000
C	-3.294020000	-2.027536000	3.638225000	N	1.276544000	-1.810710000	2.350357000
C	-3.253324000	-0.641016000	3.795506000	N	0.147361000	1.987863000	2.689377000
C	-1.174441000	1.599027000	5.453811000	N	-0.907949000	-0.654772000	3.391347000
C	-0.942412000	3.002292000	6.013536000	N	-4.277437000	2.549583000	4.417280000
C	-0.318430000	2.966739000	7.413753000	Co	0.974493000	0.185994000	3.044880000
C	-0.058129000	4.356725000	7.992697000	Br	2.291830000	-0.169889000	5.130945000
H	1.342640000	-4.251781000	-4.082756000	7a low spin			
H	2.712652000	-4.833641000	-3.107735000	C	1.466066000	-4.195029000	-3.076693000
H	2.575224000	-2.300429000	-3.104721000	C	1.693633000	-2.815740000	-2.459653000
H	1.059322000	-4.918135000	-2.457293000	C	2.351828000	-2.874536000	-1.075742000
H	0.937439000	-2.386135000	-2.454285000	C	2.549999000	-1.481581000	-0.479295000
H	3.464751000	-3.422874000	-1.043107000	C	4.613669000	2.193110000	0.860028000
H	3.202280000	-0.889487000	-1.144411000	C	4.652598000	-1.972991000	0.714855000
H	1.823574000	-3.540851000	-0.396535000	C	4.600106000	0.790924000	0.856316000
H	1.621506000	-1.044740000	-0.361552000	C	3.306922000	-1.401258000	0.913466000
H	5.352186000	2.813402000	0.339957000	C	3.445165000	2.866792000	1.172915000
H	5.412214000	0.318928000	0.457968000	C	3.442625000	0.103423000	1.211778000
H	3.240320000	4.016271000	0.903746000	C	2.315440000	2.124348000	1.549672000
H	1.109116000	4.650214000	0.786107000	C	0.681344000	4.036101000	1.591509000
H	3.836549000	-3.952939000	1.937518000	C	2.538044000	-2.263349000	1.927624000
H	-1.203055000	5.387356000	1.372850000	C	2.941455000	-3.567026000	2.201279000
H	2.233956000	-5.464712000	3.085502000	C	1.032736000	2.713607000	1.896859000
H	-2.634293000	3.906547000	2.794646000	C	-0.595811000	4.478352000	1.893150000
H	-0.060232000	-4.634757000	3.646823000	C	2.085819000	-4.437216000	2.893506000
H	-2.126110000	-3.808958000	3.255422000	C	-1.460848000	3.607018000	2.567836000

C	0.485783000	-2.649556000	2.982167000	H	-1.867437000	1.006894000	6.009242000
C	-1.042775000	2.320521000	2.903211000	H	0.370816000	5.007661000	7.299041000
C	0.827118000	-3.984819000	3.250244000	H	0.439833000	2.473162000	7.329367000
C	-0.794397000	-2.052288000	3.323454000	H	-1.288525000	4.966918000	7.938083000
C	-1.935555000	-2.798810000	3.649583000	H	-1.203314000	2.431181000	7.971930000
C	-1.947358000	-0.036360000	3.607058000	H	0.062100000	4.371312000	8.931665000
C	-3.231285000	2.021400000	3.965545000	N	5.698370000	-2.428407000	0.513594000
C	-1.862177000	1.473839000	3.889376000	N	2.330668000	0.760817000	1.622422000
C	-3.124909000	-2.134418000	3.897885000	N	1.352401000	-1.783563000	2.378904000
C	-3.121061000	-0.733366000	3.886613000	N	0.164312000	1.844043000	2.503837000
C	-1.230095000	1.604493000	5.337348000	N	-0.806941000	-0.682964000	3.254976000
C	-1.076744000	3.020545000	5.891260000	N	-4.297220000	2.460969000	4.077806000
C	-0.524134000	3.012399000	7.322096000	Co	0.865328000	0.061337000	2.664898000
C	-0.334831000	4.412594000	7.903856000	Br	2.207618000	0.200517000	4.832927000
H	0.993786000	-4.117993000	-4.069877000	8 high spin			
H	2.416660000	-4.741282000	-3.201991000	C	-1.422374000	-1.019314000	-3.959480000
H	2.321425000	-2.207554000	-3.135661000	C	-0.134342000	-0.558607000	-3.691606000
H	0.809496000	-4.816010000	-2.443483000	C	-2.369323000	-1.090375000	-2.931620000
H	0.728854000	-2.282764000	-2.379875000	C	0.175759000	-0.161975000	-2.381987000
H	3.324028000	-3.392205000	-1.160223000	C	1.561435000	0.336113000	-2.004340000
H	3.117235000	-0.851557000	-1.182652000	C	-1.988358000	-0.680504000	-1.650538000
H	1.727393000	-3.490915000	-0.407605000	C	-0.211242000	5.044162000	-1.038512000
H	1.576559000	-0.993655000	-0.318617000	C	0.940555000	4.258017000	-0.977923000
H	5.521432000	2.737323000	0.591741000	C	-1.430270000	4.493549000	-0.635266000
H	5.489097000	0.244031000	0.544185000	C	0.842471000	2.944550000	-0.507259000
H	3.404917000	3.955909000	1.151611000	C	-4.195681000	-1.133666000	-0.463015000
H	1.397349000	4.691469000	1.095501000	C	-2.857122000	-0.721753000	-0.442560000
H	3.906566000	-3.927920000	1.848202000	C	2.058344000	2.062549000	-0.321747000
H	-0.917645000	5.489225000	1.635488000	C	-1.446704000	3.171479000	-0.193636000
H	2.399725000	-5.458874000	3.116480000	C	2.687055000	-0.273544000	0.104967000
H	-2.452116000	3.951977000	2.857946000	C	2.068376000	-1.624073000	0.404967000
H	0.120089000	-4.641514000	3.757336000	C	2.836464000	-2.793723000	0.417554000
H	-1.886737000	-3.887413000	3.678684000	C	-4.919014000	-1.148760000	0.730558000
H	-4.041529000	-2.683932000	4.121070000	C	2.236408000	-3.995305000	0.796531000
H	-4.034534000	-0.190887000	4.126820000	C	0.184794000	-2.790563000	1.090103000
H	-0.395890000	3.606237000	5.250824000	C	0.883686000	-3.995723000	1.145291000
H	-0.246058000	1.112083000	5.287867000	C	-2.956629000	-0.354130000	1.855682000
H	-2.047620000	3.548257000	5.879628000	C	-4.292302000	-0.753944000	1.913977000

H	-1.693220000	-1.334375000	-4.969921000	C	0.793413000	2.847984000	-0.501868000
H	0.623173000	-0.507837000	-4.476681000	C	-4.128190000	-1.055205000	-0.493205000
H	-3.373288000	-1.464785000	-3.131569000	C	-2.780747000	-0.667961000	-0.467467000
H	1.779792000	1.232538000	-2.607329000	C	2.083004000	2.055489000	-0.432327000
H	2.296202000	-0.420441000	-2.324991000	C	-1.487897000	2.905750000	-0.055239000
H	-0.157974000	6.074165000	-1.399771000	C	2.756934000	-0.289880000	0.022721000
H	-4.670319000	-1.436370000	-1.396648000	C	2.066011000	-1.588635000	0.388047000
H	1.910345000	4.652656000	-1.288213000	C	2.778185000	-2.785001000	0.516647000
H	2.891910000	2.422622000	-0.949991000	C	-4.861890000	-1.021031000	0.693704000
H	-2.355849000	5.071581000	-0.666639000	C	2.115935000	-3.932836000	0.952327000
H	3.622054000	-0.404563000	-0.467180000	C	0.105059000	-2.631884000	1.076002000
H	-2.378311000	2.695077000	0.124841000	C	0.752328000	-3.853965000	1.242721000
H	2.370552000	2.158073000	0.730564000	C	-2.893138000	-0.231956000	1.812496000
H	3.890803000	-2.753752000	0.135596000	C	-4.237976000	-0.603290000	1.871308000
H	-5.964341000	-1.466148000	0.732613000	H	-1.684351000	-1.309544000	-4.998617000
H	2.817310000	-4.920785000	0.815778000	H	0.657885000	-0.521246000	-4.544472000
H	-0.877649000	-2.746241000	1.345167000	H	-3.327147000	-1.396405000	-3.125163000
H	0.372096000	-4.911567000	1.447820000	H	1.878220000	1.176129000	-2.739086000
H	2.955150000	0.179594000	1.072630000	H	2.383259000	-0.477154000	-2.425373000
H	-2.410651000	-0.028770000	2.746141000	H	-0.451250000	5.954915000	-1.139513000
H	-4.822721000	-0.751498000	2.867953000	H	-4.602882000	-1.377257000	-1.420264000
N	-0.744129000	-0.220652000	-1.422392000	H	1.704148000	4.664726000	-1.222402000
N	1.750278000	0.642409000	-0.565334000	H	2.834318000	2.501837000	-1.107784000
N	-0.338480000	2.421090000	-0.132644000	H	-2.537162000	4.764030000	-0.355459000
N	0.763533000	-1.637351000	0.729917000	H	3.684094000	-0.504057000	-0.538072000
N	-2.262453000	-0.339719000	0.711721000	H	-2.368379000	2.354829000	0.280889000
Cl	0.293515000	0.967865000	2.760193000	H	2.461056000	2.155054000	0.597248000
Co	-0.223264000	0.357114000	0.548777000	H	3.843753000	-2.804193000	0.278503000
8 low spin				H	-5.913050000	-1.318746000	0.695337000
C	-1.384813000	-1.006958000	-3.992630000	H	2.656592000	-4.876096000	1.061745000
C	-0.085452000	-0.571075000	-3.746016000	H	-0.961258000	-2.527571000	1.285543000
C	-2.307903000	-1.056180000	-2.944569000	H	0.189622000	-4.723704000	1.586989000
C	0.263870000	-0.192259000	-2.443219000	H	3.047467000	0.192163000	0.969162000
C	1.663432000	0.296263000	-2.109942000	H	-2.347243000	0.105296000	2.699110000
C	-1.900204000	-0.664500000	-1.666431000	H	-4.777932000	-0.563154000	2.819309000
C	-0.420165000	4.903864000	-0.842325000	N	-0.630560000	-0.246230000	-1.450639000
C	0.778018000	4.190859000	-0.890265000	N	1.866000000	0.629139000	-0.691214000
C	-1.575989000	4.249671000	-0.411259000	N	-0.334236000	2.222581000	-0.101643000

N	0.744740000	-1.528972000	0.657948000
N	-2.190295000	-0.264449000	0.676930000
Cl	0.480758000	0.882687000	2.533620000
Co	-0.081943000	0.282515000	0.368709000

8a high spin

C	-1.652862000	-1.145054000	-4.614498000
C	-0.395188000	-0.538587000	-4.348586000
C	-2.569186000	-1.313704000	-3.591435000
C	-0.126890000	-0.126893000	-3.053908000
C	1.126734000	0.625549000	-2.647898000
C	-2.239176000	-0.886904000	-2.279687000
C	0.502632000	4.839030000	0.386553000
C	1.457983000	3.929185000	-0.067912000
C	-0.773642000	4.375203000	0.716687000
C	1.117932000	2.576646000	-0.171516000
C	-4.386044000	-1.537180000	-1.104431000
C	-3.073741000	-1.001849000	-1.103736000
C	2.124384000	1.525656000	-0.589217000
C	-1.041264000	3.016330000	0.574458000
C	2.192947000	-0.882114000	-1.034244000
C	1.971826000	-1.434620000	0.357181000
C	2.942386000	-2.188344000	1.023400000
C	-5.113317000	-1.601278000	0.069366000
C	2.646659000	-2.721547000	2.279204000
C	0.475770000	-1.719084000	2.115155000
C	1.387993000	-2.485236000	2.837448000
C	-3.241987000	-0.613606000	1.214236000
C	-4.526413000	-1.123190000	1.269327000
H	-1.894186000	-1.479880000	-5.626331000
H	0.341777000	-0.391810000	-5.140807000
H	-3.534497000	-1.781901000	-3.791243000
H	0.919555000	1.702525000	-2.760426000
H	1.964765000	0.393286000	-3.329121000
H	0.748994000	5.900017000	0.475182000
H	-4.821461000	-1.894789000	-2.039112000
H	2.462921000	4.256279000	-0.342999000
H	2.910693000	1.980210000	-1.218547000
H	-1.554057000	5.051615000	1.070279000

H	1.793183000	-1.617387000	-1.752417000
H	-2.028845000	2.607782000	0.804794000
H	2.626568000	1.165709000	0.324332000
H	3.916609000	-2.348916000	0.556973000
H	-6.125769000	-2.012332000	0.070432000
H	3.392604000	-3.311278000	2.817721000
H	-0.521343000	-1.507826000	2.510990000
H	1.113445000	-2.882233000	3.816540000
H	3.274579000	-0.792808000	-1.242397000
H	-2.755160000	-0.234533000	2.118693000
H	-5.065009000	-1.151721000	2.218495000
N	-1.013971000	-0.308028000	-2.052388000
N	1.478840000	0.381225000	-1.238060000
N	-0.117090000	2.140809000	0.144059000
N	0.764062000	-1.205141000	0.908692000
N	-2.510836000	-0.544017000	0.078141000
Co	-0.551370000	0.093260000	-0.147068000

8a low spin

C	-1.446491000	-1.258649000	-4.813978000
C	-0.199422000	-0.651524000	-4.512584000
C	-2.396252000	-1.406793000	-3.811439000
C	0.047938000	-0.228224000	-3.222628000
C	1.228678000	0.570870000	-2.731353000
C	-2.092454000	-0.977560000	-2.505447000
C	0.251464000	4.639080000	0.715925000
C	1.237439000	3.829835000	0.146821000
C	-0.974652000	4.063432000	1.055596000
C	0.970671000	2.474728000	-0.058704000
C	-4.229873000	-1.499563000	-1.229496000
C	-2.908822000	-1.020977000	-1.312791000
C	2.018031000	1.520366000	-0.581996000
C	-1.169577000	2.706145000	0.805340000
C	2.139569000	-0.900561000	-0.978772000
C	1.857897000	-1.352303000	0.431794000
C	2.765747000	-2.098901000	1.183661000
C	-4.903718000	-1.453637000	-0.017868000
C	2.400069000	-2.522556000	2.463715000
C	0.295517000	-1.410188000	2.144343000

C	1.140774000	-2.169546000	2.952450000	C	-2.574090000	-0.851886000	-1.184079000
C	-2.941829000	-0.466980000	0.967014000	C	0.434587000	-1.085322000	-1.229617000
C	-4.245492000	-0.919151000	1.105928000	C	1.121823000	0.257580000	-1.251005000
H	-1.659478000	-1.594068000	-5.831013000	C	1.063540000	2.501240000	-0.661284000
H	0.551817000	-0.499622000	-5.290903000	C	-1.732842000	-1.887563000	-0.479822000
H	-3.369352000	-1.853448000	-4.025683000	C	0.200210000	-2.152251000	0.986710000
H	1.004136000	1.640403000	-2.875130000	C	2.668270000	-2.391098000	1.502773000
H	2.158558000	0.351116000	-3.281527000	C	1.505687000	-1.609664000	1.510997000
H	0.437548000	5.702034000	0.887270000	C	3.865684000	-1.928411000	2.060403000
H	-4.712536000	-1.897755000	-2.123815000	C	1.544499000	-0.309326000	2.092272000
H	2.209485000	4.239127000	-0.136665000	C	3.901952000	-0.652615000	2.638315000
H	2.736378000	2.033428000	-1.240875000	C	2.760391000	0.148369000	2.653640000
H	-1.777498000	4.653044000	1.502796000	H	-4.970798000	-0.399757000	-3.557443000
H	1.773502000	-1.671035000	-1.676693000	H	-4.668158000	1.969707000	-2.740838000
H	-2.121650000	2.226504000	1.046291000	H	3.729635000	1.915297000	-2.684007000
H	2.593518000	1.150797000	0.281137000	H	-3.573178000	-2.216291000	-2.526123000
H	3.743611000	-2.343984000	0.763972000	H	2.738797000	-0.387724000	-2.531339000
H	-5.929967000	-1.819994000	0.059543000	H	-0.178454000	-1.142856000	-2.143347000
H	3.091090000	-3.111970000	3.071037000	H	2.593041000	3.801719000	-1.444256000
H	-0.692260000	-1.111095000	2.501592000	H	1.179895000	-1.891804000	-1.314098000
H	0.811613000	-2.468866000	3.949560000	H	-1.584642000	-2.773210000	-1.121215000
H	3.221743000	-0.783020000	-1.157593000	H	-2.990110000	2.399911000	-0.917424000
H	-2.407769000	-0.036652000	1.816834000	H	0.541982000	3.274763000	-0.092827000
H	-4.739957000	-0.852499000	2.076860000	H	-2.271388000	-2.208295000	0.424712000
N	-0.870124000	-0.420016000	-2.228345000	H	0.357989000	-3.167892000	0.582501000
N	1.400773000	0.352956000	-1.263048000	H	2.627853000	-3.388871000	1.054799000
N	-0.221900000	1.923944000	0.261570000	H	4.759404000	-2.557102000	2.044897000
N	0.637413000	-1.013321000	0.907761000	H	-0.530046000	-2.223743000	1.808194000
N	-2.262506000	-0.515840000	-0.200811000	H	4.830060000	-0.276821000	3.079101000
Co	-0.428867000	0.029014000	-0.519300000	H	2.776753000	1.146581000	3.098867000
9 high spin				N	-2.426016000	0.416614000	-0.759792000
C	-4.254204000	-0.167164000	-2.765873000	N	0.535993000	1.267372000	-0.588193000
C	-4.090071000	1.145909000	-2.317847000	N	-0.443906000	-1.304131000	-0.056648000
C	-3.482105000	-1.179787000	-2.194954000	Cl	-1.604518000	2.924562000	1.331999000
C	2.826518000	1.736112000	-2.095233000	Cl	-2.622223000	-0.345235000	2.334324000
C	2.281317000	0.457074000	-2.012183000	Fe	-1.020555000	0.697750000	0.958665000
C	2.202596000	2.782828000	-1.409311000	O	0.473876000	0.460570000	2.114448000
C	-3.159932000	1.394792000	-1.310956000				

9 intermediate spin

C	-4.252049000	-0.037757000	-2.664072000
C	-4.040612000	1.243856000	-2.152708000
C	-3.499159000	-1.098342000	-2.159134000
C	2.787884000	1.705604000	-2.084607000
C	2.228699000	0.430438000	-2.074375000
C	2.221075000	2.697077000	-1.278463000
C	-3.087932000	1.418262000	-1.152079000
C	-2.565744000	-0.855394000	-1.149321000
C	0.432381000	-1.167169000	-1.288913000
C	1.117029000	0.177379000	-1.261512000
C	1.121656000	2.369864000	-0.491976000
C	-1.741170000	-1.952425000	-0.524620000
C	0.233176000	-2.246082000	0.919575000
C	2.729347000	-2.286116000	1.381820000
C	1.500198000	-1.619459000	1.448682000
C	3.895303000	-1.725915000	1.917647000
C	1.434158000	-0.338486000	2.068602000
C	3.831014000	-0.465929000	2.525719000
C	2.620836000	0.225297000	2.592182000
H	-4.988473000	-0.209348000	-3.452830000
H	-4.599888000	2.105958000	-2.520764000
H	3.657146000	1.923797000	-2.709872000
H	-3.623072000	-2.113652000	-2.540735000
H	2.639858000	-0.374420000	-2.687227000
H	-0.184574000	-1.195439000	-2.201287000
H	2.624273000	3.711056000	-1.250157000
H	1.181705000	-1.966586000	-1.404773000
H	-1.642241000	-2.808168000	-1.214070000
H	-2.878550000	2.393921000	-0.708219000
H	0.633845000	3.098179000	0.159240000
H	-2.261684000	-2.297254000	0.381210000
H	0.451575000	-3.248825000	0.511269000
H	2.769270000	-3.270161000	0.904583000
H	4.843238000	-2.266324000	1.857988000
H	-0.498227000	-2.355342000	1.735669000
H	4.733564000	-0.013842000	2.947436000
H	2.557438000	1.208922000	3.064591000

N	-2.374181000	0.391371000	-0.662962000
N	0.583232000	1.136633000	-0.488241000
N	-0.430294000	-1.413845000	-0.117608000
Cl	-1.518355000	2.859498000	1.372307000
Cl	-2.595214000	-0.442154000	2.254210000
Fe	-0.984396000	0.570018000	0.869484000
O	0.283033000	0.301233000	2.216211000

9 low spin

C	-4.226834000	-0.041259000	-2.694205000
C	-3.985404000	1.248906000	-2.217316000
C	-3.492792000	-1.106025000	-2.169077000
C	2.711136000	1.785720000	-2.113909000
C	2.207437000	0.487284000	-2.088966000
C	2.098081000	2.764866000	-1.326304000
C	-3.021014000	1.431478000	-1.228991000
C	-2.546650000	-0.849685000	-1.176056000
C	0.447035000	-1.144041000	-1.265542000
C	1.101560000	0.204685000	-1.281410000
C	1.008267000	2.409018000	-0.539588000
C	-1.731612000	-1.918883000	-0.505311000
C	0.214418000	-2.192533000	0.961376000
C	2.689214000	-2.369822000	1.479338000
C	1.506305000	-1.619622000	1.478195000
C	3.870589000	-1.868589000	2.037115000
C	1.495893000	-0.312424000	2.043725000
C	3.863485000	-0.586536000	2.603086000
C	2.699585000	0.182289000	2.603909000
H	-4.974027000	-0.216644000	-3.471933000
H	-4.532180000	2.111061000	-2.603671000
H	3.574976000	2.031344000	-2.736353000
H	-3.642979000	-2.128494000	-2.520692000
H	2.657029000	-0.309352000	-2.684711000
H	-0.165017000	-1.227310000	-2.177005000
H	2.460198000	3.794423000	-1.311995000
H	1.196744000	-1.946729000	-1.321624000
H	-1.573918000	-2.788513000	-1.162709000
H	-2.791770000	2.411823000	-0.806721000
H	0.488597000	3.121299000	0.104119000

H	-2.265917000	-2.246216000	0.397934000
H	0.381730000	-3.195348000	0.534531000
H	2.676704000	-3.372955000	1.041312000
H	4.782922000	-2.470092000	2.031145000
H	-0.519889000	-2.275909000	1.777140000
H	4.777564000	-0.178638000	3.045243000
H	2.686193000	1.183648000	3.042523000
N	-2.324334000	0.402495000	-0.721905000
N	0.520816000	1.154563000	-0.525644000
N	-0.434625000	-1.331279000	-0.074379000
Cl	-1.538469000	2.653282000	1.397580000
Cl	-2.500475000	-0.405629000	2.195679000
Fe	-0.904883000	0.501058000	0.749168000
O	0.401427000	0.423214000	2.090798000

9a' high spin

C	-4.390158000	-0.310255000	-2.675135000
C	-4.339388000	0.965778000	-2.109144000
C	-3.514924000	-1.292788000	-2.208392000
C	2.932593000	1.731959000	-1.978413000
C	2.355863000	0.462803000	-2.005573000
C	2.321352000	2.743496000	-1.229930000
C	-3.412911000	1.207283000	-1.096403000
C	-2.618892000	-0.974486000	-1.183092000
C	0.444159000	-1.090411000	-1.371472000
C	1.175514000	0.234559000	-1.285599000
C	1.158999000	2.434450000	-0.529547000
C	-1.681066000	-1.995572000	-0.583604000
C	0.299825000	-2.272886000	0.786624000
C	2.777406000	-2.310438000	1.321825000
C	1.531998000	-1.676282000	1.413785000
C	3.904478000	-1.817666000	1.991323000
C	1.388503000	-0.491058000	2.202851000
C	3.771071000	-0.663499000	2.775901000
C	2.541478000	-0.012253000	2.881286000
H	-5.098135000	-0.536968000	-3.476245000
H	-5.000867000	1.766447000	-2.446008000
H	3.853375000	1.930815000	-2.532802000
H	-3.518480000	-2.299457000	-2.631622000

H	2.808820000	-0.349618000	-2.577912000
H	-0.205965000	-1.029128000	-2.260157000
H	2.740137000	3.750587000	-1.181729000
H	1.164866000	-1.900301000	-1.578706000
H	-1.560403000	-2.851623000	-1.273188000
H	-3.320251000	2.183695000	-0.612453000
H	0.636071000	3.175662000	0.082265000
H	-2.153171000	-2.388970000	0.332040000
H	0.553516000	-3.241418000	0.314266000
H	2.860289000	-3.219919000	0.716975000
H	4.867251000	-2.328155000	1.906817000
H	-0.439554000	-2.475562000	1.579072000
H	4.638501000	-0.264700000	3.311781000
H	2.434810000	0.889053000	3.492203000
N	-2.576630000	0.258764000	-0.645408000
N	0.604658000	1.211953000	-0.561987000
N	-0.392173000	-1.403448000	-0.198691000
Cl	-1.859744000	2.747575000	1.549538000
Fe	-0.970959000	0.650810000	0.827390000
O	0.237773000	0.126544000	2.303175000

9a' intermediate spin

C	-4.184424000	-0.047189000	-2.712283000
C	-3.984315000	1.230351000	-2.183360000
C	-3.437107000	-1.113047000	-2.206005000
C	2.670423000	1.738783000	-2.253123000
C	2.193525000	0.430891000	-2.190669000
C	2.064978000	2.721186000	-1.462020000
C	-3.042004000	1.394206000	-1.170324000
C	-2.513696000	-0.874186000	-1.186154000
C	0.512533000	-1.254418000	-1.291551000
C	1.115411000	0.136028000	-1.346174000
C	1.008964000	2.347163000	-0.637067000
C	-1.705589000	-1.965034000	-0.522233000
C	0.237214000	-2.214755000	0.974519000
C	2.693786000	-2.334478000	1.538682000
C	1.502256000	-1.595444000	1.522361000
C	3.866119000	-1.846948000	2.127866000
C	1.467562000	-0.286741000	2.115008000

C	3.837977000	-0.578364000	2.724447000	C	-1.690831000	-1.920068000	-0.506022000
C	2.670340000	0.182123000	2.717360000	C	0.224021000	-2.158971000	1.010504000
H	-4.912523000	-0.212073000	-3.510195000	C	2.648022000	-2.431188000	1.650990000
H	-4.547554000	2.092250000	-2.546318000	C	1.517718000	-1.608314000	1.554453000
H	3.509535000	1.990505000	-2.906463000	C	3.830790000	-2.002767000	2.266103000
H	-3.563344000	-2.126334000	-2.592896000	C	1.557544000	-0.269207000	2.077977000
H	2.645854000	-0.364213000	-2.787636000	C	3.873580000	-0.706840000	2.802605000
H	-0.056982000	-1.402781000	-2.223762000	C	2.770047000	0.138282000	2.711439000
H	2.408615000	3.757245000	-1.475098000	H	-4.950897000	-0.211588000	-3.468992000
H	1.320237000	-2.004856000	-1.311635000	H	-4.502646000	2.111985000	-2.593053000
H	-1.655752000	-2.862257000	-1.165882000	H	3.398289000	2.122990000	-2.970895000
H	-2.857463000	2.372181000	-0.718249000	H	-3.613552000	-2.128657000	-2.536253000
H	0.515347000	3.072838000	0.015256000	H	2.632016000	-0.265978000	-2.815167000
H	-2.230536000	-2.250489000	0.404539000	H	-0.027168000	-1.420529000	-2.183777000
H	0.443265000	-3.256157000	0.661900000	H	2.230616000	3.861317000	-1.560086000
H	2.694098000	-3.330862000	1.083586000	H	1.347319000	-1.938178000	-1.211138000
H	4.779954000	-2.446491000	2.126348000	H	-1.564846000	-2.815749000	-1.136728000
H	-0.525955000	-2.252217000	1.770740000	H	-2.737089000	2.414488000	-0.839458000
H	4.739487000	-0.175599000	3.197683000	H	0.363773000	3.125494000	-0.055114000
H	2.645038000	1.172981000	3.180718000	H	-2.224440000	-2.205949000	0.413066000
N	-2.321121000	0.368219000	-0.691251000	H	0.377762000	-3.192340000	0.652657000
N	0.544724000	1.086637000	-0.589620000	H	2.589782000	-3.446515000	1.243466000
N	-0.379767000	-1.456887000	-0.139724000	H	4.696623000	-2.666555000	2.330503000
Cl	-2.668363000	0.466855000	2.316957000	H	-0.539697000	-2.177152000	1.803776000
Fe	-0.945037000	0.510449000	0.750995000	H	4.784228000	-0.349499000	3.294887000
O	0.393923000	0.456298000	2.146633000	H	2.805249000	1.151169000	3.124153000
9a' low spin				N	-2.266874000	0.395927000	-0.742646000
C	-4.195538000	-0.039941000	-2.698362000	N	0.479917000	1.134089000	-0.627047000
C	-3.949912000	1.248919000	-2.216685000	N	-0.382790000	-1.346789000	-0.088788000
C	-3.455986000	-1.107509000	-2.182824000	Cl	-2.468720000	-0.170761000	2.251200000
C	2.573320000	1.845968000	-2.310106000	Fe	-0.853041000	0.452732000	0.638026000
C	2.150883000	0.518967000	-2.227654000	O	0.550476000	0.545158000	1.996890000
C	1.929830000	2.812366000	-1.529690000	9a'' high spin			
C	-2.970433000	1.424434000	-1.241090000	C	-4.349344000	-0.181645000	-2.699748000
C	-2.502980000	-0.855091000	-1.195163000	C	-4.245400000	1.120609000	-2.205060000
C	0.532580000	-1.200192000	-1.261272000	C	-3.519066000	-1.173709000	-2.174593000
C	1.092723000	0.195176000	-1.373172000	C	2.985771000	1.634751000	-2.129468000
C	0.889965000	2.412236000	-0.695608000	C	2.379077000	0.380802000	-2.073142000

C	2.406772000	2.704828000	-1.438688000
C	-3.313298000	1.377713000	-1.201381000
C	-2.613544000	-0.837515000	-1.163366000
C	0.439708000	-1.085022000	-1.330420000
C	1.201306000	0.225654000	-1.329853000
C	1.245589000	2.467202000	-0.709187000
C	-1.721191000	-1.861351000	-0.501881000
C	0.245445000	-2.144975000	0.888368000
C	2.721038000	-2.273230000	1.415012000
C	1.509428000	-1.572745000	1.473262000
C	3.877213000	-1.796524000	2.045059000
C	1.432093000	-0.334659000	2.186681000
C	3.808861000	-0.589179000	2.754498000
C	2.614385000	0.128410000	2.824970000
H	-5.064144000	-0.421764000	-3.490824000
H	-4.870847000	1.928891000	-2.589290000
H	3.904837000	1.776900000	-2.703734000
H	-3.565384000	-2.201290000	-2.541274000
H	2.806210000	-0.476003000	-2.598851000
H	-0.204082000	-1.069776000	-2.225736000
H	2.849822000	3.702469000	-1.456727000
H	1.142906000	-1.922420000	-1.478873000
H	-1.632862000	-2.759011000	-1.141498000
H	-3.182652000	2.373610000	-0.768707000
H	0.748387000	3.256802000	-0.137798000
H	-2.212103000	-2.182616000	0.431924000
H	0.449152000	-3.150446000	0.472470000
H	2.753077000	-3.222043000	0.868563000
H	4.812301000	-2.359598000	1.988195000
H	-0.498438000	-2.265125000	1.693465000
H	4.700074000	-0.201068000	3.258230000
H	2.557985000	1.070995000	3.377517000
N	-2.520585000	0.420407000	-0.694470000
N	0.662001000	1.258834000	-0.661799000
N	-0.409729000	-1.301358000	-0.144207000
Cl	-1.771073000	2.939061000	1.434874000
Fe	-0.907256000	0.815313000	0.774049000
O	0.314903000	0.344988000	2.257012000

9a'' intermediate spin

C	-4.392209000	-0.125522000	-2.616690000
C	-4.222984000	1.168302000	-2.118668000
C	-3.582032000	-1.151076000	-2.123375000
C	3.061295000	1.540653000	-2.089884000
C	2.428100000	0.296698000	-2.067350000
C	2.478092000	2.617261000	-1.413813000
C	-3.253347000	1.391603000	-1.143363000
C	-2.634780000	-0.852523000	-1.143111000
C	0.405007000	-1.102547000	-1.379428000
C	1.220868000	0.169359000	-1.370727000
C	1.281322000	2.400458000	-0.732724000
C	-1.740265000	-1.881649000	-0.507696000
C	0.252323000	-2.125669000	0.861814000
C	2.730199000	-2.197221000	1.399556000
C	1.503625000	-1.522800000	1.434649000
C	3.865986000	-1.682037000	2.036340000
C	1.385367000	-0.275832000	2.123953000
C	3.758288000	-0.467355000	2.728950000
C	2.546723000	0.223042000	2.773577000
H	-5.140727000	-0.333940000	-3.385015000
H	-4.831033000	2.000739000	-2.478323000
H	4.005138000	1.668214000	-2.626124000
H	-3.675638000	-2.174456000	-2.492057000
H	2.859112000	-0.566050000	-2.579906000
H	-0.266464000	-1.044553000	-2.251349000
H	2.943824000	3.604843000	-1.406848000
H	1.049803000	-1.981182000	-1.542268000
H	-1.626975000	-2.768979000	-1.153876000
H	-3.076342000	2.376692000	-0.705482000
H	0.779585000	3.194523000	-0.170980000
H	-2.209796000	-2.218112000	0.430803000
H	0.468132000	-3.117391000	0.425803000
H	2.790967000	-3.153592000	0.869109000
H	4.815846000	-2.221413000	1.998385000
H	-0.483838000	-2.266961000	1.670200000
H	4.633241000	-0.051153000	3.238732000
H	2.460331000	1.171390000	3.312078000

N	-2.478198000	0.402185000	-0.665267000
N	0.673695000	1.207163000	-0.721158000
N	-0.430583000	-1.278626000	-0.160269000
Cl	-1.703239000	2.672716000	1.467285000
Fe	-0.933200000	0.621984000	0.652997000
O	0.252119000	0.377981000	2.175098000
9a'' low spin			
C	-4.218098000	-0.060063000	-2.692378000
C	-3.961098000	1.244193000	-2.261603000
C	-3.485807000	-1.110511000	-2.134556000
C	2.670262000	1.781180000	-2.290109000
C	2.188890000	0.473929000	-2.214738000
C	2.059046000	2.771095000	-1.514404000
C	-2.983147000	1.453979000	-1.291805000
C	-2.528988000	-0.823630000	-1.160022000
C	0.487705000	-1.177214000	-1.279019000
C	1.109940000	0.192913000	-1.372495000
C	0.993038000	2.419347000	-0.692253000
C	-1.714787000	-1.873031000	-0.452102000
C	0.232913000	-2.152281000	0.983467000
C	2.690017000	-2.370803000	1.554382000
C	1.520055000	-1.601293000	1.526922000
C	3.858685000	-1.907028000	2.170513000
C	1.496059000	-0.298218000	2.121461000
C	3.841991000	-0.642779000	2.779129000
C	2.691210000	0.143940000	2.757875000
H	-4.974557000	-0.257036000	-3.455905000
H	-4.507421000	2.095923000	-2.671954000
H	3.513822000	2.023676000	-2.940885000
H	-3.648249000	-2.144248000	-2.446524000
H	2.640624000	-0.330543000	-2.799019000
H	-0.115445000	-1.337821000	-2.186606000
H	2.403957000	3.806717000	-1.537995000
H	1.266259000	-1.955286000	-1.285786000
H	-1.619601000	-2.790357000	-1.057801000
H	-2.748367000	2.445946000	-0.899958000
H	0.474803000	3.139651000	-0.055720000
H	-2.229455000	-2.149546000	0.482890000

H	0.383926000	-3.177266000	0.600531000
H	2.677229000	-3.364102000	1.092529000
H	4.762494000	-2.521522000	2.181591000
H	-0.516172000	-2.204698000	1.792137000
H	4.742906000	-0.264063000	3.273012000
H	2.677727000	1.132015000	3.227665000
N	-2.282685000	0.441220000	-0.750070000
N	0.527585000	1.156364000	-0.628697000
N	-0.390922000	-1.313966000	-0.081324000
Cl	-1.625673000	2.632224000	1.446501000
Fe	-0.823942000	0.565417000	0.611550000
O	0.430608000	0.452741000	2.105149000

10 high spin			
C	-1.827758000	-1.434352000	-3.526032000
C	-2.902783000	-2.267005000	-3.201725000
C	-0.728541000	-1.355421000	-2.673005000
C	-2.851715000	-3.032906000	-2.033746000
C	-0.656362000	-2.103428000	-1.482366000
C	-1.736969000	-2.954932000	-1.192606000
C	0.553968000	-2.088833000	-0.567689000
C	-2.931511000	2.556221000	0.301918000
C	-1.553125000	2.475172000	0.126485000
C	-3.612589000	1.427949000	0.766908000
C	-2.888086000	0.270797000	1.047588000
C	-1.500699000	0.273194000	0.860910000
C	-0.657460000	-0.907748000	1.267397000
C	1.711073000	-1.399415000	1.427154000
C	2.047341000	-0.257161000	2.349942000
C	2.181331000	2.048083000	2.613474000
C	2.523999000	-0.465999000	3.647578000
C	2.665491000	1.920818000	3.913174000
C	2.844296000	0.638411000	4.437543000
H	-1.817679000	-0.837755000	-4.441793000
H	-3.769433000	-2.327518000	-3.865482000
H	-3.675965000	-3.704083000	-1.779283000
H	1.477241000	-1.970274000	-1.153443000
H	-3.456129000	3.484824000	0.069061000
H	-0.970433000	3.321344000	-0.244323000

H	-1.697035000	-3.578123000	-0.294919000
H	-4.696256000	1.448680000	0.906448000
H	0.605796000	-3.074556000	-0.073889000
H	2.598588000	-1.627311000	0.818163000
H	-3.382637000	-0.631801000	1.412132000
H	-1.249055000	-1.833579000	1.228250000
H	1.459006000	-2.302088000	2.010004000
H	2.024958000	3.024550000	2.149749000
H	-0.408750000	-0.759872000	2.330256000
H	2.633681000	-1.484213000	4.026099000
H	2.893089000	2.813870000	4.498302000
H	3.219806000	0.499571000	5.454347000
N	-0.857667000	1.359790000	0.402925000
N	0.608531000	-1.039809000	0.505118000
N	1.887632000	0.982756000	1.851594000
O	0.216321000	0.336275000	-4.488483000
O	0.466083000	0.826198000	-2.016532000
S	0.662705000	-0.262875000	-3.185112000
Cl	3.355284000	0.246069000	-0.906055000
Cl	1.650555000	3.382510000	-0.419290000
Fe	1.257182000	1.093725000	-0.297542000

10 intermediate spin

C	-1.720095000	-1.608652000	-3.627306000
C	-2.787742000	-2.467547000	-3.355469000
C	-0.718506000	-1.450435000	-2.667345000
C	-2.824197000	-3.163087000	-2.144570000
C	-0.708396000	-2.146781000	-1.444009000
C	-1.793036000	-3.010537000	-1.213057000
C	0.453223000	-2.124503000	-0.467264000
C	-2.941401000	2.658472000	0.435522000
C	-1.568792000	2.549642000	0.227176000
C	-3.633227000	1.538812000	0.906961000
C	-2.924280000	0.365859000	1.162835000
C	-1.540418000	0.343928000	0.945121000
C	-0.711922000	-0.863648000	1.326214000
C	1.680463000	-1.343085000	1.418135000
C	2.054837000	-0.203656000	2.332087000
C	2.344767000	2.089123000	2.554505000

C	2.489905000	-0.418395000	3.644295000
C	2.799090000	1.956878000	3.865430000
C	2.873915000	0.676905000	4.419712000
H	-1.663122000	-1.063920000	-4.571309000
H	-3.583118000	-2.593577000	-4.094124000
H	-3.650267000	-3.844918000	-1.928516000
H	1.397156000	-2.087433000	-1.028898000
H	-3.454342000	3.598623000	0.222924000
H	-0.973114000	3.385873000	-0.149940000
H	-1.811064000	-3.594085000	-0.289081000
H	-4.713064000	1.578727000	1.071031000
H	0.432414000	-3.088125000	0.072796000
H	2.542198000	-1.545421000	0.762564000
H	-3.429407000	-0.529334000	1.532172000
H	-1.334589000	-1.770786000	1.292629000
H	1.487422000	-2.255338000	2.010711000
H	2.260231000	3.062988000	2.064538000
H	-0.441426000	-0.732065000	2.386696000
H	2.522594000	-1.433633000	4.044991000
H	3.081722000	2.843446000	4.436626000
H	3.219498000	0.532924000	5.446461000
N	-0.888153000	1.419789000	0.478064000
N	0.531261000	-1.024506000	0.538789000
N	1.989321000	1.033158000	1.806841000
O	0.580794000	0.037015000	-4.489713000
O	0.180131000	0.953905000	-2.140884000
S	0.583125000	-0.215076000	-3.021999000
Cl	3.073630000	0.003428000	-1.432269000
Cl	1.743250000	3.484595000	-0.517454000
Fe	1.208047000	1.194202000	-0.243418000

10 low spin

C	-1.799740000	-1.576457000	-3.583910000
C	-2.819116000	-2.497374000	-3.320251000
C	-0.738083000	-1.444653000	-2.692218000
C	-2.751301000	-3.290717000	-2.171683000
C	-0.649936000	-2.222190000	-1.522904000
C	-1.673720000	-3.156033000	-1.288870000
C	0.534569000	-2.150874000	-0.581400000

C	-2.645186000	2.829528000	0.600336000	Fe	1.110353000	0.883590000	-0.188992000
C	-1.304612000	2.607016000	0.304241000	10a' high spin			
C	-3.416951000	1.763142000	1.070036000	C	-1.819093000	-1.395897000	-3.496435000
C	-2.815067000	0.517865000	1.236651000	C	-2.916541000	-2.203802000	-3.187289000
C	-1.456467000	0.371667000	0.936865000	C	-0.713254000	-1.351556000	-2.647407000
C	-0.743536000	-0.928021000	1.192684000	C	-2.885332000	-2.991539000	-2.032655000
C	1.632217000	-1.426600000	1.428908000	C	-0.665684000	-2.122762000	-1.468758000
C	1.954881000	-0.255822000	2.307359000	C	-1.767776000	-2.953475000	-1.193521000
C	2.063066000	2.067576000	2.427513000	C	0.531985000	-2.153081000	-0.535238000
C	2.425268000	-0.382144000	3.615535000	C	-2.912983000	2.541066000	0.269403000
C	2.543715000	2.017950000	3.732883000	C	-1.537203000	2.432748000	0.082182000
C	2.730491000	0.772292000	4.336866000	C	-3.601833000	1.434732000	0.776192000
H	-1.806465000	-0.948551000	-4.478628000	C	-2.889980000	0.274974000	1.079043000
H	-3.657267000	-2.601724000	-4.014633000	C	-1.503781000	0.252572000	0.874961000
H	-3.533192000	-4.025549000	-1.963613000	C	-0.676020000	-0.946988000	1.289429000
H	1.471681000	-2.033184000	-1.143641000	C	1.716397000	-1.415475000	1.434909000
H	-3.073600000	3.822465000	0.451773000	C	2.033488000	-0.261570000	2.359023000
H	-0.651093000	3.390100000	-0.084717000	C	2.148533000	2.046277000	2.594157000
H	-1.619087000	-3.797009000	-0.404273000	C	2.527161000	-0.452007000	3.654026000
H	-4.476568000	1.899508000	1.299541000	C	2.654718000	1.942370000	3.888874000
H	0.588396000	-3.109217000	-0.040440000	C	2.847656000	0.666394000	4.425648000
H	2.529816000	-1.679022000	0.846147000	H	-1.786514000	-0.789785000	-4.406290000
H	-3.381740000	-0.342538000	1.598012000	H	-3.784452000	-2.231556000	-3.852183000
H	-1.407679000	-1.769916000	0.958521000	H	-3.725183000	-3.647443000	-1.788842000
H	1.338355000	-2.307335000	2.022001000	H	1.463409000	-2.049008000	-1.111875000
H	1.909664000	3.008645000	1.896709000	H	-3.430502000	3.468786000	0.017202000
H	-0.553684000	-0.989981000	2.275778000	H	-0.957265000	3.266401000	-0.324330000
H	2.543588000	-1.375011000	4.053361000	H	-1.741263000	-3.592455000	-0.306199000
H	2.763394000	2.946854000	4.262350000	H	-4.683352000	1.474324000	0.928932000
H	3.102760000	0.700396000	5.361623000	H	0.554318000	-3.146836000	-0.052192000
N	-0.728052000	1.405260000	0.477098000	H	2.603171000	-1.589002000	0.803658000
N	0.557669000	-1.059639000	0.463245000	H	-3.395369000	-0.610246000	1.471312000
N	1.783841000	0.951571000	1.733343000	H	-1.291720000	-1.858141000	1.253731000
O	0.118155000	0.443319000	-4.345270000	H	1.528365000	-2.333970000	2.019458000
O	0.249378000	0.757389000	-1.850269000	H	1.975131000	3.022022000	2.130282000
S	0.584130000	-0.229255000	-3.081428000	H	-0.426930000	-0.802275000	2.353004000
Cl	3.150754000	0.098374000	-0.927730000	H	2.653577000	-1.463546000	4.045656000
Cl	1.731318000	3.074062000	-0.625308000	H	2.886269000	2.842719000	4.461428000

H	3.237313000	0.543296000	5.439272000
N	-0.852937000	1.318647000	0.381777000
N	0.586024000	-1.105399000	0.530959000
N	1.852739000	0.970546000	1.854061000
O	0.299656000	0.188608000	-4.556918000
O	0.458769000	0.921143000	-2.144555000
S	0.699904000	-0.264588000	-3.174140000
Cl	3.541615000	0.552902000	-0.838558000
Fe	1.229532000	0.919114000	-0.302701000

10a' intermediate spin

C	-1.722052000	-1.341815000	-3.524586000
C	-2.843151000	-2.148634000	-3.310612000
C	-0.660204000	-1.357393000	-2.620573000
C	-2.881083000	-2.991469000	-2.195435000
C	-0.679319000	-2.191815000	-1.485039000
C	-1.805445000	-3.014593000	-1.301830000
C	0.478443000	-2.283530000	-0.506512000
C	-2.796164000	2.568543000	0.469985000
C	-1.441881000	2.394064000	0.204637000
C	-3.515163000	1.491396000	0.997716000
C	-2.849765000	0.292203000	1.245489000
C	-1.479904000	0.196413000	0.969563000
C	-0.703029000	-1.061272000	1.311948000
C	1.709926000	-1.475337000	1.412656000
C	2.002795000	-0.277739000	2.282453000
C	2.027355000	2.046870000	2.406772000
C	2.520620000	-0.382688000	3.575535000
C	2.554615000	2.020402000	3.695570000
C	2.806943000	0.781771000	4.290730000
H	-1.637212000	-0.691098000	-4.399838000
H	-3.677591000	-2.130571000	-4.017508000
H	-3.742843000	-3.642149000	-2.024886000
H	1.430001000	-2.230494000	-1.056462000
H	-3.275064000	3.526265000	0.257469000
H	-0.841173000	3.200268000	-0.224175000
H	-1.831156000	-3.695126000	-0.445733000
H	-4.583521000	1.584544000	1.207897000
H	0.437198000	-3.276027000	-0.020037000

H	2.582384000	-1.637068000	0.757863000
H	-3.378635000	-0.572598000	1.651944000
H	-1.364556000	-1.935304000	1.213879000
H	1.585256000	-2.381160000	2.034245000
H	1.812242000	2.990417000	1.898905000
H	-0.457246000	-1.000763000	2.384891000
H	2.693027000	-1.369704000	4.009515000
H	2.757960000	2.956618000	4.218971000
H	3.215873000	0.722545000	5.302246000
N	-0.802517000	1.238529000	0.455748000
N	0.545252000	-1.230217000	0.541360000
N	1.761345000	0.924375000	1.720175000
O	0.512510000	0.233361000	-4.391992000
O	0.391104000	0.924460000	-1.970582000
S	0.779242000	-0.240702000	-2.983519000
Cl	3.314896000	0.915116000	-0.868681000
Fe	1.114453000	0.898348000	-0.171669000

10a' low spin

C	-1.794973000	-1.351390000	-3.517894000
C	-2.858772000	-2.223389000	-3.267733000
C	-0.706863000	-1.300030000	-2.647793000
C	-2.811993000	-3.062143000	-2.150015000
C	-0.643974000	-2.124654000	-1.508151000
C	-1.710908000	-3.015122000	-1.288818000
C	0.547461000	-2.145609000	-0.569512000
C	-2.753906000	2.575879000	0.410223000
C	-1.396728000	2.373171000	0.175134000
C	-3.509122000	1.519593000	0.928785000
C	-2.877562000	0.304654000	1.200375000
C	-1.507516000	0.183609000	0.953429000
C	-0.714631000	-1.050174000	1.295255000
C	1.688539000	-1.472227000	1.457040000
C	1.999459000	-0.293390000	2.337924000
C	2.014851000	2.032232000	2.429428000
C	2.536551000	-0.385617000	3.622374000
C	2.565338000	2.021421000	3.709363000
C	2.830049000	0.790811000	4.316968000
H	-1.777224000	-0.696210000	-4.393714000

H	-3.714091000	-2.258485000	-3.948606000	C	-0.652537000	-0.933065000	1.412021000
H	-3.626489000	-3.763906000	-1.952090000	C	1.751282000	-1.360854000	1.381437000
H	1.481209000	-1.995461000	-1.129423000	C	2.122068000	-0.214059000	2.288942000
H	-3.207668000	3.541869000	0.180384000	C	2.270905000	2.089979000	2.546163000
H	-0.766076000	3.159171000	-0.248179000	C	2.656230000	-0.423010000	3.564518000
H	-1.670981000	-3.692788000	-0.430968000	C	2.812398000	1.963796000	3.823807000
H	-4.579165000	1.639597000	1.114851000	C	3.011962000	0.681430000	4.340353000
H	0.590717000	-3.142505000	-0.098979000	H	-1.441190000	-0.766976000	-4.511254000
H	2.572844000	-1.674969000	0.834603000	H	-3.660611000	-1.870575000	-4.020582000
H	-3.433952000	-0.545713000	1.599928000	H	-3.946750000	-3.129692000	-1.879923000
H	-1.316373000	-1.958817000	1.155733000	H	1.368578000	-2.206619000	-0.984585000
H	1.454346000	-2.374569000	2.046283000	H	-3.804957000	3.155148000	-0.023946000
H	1.784540000	2.968499000	1.913309000	H	-1.317512000	3.127980000	-0.425563000
H	-0.480439000	-1.004057000	2.370199000	H	-2.078129000	-3.258396000	-0.253477000
H	2.720488000	-1.366403000	4.065793000	H	-4.861443000	1.130195000	1.051973000
H	2.776304000	2.964095000	4.218074000	H	0.311803000	-3.127426000	0.098637000
H	3.255104000	0.746984000	5.322568000	H	2.587458000	-1.536012000	0.683867000
N	-0.792028000	1.205708000	0.448606000	H	-3.395175000	-0.806086000	1.680534000
N	0.571324000	-1.120514000	0.531792000	H	-1.194110000	-1.887735000	1.515368000
N	1.743658000	0.899803000	1.762635000	H	1.632502000	-2.284477000	1.978148000
O	0.233896000	0.474300000	-4.384146000	H	2.096217000	3.062783000	2.078876000
O	0.375784000	0.937963000	-1.912467000	H	-0.336802000	-0.658855000	2.431844000
S	0.665401000	-0.115262000	-3.060380000	H	2.784378000	-1.441064000	3.937849000
Cl	3.259189000	0.378087000	-0.820638000	H	3.068102000	2.856551000	4.397992000
Fe	1.049148000	0.763197000	-0.073055000	H	3.431704000	0.541977000	5.339751000
10a'' high spin				N	-1.057393000	1.236081000	0.368146000
C	-1.621207000	-1.297959000	-3.572373000	N	0.553367000	-1.076737000	0.570303000
C	-2.842676000	-1.919497000	-3.296292000	N	1.939144000	1.025412000	1.798024000
C	-0.583740000	-1.357008000	-2.643071000	O	0.809354000	-0.092248000	-4.509101000
C	-3.003812000	-2.620972000	-2.097029000	O	0.924970000	0.704756000	-2.118872000
C	-0.726326000	-2.045179000	-1.424256000	S	1.019311000	-0.546519000	-3.086580000
C	-1.951691000	-2.687690000	-1.177733000	Cl	1.644322000	3.475876000	-0.444533000
C	0.416432000	-2.164369000	-0.435816000	Fe	1.024345000	1.171412000	-0.218572000
C	-3.206284000	2.288370000	0.262647000	10a'' intermediate spin			
C	-1.833533000	2.278836000	0.031866000	C	-1.132341000	-0.919867000	-3.622210000
C	-3.785844000	1.165129000	0.861009000	C	-2.487526000	-1.257138000	-3.540202000
C	-2.974826000	0.085723000	1.210971000	C	-0.261405000	-1.249131000	-2.582832000
C	-1.600249000	0.155325000	0.953771000	C	-2.960303000	-1.946783000	-2.420330000

C	-0.723736000	-1.929389000	-1.437241000
C	-2.082349000	-2.278765000	-1.382550000
C	0.201679000	-2.289095000	-0.293637000
C	-3.514449000	1.896557000	0.464662000
C	-2.183169000	1.882743000	0.057304000
C	-3.976225000	0.859509000	1.280184000
C	-3.090757000	-0.149457000	1.660874000
C	-1.766817000	-0.090607000	1.216622000
C	-0.721705000	-1.082344000	1.657004000
C	1.685132000	-1.426693000	1.431787000
C	2.118974000	-0.193867000	2.186586000
C	2.189926000	2.128775000	2.156677000
C	2.831113000	-0.239137000	3.388139000
C	2.909870000	2.169991000	3.350234000
C	3.235395000	0.962862000	3.974589000
H	-0.724503000	-0.394233000	-4.489344000
H	-3.168682000	-0.992161000	-4.353578000
H	-4.013649000	-2.231179000	-2.352657000
H	1.188442000	-2.556789000	-0.688173000
H	-4.173706000	2.705066000	0.142884000
H	-1.754748000	2.665405000	-0.573433000
H	-2.456287000	-2.823564000	-0.511176000
H	-5.016477000	0.835007000	1.614100000
H	-0.190423000	-3.174110000	0.234448000
H	2.451386000	-1.645980000	0.673183000
H	-3.414309000	-0.976979000	2.295543000
H	-1.172733000	-2.068325000	1.853717000
H	1.612285000	-2.299283000	2.103309000
H	1.901775000	3.035399000	1.616584000
H	-0.328701000	-0.724782000	2.622176000
H	3.060725000	-1.200427000	3.852497000
H	3.204202000	3.129956000	3.779181000
H	3.794128000	0.956368000	4.913821000
N	-1.332258000	0.910331000	0.427713000
N	0.413474000	-1.189244000	0.702334000
N	1.809496000	0.973656000	1.594602000
O	1.518550000	0.113643000	-3.998029000
O	1.884850000	-0.180433000	-1.462031000

S	1.541018000	-0.866747000	-2.847337000
Cl	0.819517000	2.902896000	-1.004047000
Fe	0.635356000	0.732029000	-0.206686000

10a" low spin

C	-1.718397000	-1.421696000	-3.574488000
C	-2.837431000	-2.219693000	-3.315190000
C	-0.668499000	-1.378246000	-2.659694000
C	-2.881937000	-2.987545000	-2.146841000
C	-0.694750000	-2.133203000	-1.473987000
C	-1.814883000	-2.949887000	-1.242222000
C	0.481785000	-2.152449000	-0.519830000
C	-2.824328000	2.577281000	0.368295000
C	-1.459845000	2.420527000	0.139786000
C	-3.546250000	1.507912000	0.905454000
C	-2.874205000	0.320975000	1.201599000
C	-1.501165000	0.238946000	0.958811000
C	-0.675422000	-0.966148000	1.326460000
C	1.739686000	-1.385297000	1.369029000
C	2.034521000	-0.239621000	2.296646000
C	1.948701000	2.069590000	2.550146000
C	2.575780000	-0.400462000	3.572887000
C	2.487823000	1.988884000	3.832011000
C	2.812903000	0.733665000	4.352395000
H	-1.630888000	-0.823210000	-4.485846000
H	-3.667051000	-2.252469000	-4.027221000
H	-3.743326000	-3.628921000	-1.942716000
H	1.419400000	-2.107708000	-1.092249000
H	-3.309221000	3.523298000	0.119324000
H	-0.837903000	3.211625000	-0.283885000
H	-1.845263000	-3.575752000	-0.345463000
H	-4.620195000	1.595067000	1.087278000
H	0.473006000	-3.116605000	0.017328000
H	2.602927000	-1.547731000	0.702589000
H	-3.401264000	-0.540371000	1.617027000
H	-1.272986000	-1.886416000	1.260930000
H	1.580137000	-2.320525000	1.932991000
H	1.700181000	3.021993000	2.078808000
H	-0.395878000	-0.863215000	2.386715000

H	2.798689000	-1.402499000	3.944818000
H	2.647091000	2.901806000	4.409409000
H	3.235911000	0.637205000	5.355269000
N	-0.816830000	1.276659000	0.436023000
N	0.569978000	-1.062466000	0.507593000
N	1.733446000	0.977132000	1.794880000
O	0.501377000	0.241349000	-4.400480000
O	0.431292000	0.852885000	-1.959530000
S	0.772197000	-0.274744000	-3.006557000
Cl	1.837464000	3.098440000	-0.495333000
Fe	1.013657000	0.925323000	-0.067710000

11 high spin

C	-4.313806000	-0.172872000	-2.655150000
C	-4.132931000	1.142729000	-2.221314000
C	-3.533011000	-1.185221000	-2.095756000
C	2.777446000	1.710555000	-2.188436000
C	2.229947000	0.434117000	-2.083722000
C	2.182402000	2.761458000	-1.483773000
C	-3.178037000	1.395437000	-1.239400000
C	-2.599394000	-0.854737000	-1.109963000
C	0.406638000	-1.098627000	-1.233213000
C	1.096827000	0.241499000	-1.282824000
C	1.068765000	2.487397000	-0.696216000
C	-1.744458000	-1.888113000	-0.419891000
C	0.223530000	-2.149386000	0.995551000
C	2.687332000	-2.399454000	1.459217000
C	1.542655000	-1.610941000	1.488664000
C	3.888885000	-1.928047000	2.006471000
C	1.601019000	-0.303441000	2.072365000
C	3.964959000	-0.656041000	2.594581000
C	2.834538000	0.142647000	2.623967000
H	-5.050365000	-0.407724000	-3.427400000
H	-4.717155000	1.966132000	-2.636386000
H	3.660300000	1.884387000	-2.808593000
H	-3.636508000	-2.223592000	-2.416966000
H	2.664856000	-0.414042000	-2.616550000
H	-0.229394000	-1.162338000	-2.130416000
H	2.575819000	3.778478000	-1.534459000

H	1.146293000	-1.908888000	-1.328761000
H	-1.612622000	-2.777643000	-1.058842000
H	-2.994480000	2.402997000	-0.859210000
H	0.571354000	3.265586000	-0.113210000
H	-2.259736000	-2.203457000	0.499931000
H	0.369630000	-3.166638000	0.592880000
H	2.657793000	-3.396786000	1.019253000
H	-0.482721000	-2.215284000	1.837848000
H	4.909878000	-0.311840000	3.015171000
H	2.865115000	1.138559000	3.071329000
N	-2.435681000	0.416843000	-0.698961000
N	0.538744000	1.255434000	-0.601941000
N	-0.442243000	-1.303626000	-0.034723000
Cl	-1.543863000	2.925794000	1.351977000
Cl	-2.522262000	-0.315084000	2.411774000
Fe	-0.993898000	0.706352000	0.965647000
O	0.554791000	0.470707000	2.106550000
N	5.069354000	-2.770691000	1.964464000
O	4.982270000	-3.875065000	1.431951000
O	6.108760000	-2.344989000	2.462707000

11 intermediate spin

C	-4.260679000	-0.044268000	-2.652000000
C	-4.032584000	1.243686000	-2.164224000
C	-3.512355000	-1.103103000	-2.137450000
C	2.751350000	1.708600000	-2.139686000
C	2.201737000	0.430018000	-2.112176000
C	2.184405000	2.702968000	-1.337476000
C	-3.069257000	1.426247000	-1.175922000
C	-2.566667000	-0.852473000	-1.141167000
C	0.430745000	-1.177415000	-1.296228000
C	1.098188000	0.174729000	-1.289466000
C	1.094404000	2.376898000	-0.538742000
C	-1.742890000	-1.946675000	-0.511597000
C	0.228979000	-2.243108000	0.920131000
C	2.693863000	-2.362464000	1.432533000
C	1.505378000	-1.641833000	1.455662000
C	3.856355000	-1.839511000	2.016534000
C	1.475972000	-0.347601000	2.072616000

C	3.846933000	-0.580409000	2.636711000
C	2.673578000	0.153290000	2.657621000
H	-5.006515000	-0.222005000	-3.430425000
H	-4.586822000	2.105109000	-2.541207000
H	3.613662000	1.927048000	-2.774271000
H	-3.648404000	-2.123465000	-2.500930000
H	2.613956000	-0.378509000	-2.719341000
H	-0.185615000	-1.229802000	-2.207964000
H	2.580140000	3.720041000	-1.320794000
H	1.190280000	-1.968855000	-1.398544000
H	-1.652001000	-2.807990000	-1.195013000
H	-2.849116000	2.407343000	-0.750623000
H	0.609542000	3.108906000	0.109856000
H	-2.258711000	-2.285973000	0.398970000
H	0.434052000	-3.251453000	0.519669000
H	2.728924000	-3.349657000	0.970528000
H	-0.499743000	-2.340866000	1.740049000
H	4.761644000	-0.192455000	3.085199000
H	2.638257000	1.137364000	3.130024000
N	-2.360369000	0.399745000	-0.677202000
N	0.562811000	1.139537000	-0.521059000
N	-0.426788000	-1.411960000	-0.118883000
Cl	-1.511786000	2.880325000	1.345762000
Cl	-2.503063000	-0.364625000	2.260871000
Fe	-0.965522000	0.607657000	0.837270000
O	0.383900000	0.360891000	2.151185000
N	5.082156000	-2.612528000	1.979273000
O	5.068862000	-3.706372000	1.417945000
O	6.086149000	-2.142483000	2.510206000
11 low spin			
C	-4.270300000	-0.043693000	-2.639140000
C	-4.015216000	1.246657000	-2.170524000
C	-3.528352000	-1.109301000	-2.127136000
C	2.704478000	1.769544000	-2.180512000
C	2.191989000	0.474683000	-2.148727000
C	2.110465000	2.752360000	-1.383206000
C	-3.031108000	1.429611000	-1.202303000
C	-2.561838000	-0.853713000	-1.154570000

C	0.434623000	-1.145173000	-1.299878000
C	1.095825000	0.199864000	-1.325954000
C	1.030041000	2.404268000	-0.580491000
C	-1.732693000	-1.921169000	-0.501062000
C	0.230154000	-2.186031000	0.934983000
C	2.681616000	-2.389252000	1.471194000
C	1.523645000	-1.621768000	1.458067000
C	3.851034000	-1.900773000	2.072232000
C	1.524947000	-0.312926000	2.045990000
C	3.871775000	-0.632660000	2.676830000
C	2.727589000	0.144339000	2.661579000
H	-5.033768000	-0.218661000	-3.400891000
H	-4.566428000	2.109881000	-2.547848000
H	3.560511000	2.009394000	-2.815756000
H	-3.687374000	-2.132137000	-2.473499000
H	2.627043000	-0.325113000	-2.750947000
H	-0.191654000	-1.226791000	-2.201626000
H	2.479986000	3.779282000	-1.373536000
H	1.178480000	-1.952628000	-1.365258000
H	-1.581722000	-2.788672000	-1.162354000
H	-2.790844000	2.411106000	-0.790062000
H	0.526699000	3.121244000	0.070433000
H	-2.248507000	-2.254209000	0.410592000
H	0.398333000	-3.186689000	0.505097000
H	2.687171000	-3.385833000	1.028335000
H	-0.495742000	-2.275475000	1.757314000
H	4.789694000	-0.274109000	3.143084000
H	2.719419000	1.135707000	3.120058000
N	-2.327838000	0.398852000	-0.706303000
N	0.533052000	1.153365000	-0.560784000
N	-0.429768000	-1.326729000	-0.094325000
Cl	-1.490278000	2.651929000	1.383218000
Cl	-2.427056000	-0.391398000	2.215788000
Fe	-0.892864000	0.507335000	0.725534000
O	0.472960000	0.448746000	2.056454000
N	5.046343000	-2.716572000	2.072248000
O	5.006680000	-3.817551000	1.524363000
O	6.056130000	-2.276597000	2.619526000

11a' high spin

C	-4.434382000	-0.283979000	-2.579166000
C	-4.351271000	0.998355000	-2.031457000
C	-3.566951000	-1.275569000	-2.116803000
C	2.882700000	1.685771000	-2.080313000
C	2.295431000	0.421248000	-2.081250000
C	2.315295000	2.701275000	-1.303253000
C	-3.401511000	1.237568000	-1.040168000
C	-2.646241000	-0.959303000	-1.113461000
C	0.407055000	-1.118938000	-1.358913000
C	1.148426000	0.201895000	-1.307236000
C	1.184514000	2.401517000	-0.549661000
C	-1.714821000	-1.987297000	-0.516551000
C	0.290119000	-2.289737000	0.806411000
C	2.761448000	-2.365417000	1.302162000
C	1.542377000	-1.711912000	1.411693000
C	3.896594000	-1.876941000	1.971236000
C	1.432155000	-0.517104000	2.209221000
C	3.813874000	-0.723328000	2.771696000
C	2.605439000	-0.061295000	2.887618000
H	-5.161819000	-0.508941000	-3.363081000
H	-5.005887000	1.805532000	-2.366003000
H	3.777723000	1.878053000	-2.677432000
H	-3.595962000	-2.287479000	-2.526184000
H	2.713882000	-0.394208000	-2.675148000
H	-0.259753000	-1.068219000	-2.235554000
H	2.743699000	3.705002000	-1.274440000
H	1.117630000	-1.937107000	-1.566945000
H	-1.616662000	-2.853151000	-1.196564000
H	-3.284424000	2.218652000	-0.571423000
H	0.695921000	3.146979000	0.084689000
H	-2.176110000	-2.361352000	0.412441000
H	0.523892000	-3.260489000	0.330603000
H	2.848772000	-3.274630000	0.705743000
H	-0.431396000	-2.483742000	1.616777000
H	4.705436000	-0.365084000	3.287181000
H	2.519496000	0.838327000	3.502083000
N	-2.572986000	0.280160000	-0.593534000

N	0.619397000	1.182946000	-0.557162000
N	-0.407838000	-1.409384000	-0.163096000
Cl	-1.767027000	2.743607000	1.610637000
Fe	-0.950186000	0.649998000	0.843112000
O	0.313893000	0.119905000	2.315186000
N	5.154098000	-2.572297000	1.842154000
O	5.203668000	-3.575813000	1.128935000
O	6.133489000	-2.137326000	2.449462000

11a' intermediate spin

C	-4.258453000	-0.029244000	-2.576038000
C	-4.032006000	1.248205000	-2.057763000
C	-3.495076000	-1.097436000	-2.099950000
C	2.575706000	1.742138000	-2.407981000
C	2.116841000	0.430458000	-2.305953000
C	1.996614000	2.729778000	-1.603580000
C	-3.047452000	1.410196000	-1.085581000
C	-2.531383000	-0.861318000	-1.117644000
C	0.500742000	-1.261985000	-1.308660000
C	1.081170000	0.136103000	-1.409806000
C	0.984181000	2.357344000	-0.725728000
C	-1.706144000	-1.956355000	-0.482821000
C	0.264277000	-2.211827000	0.969430000
C	2.705492000	-2.376968000	1.513014000
C	1.547995000	-1.610375000	1.496995000
C	3.885890000	-1.905071000	2.112350000
C	1.557146000	-0.287783000	2.088440000
C	3.910944000	-0.640329000	2.730216000
C	2.772824000	0.139439000	2.719940000
H	-5.019224000	-0.192217000	-3.343231000
H	-4.605989000	2.111903000	-2.398767000
H	3.380807000	1.993178000	-3.102921000
H	-3.640220000	-2.110536000	-2.480532000
H	2.549368000	-0.368150000	-2.912774000
H	-0.081034000	-1.445602000	-2.226640000
H	2.327820000	3.769015000	-1.647007000
H	1.320376000	-1.999045000	-1.322212000
H	-1.672710000	-2.849765000	-1.131708000
H	-2.836647000	2.388921000	-0.646765000

H	0.512530000	3.086807000	-0.061566000
H	-2.206332000	-2.245194000	0.456165000
H	0.455231000	-3.256009000	0.659592000
H	2.706330000	-3.373652000	1.069569000
H	-0.479223000	-2.237777000	1.783898000
H	4.830437000	-0.291681000	3.201352000
H	2.770659000	1.127483000	3.187015000
N	-2.314149000	0.381096000	-0.632855000
N	0.536733000	1.092165000	-0.640883000
N	-0.367447000	-1.452448000	-0.133920000
Cl	-2.523742000	0.302919000	2.388037000
Fe	-0.894591000	0.512748000	0.754153000
O	0.540384000	0.499488000	2.083985000
N	5.069108000	-2.723305000	2.101109000
O	5.025656000	-3.822383000	1.542646000
O	6.087759000	-2.296181000	2.649625000

11a' low spin

C	-4.268385000	-0.030071000	-2.545018000
C	-4.012085000	1.256000000	-2.061592000
C	-3.500876000	-1.097290000	-2.071916000
C	2.436964000	1.883439000	-2.499733000
C	2.048839000	0.549168000	-2.379796000
C	1.822948000	2.844908000	-1.689783000
C	-2.993533000	1.429933000	-1.126732000
C	-2.508865000	-0.846835000	-1.123021000
C	0.538446000	-1.196271000	-1.295663000
C	1.053403000	0.211960000	-1.457583000
C	0.845867000	2.432276000	-0.789285000
C	-1.667052000	-1.913380000	-0.474529000
C	0.284615000	-2.166711000	0.977774000
C	2.697183000	-2.460673000	1.595018000
C	1.591116000	-1.629325000	1.505078000
C	3.882529000	-2.028359000	2.217735000
C	1.655511000	-0.282740000	2.034422000
C	3.960847000	-0.735839000	2.774142000
C	2.874176000	0.108859000	2.686063000
H	-5.054580000	-0.199981000	-3.284527000
H	-4.586806000	2.118199000	-2.405393000

H	3.212686000	2.170748000	-3.213544000
H	-3.666473000	-2.116268000	-2.427698000
H	2.508119000	-0.231244000	-2.990365000
H	-0.030604000	-1.464212000	-2.199556000
H	2.098588000	3.899508000	-1.748756000
H	1.378793000	-1.904475000	-1.240792000
H	-1.558537000	-2.801960000	-1.117752000
H	-2.750269000	2.417446000	-0.725020000
H	0.343965000	3.140885000	-0.124583000
H	-2.167618000	-2.212324000	0.458818000
H	0.429581000	-3.196339000	0.608158000
H	2.654478000	-3.475824000	1.197785000
H	-0.454849000	-2.191329000	1.793160000
H	4.883523000	-0.419538000	3.261751000
H	2.916857000	1.117730000	3.104379000
N	-2.263199000	0.401165000	-0.669568000
N	0.469804000	1.145865000	-0.683352000
N	-0.345055000	-1.341274000	-0.096325000
Cl	-2.312567000	-0.160874000	2.337618000
Fe	-0.794887000	0.458414000	0.647583000
O	0.681656000	0.542937000	1.940344000
N	5.011027000	-2.912993000	2.294315000
O	4.920319000	-4.037880000	1.793468000
O	6.035595000	-2.518679000	2.858516000

11a'' high spin

C	-4.418715000	-0.176893000	-2.596675000
C	-4.285066000	1.130960000	-2.124428000
C	-3.584774000	-1.171483000	-2.082194000
C	2.974940000	1.558315000	-2.202580000
C	2.343014000	0.317205000	-2.136054000
C	2.444272000	2.633992000	-1.482597000
C	-3.320037000	1.391965000	-1.153598000
C	-2.646533000	-0.832052000	-1.102863000
C	0.397754000	-1.111103000	-1.337385000
C	1.188880000	0.181367000	-1.353676000
C	1.304027000	2.415823000	-0.715181000
C	-1.751148000	-1.859197000	-0.450595000
C	0.246702000	-2.161562000	0.886636000

C	2.717652000	-2.289235000	1.374382000
C	1.519851000	-1.593779000	1.457342000
C	3.872227000	-1.802345000	2.010526000
C	1.452316000	-0.356426000	2.192490000
C	3.830339000	-0.608007000	2.752277000
C	2.643535000	0.095933000	2.841280000
H	-5.159783000	-0.419784000	-3.362255000
H	-4.912812000	1.940812000	-2.501340000
H	3.875865000	1.686009000	-2.808051000
H	-3.653741000	-2.203556000	-2.432217000
H	2.731432000	-0.543564000	-2.684741000
H	-0.270278000	-1.078252000	-2.213929000
H	2.908010000	3.622000000	-1.507687000
H	1.074981000	-1.965753000	-1.505875000
H	-1.683915000	-2.762987000	-1.083328000
H	-3.164138000	2.393131000	-0.742149000
H	0.842200000	3.211067000	-0.122575000
H	-2.224837000	-2.166709000	0.496494000
H	0.446887000	-3.162738000	0.461315000
H	2.772993000	-3.229345000	0.823818000
H	-0.478255000	-2.289020000	1.707046000
H	4.736111000	-0.251515000	3.243599000
H	2.589531000	1.027809000	3.409574000
N	-2.524002000	0.432030000	-0.656373000
N	0.696101000	1.219540000	-0.657847000
N	-0.424360000	-1.309761000	-0.126931000
Cl	-1.629583000	2.974485000	1.401156000
Fe	-0.888976000	0.810698000	0.765626000
O	0.355805000	0.321566000	2.269239000
N	5.107928000	-2.539801000	1.906817000
O	5.122469000	-3.577851000	1.243162000
O	6.104726000	-2.104364000	2.484790000

11a'' intermediate spin

C	-4.469810000	-0.110062000	-2.486849000
C	-4.264384000	1.188691000	-2.015783000
C	-3.656841000	-1.140473000	-2.008840000
C	3.030670000	1.459752000	-2.211380000
C	2.375491000	0.228186000	-2.161117000

C	2.500783000	2.545562000	-1.506848000
C	-3.256832000	1.412374000	-1.079970000
C	-2.670140000	-0.840993000	-1.068698000
C	0.360392000	-1.132734000	-1.385099000
C	1.200477000	0.122387000	-1.408657000
C	1.334136000	2.350727000	-0.769469000
C	-1.770812000	-1.874106000	-0.446945000
C	0.251242000	-2.135684000	0.867930000
C	2.723879000	-2.237926000	1.358386000
C	1.521085000	-1.549883000	1.418735000
C	3.866622000	-1.728708000	1.998440000
C	1.431811000	-0.300849000	2.129284000
C	3.803985000	-0.524133000	2.722957000
C	2.610148000	0.170100000	2.788825000
H	-5.249903000	-0.318895000	-3.222939000
H	-4.873775000	2.024198000	-2.365711000
H	3.949737000	1.570538000	-2.792423000
H	-3.779120000	-2.167749000	-2.357581000
H	2.763369000	-0.641104000	-2.696514000
H	-0.335129000	-1.067210000	-2.237208000
H	2.984641000	3.524216000	-1.521530000
H	0.981289000	-2.026119000	-1.559203000
H	-1.682810000	-2.768563000	-1.086591000
H	-3.050194000	2.401154000	-0.664223000
H	0.873766000	3.153729000	-0.185807000
H	-2.219817000	-2.195966000	0.506364000
H	0.449556000	-3.129650000	0.430973000
H	2.792289000	-3.188082000	0.826960000
H	-0.464217000	-2.268872000	1.695394000
H	4.700988000	-0.151712000	3.218617000
H	2.540928000	1.109636000	3.342572000
N	-2.479901000	0.417896000	-0.616507000
N	0.705507000	1.168307000	-0.729933000
N	-0.443515000	-1.283318000	-0.140068000
Cl	-1.591052000	2.693229000	1.472146000
Fe	-0.895482000	0.626844000	0.657807000
O	0.330377000	0.369661000	2.185006000
N	5.110620000	-2.454428000	1.918642000

O	5.142860000	-3.501950000	1.270471000
O	6.096681000	-2.000394000	2.500833000
11a" low spin			
C	-4.287100000	-0.064281000	-2.571127000
C	-4.017417000	1.240660000	-2.150817000
C	-3.539916000	-1.114589000	-2.033264000
C	2.593451000	1.780348000	-2.398705000
C	2.122299000	0.471374000	-2.299207000
C	2.001862000	2.773281000	-1.611715000
C	-3.012379000	1.451767000	-1.209600000
C	-2.554870000	-0.826538000	-1.087884000
C	0.460778000	-1.181408000	-1.298251000
C	1.070935000	0.191562000	-1.422059000
C	0.964440000	2.422126000	-0.753813000
C	-1.717826000	-1.874129000	-0.404371000
C	0.265080000	-2.140844000	0.978088000
C	2.706843000	-2.400934000	1.510913000
C	1.574069000	-1.601318000	1.484008000
C	3.890869000	-1.948256000	2.118878000
C	1.602653000	-0.278268000	2.061914000
C	3.937832000	-0.678681000	2.727897000
C	2.819296000	0.129912000	2.703343000
H	-5.065193000	-0.262041000	-3.312348000
H	-4.574629000	2.091930000	-2.547068000
H	3.415379000	2.022162000	-3.076798000
H	-3.711568000	-2.148530000	-2.339262000
H	2.560177000	-0.335200000	-2.890988000
H	-0.165971000	-1.355854000	-2.186908000
H	2.340980000	3.810184000	-1.653215000
H	1.243351000	-1.955118000	-1.317996000
H	-1.636589000	-2.790536000	-1.012897000
H	-2.766017000	2.444372000	-0.826982000
H	0.465327000	3.144205000	-0.104339000
H	-2.204200000	-2.152118000	0.544942000
H	0.401261000	-3.170480000	0.604048000
H	2.685591000	-3.401535000	1.076700000
H	-0.455654000	-2.182799000	1.812279000
H	4.861668000	-0.349651000	3.204750000

H	2.837032000	1.121075000	3.163461000
N	-2.297889000	0.438847000	-0.687458000
N	0.508156000	1.157524000	-0.667966000
N	-0.383775000	-1.310356000	-0.074458000
Cl	-1.571597000	2.624139000	1.488214000
Fe	-0.802787000	0.568361000	0.624387000
O	0.591543000	0.512538000	2.026418000
N	5.055071000	-2.793415000	2.128662000
O	4.992754000	-3.895358000	1.577494000
O	6.076275000	-2.386506000	2.687547000

12 high spin			
C	0.997492000	2.293858000	-4.031899000
C	-0.004152000	3.154144000	-3.575571000
C	4.387849000	-2.763949000	-2.903030000
C	1.682932000	1.517718000	-3.099612000
C	-0.280416000	3.211401000	-2.208526000
C	3.804349000	-1.737555000	-2.062970000
C	0.445178000	2.395148000	-1.336579000
C	6.306415000	2.405976000	-0.382681000
C	5.239761000	1.535944000	-0.584595000
C	-0.353223000	-1.049012000	-0.856920000
C	-1.282140000	-2.076374000	-0.709875000
C	6.073363000	3.596722000	0.311888000
C	0.175751000	2.363916000	0.152999000
C	4.784404000	3.873313000	0.762468000
C	-1.065795000	-3.034874000	0.282989000
C	3.760426000	2.954275000	0.502683000
C	2.333244000	3.269481000	0.879744000
C	0.965244000	-1.879920000	0.860208000
C	0.073585000	-2.934087000	1.081034000
C	2.262316000	-1.764018000	1.617188000
C	4.107310000	-0.306364000	2.207272000
C	1.203605000	1.581769000	2.248707000
C	1.828760000	0.395564000	2.674378000
C	0.376806000	2.287304000	3.136691000
C	1.620217000	-0.052652000	3.988546000
C	0.168092000	1.826443000	4.435503000
C	0.796474000	0.653036000	4.864243000

H	1.251344000	2.224603000	-5.091187000	C	1.737054000	1.391106000	-2.696167000
H	-0.559118000	3.782308000	-4.276580000	C	0.074726000	3.479816000	-2.067138000
H	3.796076000	-2.866568000	-3.825426000	C	0.614938000	2.657892000	-1.074184000
H	5.421394000	-2.486685000	-3.160814000	C	5.861936000	2.371562000	-0.939930000
H	2.478923000	0.835104000	-3.407598000	C	4.784261000	1.516891000	-0.747084000
H	4.391200000	-3.723319000	-2.363459000	C	-0.179599000	-0.902188000	-0.802369000
H	-1.046294000	3.881699000	-1.813440000	C	-1.005396000	-2.021544000	-0.765108000
H	7.298684000	2.147398000	-0.756654000	C	5.814900000	3.645717000	-0.363074000
H	5.381025000	0.588148000	-1.107494000	C	0.258885000	2.846196000	0.393078000
H	-0.490149000	-0.279853000	-1.619902000	C	4.699137000	4.010476000	0.385256000
H	-2.157100000	-2.115320000	-1.361256000	C	-0.709648000	-3.051777000	0.130140000
H	6.887764000	4.300306000	0.500771000	C	3.650282000	3.096818000	0.545858000
H	-1.777023000	-3.850395000	0.434770000	C	2.441644000	3.436996000	1.401463000
H	-0.540025000	1.558083000	0.374596000	C	1.189251000	-1.779052000	0.866935000
H	1.949864000	3.984695000	0.134701000	C	0.401800000	-2.924749000	0.964264000
H	-0.289159000	3.310493000	0.470708000	C	2.427600000	-1.542121000	1.673507000
H	4.560615000	4.793189000	1.306740000	C	3.974408000	0.162160000	2.431027000
H	3.047737000	-2.283552000	1.044259000	C	1.002783000	1.765133000	2.500220000
H	4.742554000	-0.758785000	1.433365000	C	1.598343000	0.515770000	2.797118000
H	0.280765000	-3.662081000	1.867816000	C	0.061733000	2.299015000	3.393986000
H	2.305948000	3.793610000	1.846220000	C	1.257890000	-0.143220000	3.985915000
H	4.412899000	0.735123000	2.361981000	C	-0.286795000	1.625257000	4.564515000
H	2.189661000	-2.277870000	2.588591000	C	0.319759000	0.403077000	4.863419000
H	-0.103347000	3.210320000	2.805462000	H	1.488773000	1.940803000	-4.762642000
H	4.249112000	-0.860822000	3.150400000	H	-0.041635000	3.866287000	-4.191232000
H	2.110968000	-0.966058000	4.330757000	H	2.410142000	0.553543000	-2.891512000
H	-0.481609000	2.385993000	5.112725000	H	-0.575061000	4.308427000	-1.779318000
H	0.646762000	0.285656000	5.882319000	H	6.716094000	2.043684000	-1.534683000
N	1.406185000	1.565635000	-1.788318000	H	4.767703000	0.515091000	-1.182123000
N	3.340664000	-0.918043000	-1.392388000	H	-0.385267000	-0.077570000	-1.484550000
N	3.996377000	1.804981000	-0.150292000	H	-1.868711000	-2.073571000	-1.430518000
N	0.740755000	-0.948720000	-0.085048000	H	6.641200000	4.347508000	-0.499213000
N	1.428967000	2.082249000	0.900446000	H	-1.342190000	-3.940773000	0.184194000
N	2.694038000	-0.353819000	1.763116000	H	-0.605408000	2.197525000	0.608383000
Ni	2.341075000	0.495251000	-0.230231000	H	2.093173000	4.450591000	1.137989000
12 low spin				H	-0.073885000	3.888107000	0.542424000
C	1.221906000	2.167310000	-3.729136000	H	4.626633000	4.996365000	0.849363000
C	0.375470000	3.230853000	-3.406382000	H	3.304011000	-1.885892000	1.101607000

H	4.721738000	-0.175602000	1.701944000
H	0.663333000	-3.699090000	1.687301000
H	2.782153000	3.497798000	2.447619000
H	4.115469000	1.227411000	2.642452000
H	2.420081000	-2.103722000	2.617849000
H	-0.397281000	3.261786000	3.158306000
H	4.099938000	-0.402941000	3.368177000
H	1.723726000	-1.097077000	4.236703000
H	-1.023939000	2.058669000	5.244772000
H	0.066115000	-0.132407000	5.781344000
N	1.431880000	1.633464000	-1.409754000
N	3.710401000	1.879515000	-0.017872000
N	0.900661000	-0.788218000	-0.007069000
N	1.347490000	2.471357000	1.299184000
N	2.607632000	-0.074586000	1.885514000
Ni	2.173952000	0.674435000	0.082607000

12a

C	1.347938000	2.424844000	-3.863273000
C	0.583384000	3.511182000	-3.431719000
C	1.784607000	1.501898000	-2.913106000
C	0.284347000	3.628713000	-2.072767000
C	0.748829000	2.652104000	-1.185540000
C	5.971306000	2.729286000	-1.131115000
C	5.056185000	1.705960000	-0.896252000
C	0.531027000	-1.539148000	-1.134481000
C	-0.257610000	-2.681147000	-1.052253000
C	5.734655000	3.979073000	-0.551159000
C	0.379464000	2.675045000	0.285558000
C	4.598875000	4.148924000	0.239071000
C	-0.117848000	-3.529936000	0.052780000
C	3.731365000	3.066083000	0.434416000
C	2.536125000	3.207130000	1.364000000
C	1.592211000	-2.036008000	0.874016000
C	0.823284000	-3.187683000	1.030359000
C	2.690132000	-1.655605000	1.830174000
C	4.049339000	0.171982000	2.648793000
C	1.023512000	1.559797000	2.375481000
C	1.642609000	0.359898000	2.807089000

C	-0.034531000	2.091825000	3.129545000
C	1.185338000	-0.257567000	3.980320000
C	-0.487820000	1.457126000	4.287656000
C	0.125996000	0.278177000	4.716499000
H	1.610054000	2.292865000	-4.914962000
H	0.228372000	4.261239000	-4.142816000
H	2.395494000	0.642096000	-3.203611000
H	-0.305412000	4.467320000	-1.696291000
H	6.846409000	2.546955000	-1.758060000
H	5.201587000	0.715212000	-1.335202000
H	0.433494000	-0.853924000	-1.979165000
H	-0.976591000	-2.895628000	-1.846221000
H	6.424359000	4.810651000	-0.715895000
H	-0.727466000	-4.430693000	0.153295000
H	-0.470414000	1.986922000	0.417805000
H	2.132622000	4.231580000	1.283221000
H	0.027746000	3.686291000	0.555550000
H	4.377940000	5.110914000	0.707466000
H	3.654720000	-1.930792000	1.369165000
H	4.863264000	-0.125167000	1.972334000
H	0.970048000	-3.812099000	1.914797000
H	2.911623000	3.114251000	2.395219000
H	4.103057000	1.255991000	2.806834000
H	2.612381000	-2.232428000	2.767205000
H	-0.509336000	3.019007000	2.802514000
H	4.200190000	-0.326665000	3.624522000
H	1.662810000	-1.177225000	4.323309000
H	-1.316561000	1.888787000	4.854666000
H	-0.215713000	-0.227116000	5.623339000
N	1.489327000	1.610227000	-1.609323000
N	3.961976000	1.868015000	-0.131290000
N	1.451439000	-1.206037000	-0.197018000
N	1.465320000	2.210618000	1.165265000
N	2.752043000	-0.194983000	2.048747000
Ni	2.355361000	0.525307000	-0.029654000

13 high spin

C	0.684983000	4.874456000	-3.617577000
C	0.725332000	-0.960778000	-3.457738000

C	1.433067000	3.903232000	-2.846020000	H	-1.253568000	3.300141000	1.482542000
C	1.451972000	0.112943000	-2.951030000	H	-1.387267000	1.523955000	1.716036000
C	5.235401000	3.568741000	-2.326914000	H	-0.450602000	2.515464000	2.885272000
C	0.575842000	-2.098301000	-2.662775000	N	2.030080000	3.126185000	-2.233566000
C	6.381202000	1.250425000	-1.280206000	N	2.010370000	0.099446000	-1.728495000
C	1.168603000	-2.119731000	-1.400800000	N	4.088125000	3.476018000	-0.154343000
C	6.418989000	-0.252013000	-1.006433000	N	1.425194000	2.048419000	0.400797000
C	4.980298000	4.112002000	-0.940808000	S	5.038972000	1.755624000	-2.443523000
C	5.657501000	5.253513000	-0.498909000	S	4.040311000	0.012050000	0.501789000
C	1.881581000	-1.000144000	-0.958449000	Ni	3.011710000	1.810189000	-0.939931000
C	5.077069000	-0.918796000	-0.709739000	13 low spin			
C	5.402324000	5.748092000	0.779615000	C	0.667137000	-0.489928000	-2.997218000
C	2.522716000	-1.001470000	0.409357000	C	1.457677000	0.462087000	-2.365592000
C	3.855013000	3.944109000	1.083735000	C	4.815433000	3.483229000	-2.083336000
C	4.486205000	5.076538000	1.590769000	C	0.616310000	-1.776818000	-2.458178000
C	0.469862000	2.203183000	1.032244000	C	6.274638000	1.192535000	-1.280060000
C	-0.726123000	2.397081000	1.826154000	C	1.351304000	-2.057646000	-1.307784000
H	0.784254000	4.647828000	-4.690235000	C	6.507745000	-0.317738000	-1.231272000
H	1.076910000	5.883846000	-3.419549000	C	4.769839000	3.969354000	-0.665078000
H	-0.377200000	4.831941000	-3.332001000	C	5.434642000	5.123015000	-0.249258000
H	0.294401000	-0.900397000	-4.458641000	C	2.117432000	-1.053007000	-0.705481000
H	1.596252000	1.016600000	-3.545624000	C	5.325024000	-1.180502000	-0.786196000
H	4.515532000	3.984531000	-3.049792000	C	5.367222000	5.503260000	1.091381000
H	6.241974000	3.843050000	-2.672251000	C	2.861298000	-1.334809000	0.576281000
H	0.015139000	-2.963657000	-3.024330000	C	4.008918000	3.570248000	1.507513000
H	6.851571000	-0.785009000	-1.868927000	C	4.649874000	4.707610000	1.986123000
H	7.330405000	1.581160000	-1.726445000	C	0.672888000	2.144948000	1.286868000
H	4.484715000	-1.029918000	-1.629565000	C	-0.518075000	2.388896000	2.070583000
H	6.379500000	5.739382000	-1.157855000	H	0.111231000	-0.220086000	-3.896521000
H	1.089519000	-2.996646000	-0.755380000	H	1.529747000	1.480924000	-2.752817000
H	6.234426000	1.814197000	-0.347516000	H	3.945027000	3.841230000	-2.658391000
H	7.113273000	-0.401449000	-0.163432000	H	5.725776000	3.805108000	-2.607975000
H	5.234514000	-1.922540000	-0.288795000	H	0.013667000	-2.555957000	-2.930676000
H	5.921523000	6.639016000	1.141039000	H	6.817850000	-0.682424000	-2.224036000
H	2.757594000	-2.026850000	0.727315000	H	7.070897000	1.684982000	-1.857456000
H	1.841749000	-0.571691000	1.161345000	H	4.567285000	-1.227230000	-1.583254000
H	3.138239000	3.388408000	1.690791000	H	6.004436000	5.703902000	-0.976341000
H	4.263220000	5.414133000	2.604433000	H	1.338420000	-3.053136000	-0.860635000

H	6.252615000	1.633273000	-0.274456000
H	7.367359000	-0.472004000	-0.558133000
H	5.661573000	-2.210635000	-0.597896000
H	5.882156000	6.403330000	1.435069000
H	2.956768000	-2.420814000	0.712909000
H	2.284403000	-0.947608000	1.433606000
H	3.445299000	2.918162000	2.175191000
H	4.584958000	4.954156000	3.047043000
H	-1.024971000	3.291719000	1.696200000
H	-1.196615000	1.526137000	1.987179000
H	-0.239041000	2.535989000	3.125376000
N	2.165579000	0.181248000	-1.254123000
N	4.056519000	3.217278000	0.208453000
N	1.627644000	1.954419000	0.666025000
S	4.695188000	1.654380000	-2.123523000
S	4.500278000	-0.537722000	0.731697000
Ni	3.137401000	1.645332000	-0.453631000

13a

C	0.348435000	-1.068817000	-2.684139000
C	1.097662000	-0.006584000	-2.184594000
C	4.584109000	3.759067000	-2.045067000
C	0.530005000	-2.334018000	-2.119236000
C	6.184520000	1.497256000	-1.658947000
C	1.451914000	-2.481129000	-1.082925000
C	6.431590000	-0.011838000	-1.674805000
C	4.626437000	4.066652000	-0.566093000
C	5.267589000	5.219408000	-0.094561000
C	2.162076000	-1.360742000	-0.632607000
C	5.278119000	-0.892874000	-1.193100000
C	5.259675000	5.494010000	1.273021000
C	3.140720000	-1.478332000	0.513173000
C	4.008118000	3.474610000	1.588575000
C	4.616173000	4.602022000	2.135010000
C	0.287075000	2.752547000	0.512617000
C	-0.971806000	3.322666000	0.960676000
H	-0.357004000	-0.903856000	-3.500983000
H	0.988643000	1.000272000	-2.596825000
H	3.644934000	4.138499000	-2.482449000

H	5.414142000	4.259047000	-2.565340000
H	-0.034966000	-3.195507000	-2.483870000
H	6.681501000	-0.342398000	-2.697141000
H	6.996740000	2.015858000	-2.190947000
H	4.464502000	-0.895371000	-1.933041000
H	5.763391000	5.888970000	-0.800626000
H	1.626347000	-3.453883000	-0.618013000
H	6.166615000	1.870102000	-0.624548000
H	7.328954000	-0.195741000	-1.060167000
H	5.625069000	-1.930249000	-1.069859000
H	5.752911000	6.388771000	1.660819000
H	3.501564000	-2.513194000	0.605466000
H	2.642018000	-1.217612000	1.462325000
H	3.494918000	2.749054000	2.225607000
H	4.587606000	4.770166000	3.213437000
H	-1.224279000	4.208514000	0.356900000
H	-1.777276000	2.578949000	0.858069000
H	-0.895145000	3.621303000	2.017919000
N	1.984682000	-0.146781000	-1.185251000
N	4.013543000	3.209949000	0.271378000
N	1.293395000	2.297368000	0.154511000
S	4.583668000	1.974755000	-2.437588000
S	4.557479000	-0.329418000	0.407379000
Ni	2.983737000	1.537175000	-0.448826000

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C	0.400940000	1.547041000	-4.001406000
C	0.447155000	0.174248000	-3.743372000
C	-0.243392000	2.387693000	-3.092871000
C	-0.150558000	-0.301346000	-2.577591000
C	-0.830872000	1.826884000	-1.953690000
C	-1.628854000	2.664886000	-0.979507000
C	-5.944176000	-0.193114000	-0.276894000
C	-6.322588000	1.078945000	0.159024000
C	-4.593439000	-0.532289000	-0.250109000
C	-1.817894000	-2.984221000	-0.008901000
C	-5.340060000	1.965731000	0.601086000
C	-1.624608000	-4.306174000	0.384096000
C	-4.006077000	1.550630000	0.604869000

C	1.377060000	-0.051676000	0.896118000	H	5.045288000	2.128515000	2.876338000
C	-2.883520000	2.428409000	1.105026000	H	0.139529000	-3.637322000	3.224608000
C	-0.408560000	2.523996000	1.162089000	H	0.659535000	-1.186338000	3.242511000
C	-0.923244000	-4.554655000	1.566413000	H	-1.014299000	-0.613401000	3.256297000
C	2.650205000	-0.032605000	1.721849000	H	5.952010000	0.004634000	3.825902000
C	-0.663507000	-2.178978000	1.853091000	N	-0.774624000	0.507025000	-1.708415000
C	3.183341000	-1.223139000	2.247087000	N	-3.652152000	0.319444000	0.183787000
C	3.342605000	1.169255000	1.954054000	N	-1.621399000	2.115730000	0.397083000
C	-0.060330000	1.503810000	2.236957000	N	-1.357443000	-1.954010000	0.717819000
C	-0.428278000	-3.478769000	2.305864000	N	0.095175000	0.149310000	1.647947000
C	4.360995000	-1.211194000	3.001317000	Cu	-1.575364000	0.026418000	0.305371000
C	-0.199019000	-0.947721000	2.595641000				
C	4.520188000	1.184348000	2.708517000	14a			
C	5.030117000	-0.005785000	3.238322000	C	0.497463000	1.696665000	-4.072794000
H	0.867098000	1.960064000	-4.899331000	C	0.487233000	0.311114000	-3.894953000
H	0.942412000	-0.518118000	-4.426756000	C	-0.176522000	2.497826000	-3.149851000
H	-0.295961000	3.465550000	-3.259798000	C	-0.195302000	-0.210299000	-2.797060000
H	-0.127146000	-1.366016000	-2.327581000	C	-0.849026000	1.896075000	-2.079518000
H	-2.670971000	2.686018000	-1.335837000	C	-1.667541000	2.719280000	-1.102039000
H	-1.275528000	3.708567000	-0.978242000	C	-6.078710000	-0.164016000	0.081072000
H	-2.351484000	-2.736781000	-0.929848000	C	-6.387338000	1.138251000	0.483944000
H	-6.678721000	-0.915063000	-0.637972000	C	-4.736364000	-0.519569000	-0.033679000
H	-7.372442000	1.381293000	0.146868000	C	-1.661395000	-3.208287000	-0.086694000
H	-4.255432000	-1.514768000	-0.586352000	C	-5.343110000	2.021336000	0.757792000
H	-2.014979000	-5.119042000	-0.230599000	C	-1.419237000	-4.491325000	0.401755000
H	-5.595174000	2.972553000	0.937318000	C	-4.019035000	1.581393000	0.630779000
H	1.425625000	0.728262000	0.125941000	C	1.424980000	-0.090074000	0.901668000
H	1.292694000	-1.014551000	0.374204000	C	-2.859524000	2.489250000	1.003507000
H	0.417150000	2.621188000	0.444464000	C	-0.406411000	2.514246000	0.991283000
H	-3.140731000	3.495372000	0.999874000	C	-0.749253000	-4.622731000	1.620239000
H	-0.560960000	3.518119000	1.615605000	C	2.663442000	-0.078557000	1.785824000
H	-0.751978000	-5.579506000	1.904365000	C	-0.636828000	-2.213509000	1.741732000
H	2.676827000	-2.172387000	2.051926000	C	3.132040000	-1.258952000	2.390123000
H	-2.741497000	2.235782000	2.179636000	C	3.371231000	1.113676000	2.023211000
H	2.964430000	2.101971000	1.527081000	C	-0.074128000	1.494285000	2.087357000
H	4.760584000	-2.147916000	3.399058000	C	-0.349120000	-3.467198000	2.293513000
H	0.849623000	1.823301000	2.770593000	C	4.258532000	-1.246720000	3.219715000
H	-0.862153000	1.448543000	2.986304000	C	-0.281320000	-0.930933000	2.473043000
				C	4.497883000	1.130849000	2.852609000

C	4.942886000	-0.049708000	3.457377000
H	1.027546000	2.148068000	-4.915208000
H	1.002091000	-0.358183000	-4.587252000
H	-0.187734000	3.585360000	-3.251975000
H	-0.218061000	-1.288878000	-2.615533000
H	-2.712010000	2.690485000	-1.456673000
H	-1.352622000	3.779529000	-1.160603000
H	-2.178919000	-3.063496000	-1.039441000
H	-6.859962000	-0.892449000	-0.145512000
H	-7.426793000	1.462225000	0.579340000
H	-4.452515000	-1.527863000	-0.349978000
H	-1.747434000	-5.363536000	-0.167365000
H	-5.542904000	3.048939000	1.070588000
H	1.535858000	0.676581000	0.121404000
H	1.360566000	-1.058415000	0.382339000
H	0.416047000	2.550681000	0.261478000
H	-3.178590000	3.545864000	0.904687000
H	-0.449817000	3.521963000	1.453936000
H	-0.535338000	-5.609943000	2.037455000
H	2.615104000	-2.203122000	2.196969000
H	-2.661315000	2.333919000	2.076537000
H	3.045389000	2.038578000	1.539020000
H	4.607298000	-2.177082000	3.676568000
H	0.799252000	1.872695000	2.653337000
H	-0.902014000	1.455512000	2.810532000
H	5.034704000	2.068682000	3.020681000
H	0.184283000	-3.527235000	3.244927000
H	0.459446000	-1.164934000	3.261981000
H	-1.191577000	-0.591854000	2.995605000
H	5.825028000	-0.038821000	4.103331000
N	-0.848794000	0.559468000	-1.911247000
N	-3.729916000	0.329360000	0.232037000
N	-1.639079000	2.203317000	0.262994000
N	-1.284574000	-2.094582000	0.565592000
N	0.132738000	0.139208000	1.576136000
Cu	-1.689735000	-0.175758000	-0.129393000

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C	1.556860000	3.956715000	-2.960743000
C	2.934816000	3.908399000	-2.744004000
C	-0.768414000	3.047298000	-2.439793000
C	-5.019316000	2.202989000	-2.255407000
C	0.729508000	3.084402000	-2.251258000
C	-3.742180000	2.749263000	-2.115311000
C	3.447439000	3.004881000	-1.809994000
C	-5.331883000	0.987373000	-1.639485000
C	-2.767191000	2.075858000	-1.368651000
C	2.561349000	2.168401000	-1.135651000
C	-4.365282000	0.313453000	-0.891073000
C	-3.078078000	0.849428000	-0.759745000
C	1.697381000	-1.368944000	-0.864367000
C	2.051345000	-2.704082000	-0.688784000
C	1.059203000	-3.613288000	-0.313588000
C	-1.944403000	-1.284708000	-0.330724000
C	-0.528680000	-1.805343000	-0.362008000
C	-0.248949000	-3.158458000	-0.148163000
C	-1.439636000	3.721264000	-0.169629000
C	-2.255756000	0.399549000	1.482774000
C	-0.982565000	0.431769000	2.298892000
C	1.245442000	1.066160000	2.392338000
C	-0.975940000	0.071349000	3.651012000
C	1.333569000	0.748771000	3.746831000
C	0.199725000	0.238069000	4.384534000
H	1.118259000	4.663740000	-3.667429000
H	3.601419000	4.579734000	-3.290636000
H	-1.014234000	2.304527000	-3.215167000
H	-5.771987000	2.730407000	-2.846137000
H	-1.132752000	4.027392000	-2.786380000
H	-3.500820000	3.702306000	-2.590350000
H	-6.331704000	0.558700000	-1.741262000
H	4.516549000	2.946250000	-1.598979000
H	-2.350841000	-1.410353000	-1.345691000
H	2.445369000	-0.625325000	-1.145162000
H	3.086975000	-3.015925000	-0.835397000
H	-2.043343000	4.573041000	-0.524783000

H	-4.612141000	-0.634549000	-0.409480000	C	-1.423979000	3.697734000	-0.132062000
H	2.913697000	1.452236000	-0.390189000	C	-2.251348000	0.406971000	1.468804000
H	1.302060000	-4.666055000	-0.150220000	C	-0.961542000	0.390666000	2.269269000
H	-1.052673000	-3.838963000	0.139448000	C	1.269269000	0.999136000	2.419923000
H	-0.410818000	4.059827000	0.011989000	C	-0.951804000	-0.072786000	3.591155000
H	-2.563465000	-1.894329000	0.343998000	C	1.358201000	0.572709000	3.744318000
H	-1.860687000	3.345334000	0.771594000	C	0.222005000	0.020353000	4.340259000
H	-2.737535000	1.384260000	1.584436000	H	0.903480000	4.940842000	-3.587678000
H	-2.957589000	-0.345344000	1.888663000	H	3.409170000	5.006795000	-3.417787000
H	2.109194000	1.459157000	1.848275000	H	-0.987266000	2.391215000	-3.199190000
H	-1.880855000	-0.324952000	4.116307000	H	-5.670198000	2.714164000	-3.023985000
H	2.272413000	0.896304000	4.284083000	H	-1.170213000	4.100315000	-2.755895000
H	0.231512000	-0.030800000	5.443242000	H	-3.424794000	3.688024000	-2.643182000
N	1.239402000	2.203587000	-1.365591000	H	-6.274588000	0.531339000	-1.948005000
N	-1.435675000	2.632458000	-1.179874000	H	4.560162000	3.304042000	-1.945170000
N	0.438484000	-0.932748000	-0.700488000	H	-2.349818000	-1.433519000	-1.325008000
N	-2.048387000	0.162746000	0.019543000	H	2.444364000	-0.896472000	-1.082234000
N	0.113777000	0.911159000	1.691888000	H	2.978015000	-3.271566000	-0.519738000
Cu	-0.218708000	1.061440000	-0.504786000	H	-1.988903000	4.600605000	-0.439756000
15a				H	-4.617352000	-0.635264000	-0.524835000
C	1.442738000	4.218397000	-2.970743000	H	3.155691000	1.636643000	-0.729583000
C	2.834204000	4.253709000	-2.873208000	H	1.105122000	-4.769432000	0.280858000
C	-0.777561000	3.127148000	-2.405004000	H	-1.210369000	-3.809351000	0.437987000
C	-4.948954000	2.187717000	-2.393431000	H	-0.390184000	3.996307000	0.097353000
C	0.728606000	3.242577000	-2.266138000	H	-2.648592000	-1.915619000	0.350144000
C	-3.682815000	2.734037000	-2.178222000	H	-1.874617000	3.307143000	0.789607000
C	3.474406000	3.315232000	-2.060023000	H	-2.681973000	1.414704000	1.579459000
C	-5.285280000	0.970480000	-1.795013000	H	-2.971296000	-0.290220000	1.937827000
C	-2.727610000	2.083094000	-1.377958000	H	2.138361000	1.431910000	1.915210000
C	2.692725000	2.382876000	-1.381055000	H	-1.860703000	-0.499249000	4.021745000
C	-4.350073000	0.314708000	-0.993216000	H	2.299828000	0.669140000	4.288736000
C	-3.066023000	0.846192000	-0.776234000	H	0.249765000	-0.335840000	5.373094000
C	1.658239000	-1.577203000	-0.742014000	N	1.351722000	2.342648000	-1.481460000
C	1.954688000	-2.902103000	-0.426740000	N	-1.426765000	2.664600000	-1.176056000
C	0.915848000	-3.727124000	0.012005000	N	0.419832000	-1.064143000	-0.651959000
C	-1.997977000	-1.292919000	-0.290582000	N	-2.111925000	0.133037000	0.032009000
C	-0.587929000	-1.856993000	-0.248605000	N	0.140743000	0.909470000	1.698733000
C	-0.371078000	-3.195613000	0.102602000	Cu	0.169605000	1.024566000	-0.425858000

