Electronic Supplementary Information for Dalton Transactions

Ligands that Enforce Unnatural Stereospinomers

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Supporting Information

Atomic coordinates of optimized structures

d^4 Ions

Cr^{II}(**2**), S = 0

1	Cr	4.835	0.155	1.543
2	N	4.592	0.812	3.433
3	C	5.935	0.906	4.105
4	H	5.783	1.064	5.177
5	H	6.432	1.800	3.727
6	C	6.849	-0.314	3.896
7	H	6.368	-1.226	4.251
8	H	7.694	-0.173	4.575
9	C	7.472	-0.524	2.505
10	H	7.958	0.399	2.191
11	H	8.261	-1.280	2.580
12	N	6.527	-0.933	1.402
13	C	7.159	-0.703	0.055
14	H	6.590	-1.273	-0.680
15	H	8.168	-1.125	0.062
16	C	7.229	0.770	-0.384
17	H	7.856	0.785	-1.280
18	H	7.784	1.366	0.342
19	C	5.920	1.472	-0.789
20	H	6.162	2.417	-1.286
21	H	5.401	0.859	-1.525
22	N	4.944	1.760	0.326
23	C	3.577	2.051	-0.231
24	H	3.675	2.779	-1.042
25	H	2.996	2.538	0.553
26	C	2.810	0.820	-0.746
27	H	1.933	1.214	-1.268
28	H	3.377	0.305	-1.523
29	C	2.256	-0.180	0.285
30	H	1.554	-0.854	-0.215
31	H	1.684	0.364	1.037
32	N	3.277	-1.017	1.017
33	C	2.673	-1.629	2.252
34	H	3.328	-2.438	2.574
35	H	1.717	-2.090	1.985
36	C	2.457	-0.651	3.420
37	H	1.864	-1.197	4.160
38	H	1.814	0.178	3.121
39	C	3.694	-0.144	4.180
40	H	3.369	0.342	5.106
41	H	4.304	-0.998	4.476
42	C	3.928	2.150	3.298
43	H	3.736	2.566	4.293
44	H	2.948	1.955	2.863
45	C	4.649	3.232	2.460

46	H	5.349	3.780	3.095
47	H	3.875	3.961	2.214
48	C	5.453	2.879	1.185
49	H	5.545	3.789	0.581
50	H	6.470	2.605	1.467
51	C	6.092	-2.356	1.591
52	H	5.720	-2.421	2.613
53	H	6.966	-3.015	1.547
54	C	5.022	-2.920	0.625
55	H	4.621	-3.800	1.132
56	H	5.508	-3.316	-0.269
57	C	3.853	-2.051	0.097
58	H	4.182	-1.512	-0.792
59	H	3.057	-2.724	-0.240

Cr^{II}(**2**), S = 1

1	Cr	4.829	0.157	1.535
2	N	4.590	0.920	3.415
3	C	5.951	0.932	4.057
4	H	5.825	1.112	5.130
5	H	6.496	1.788	3.658
6	C	6.789	-0.349	3.864
7	H	6.249	-1.228	4.218
8	H	7.631	-0.253	4.556
9	C	7.424	-0.618	2.489
10	H	7.947	0.279	2.162
11	H	8.184	-1.398	2.598
12	N	6.484	-1.029	1.378
13	C	7.096	-0.712	0.038
14	H	6.506	-1.225	-0.723
15	H	8.098	-1.151	0.006
16	C	7.201	0.788	-0.312
17	H	7.850	0.834	-1.192
18	H	7.753	1.332	0.456
19	C	5.925	1.553	-0.712
20	H	6.214	2.503	-1.173
21	H	5.400	0.986	-1.478
22	N	4.940	1.849	0.397
23	C	3.559	2.046	-0.172
24	H	3.619	2.796	-0.968
25	H	2.937	2.477	0.614
26	C	2.878	0.779	-0.735
27	H	2.009	1.143	-1.292
28	H	3.502	0.303	-1.494
29	C	2.317	-0.269	0.245
30	H	1.647	-0.939	-0.303
31	H	1.704	0.239	0.988
32	N	3.327	-1.117	0.986
33	C	2.724	-1.645	2.261
34	H	3.384	-2.426	2.639
35	H	1.772	-2.129	2.019
36	C	2.478	-0.594	3.365
37	H	1.857	-1.098	4.111
38	H	1.847	0.218	2.998
39	C	3.680	-0.039	4.151
40	H	3.309	0.467	5.047

41	H	4.289	-0.872	4.496
42	C	3.965	2.278	3.366
43	H	3.870	2.671	4.384
44	H	2.947	2.122	3.008
45	C	4.645	3.364	2.500
46	H	5.360	3.919	3.111
47	H	3.856	4.084	2.277
48	C	5.408	3.022	1.198
49	H	5.413	3.916	0.564
50	H	6.451	2.817	1.437
51	C	6.125	-2.475	1.520
52	H	5.817	-2.602	2.558
53	H	7.026	-3.085	1.396
54	C	5.031	-3.052	0.590
55	H	4.656	-3.935	1.111
56	H	5.497	-3.444	-0.316
57	C	3.836	-2.203	0.094
58	H	4.109	-1.714	-0.841
59	H	3.015	-2.886	-0.153

Cr^{II}(**2**), S = 2

1	Cr	4.831	0.158	1.544
2	N	4.611	0.657	3.536
3	C	5.938	0.779	4.228
4	H	5.767	0.852	5.307
5	H	6.378	1.726	3.918
6	C	6.938	-0.355	3.955
7	H	6.523	-1.316	4.264
8	H	7.772	-0.188	4.643
9	C	7.580	-0.451	2.556
10	H	8.046	0.503	2.304
11	H	8.384	-1.195	2.597
12	N	6.657	-0.804	1.426
13	C	7.298	-0.614	0.081
14	H	6.773	-1.261	-0.623
15	H	8.329	-0.977	0.127
16	C	7.295	0.824	-0.461
17	H	7.926	0.809	-1.353
18	H	7.816	1.493	0.226
19	C	5.955	1.432	-0.921
20	H	6.161	2.379	-1.433
21	H	5.489	0.771	-1.653
22	N	4.938	1.681	0.156
23	C	3.582	2.012	-0.398
24	H	3.705	2.683	-1.254
25	H	3.050	2.580	0.366
26	C	2.722	0.810	-0.824
27	H	1.854	1.233	-1.336
28	H	3.232	0.229	-1.594
29	C	2.138	-0.109	0.270
30	H	1.427	-0.795	-0.202
31	H	1.572	0.491	0.984
32	N	3.131	-0.912	1.059
33	C	2.520	-1.556	2.269
34	H	3.137	-2.419	2.524
35	H	1.534	-1.948	2.002

36	C	2.384	-0.653	3.505
37	H	1.788	-1.221	4.225
38	H	1.769	0.220	3.277
39	C	3.662	-0.249	4.267
40	H	3.367	0.235	5.204
41	H	4.221	-1.147	4.538
42	C	3.967	2.003	3.316
43	H	3.805	2.479	4.290
44	H	2.975	1.803	2.915
45	C	4.660	3.061	2.409
46	H	5.379	3.627	3.006
47	H	3.865	3.776	2.192
48	C	5.437	2.752	1.095
49	H	5.513	3.695	0.543
50	H	6.457	2.476	1.355
51	C	6.137	-2.208	1.609
52	H	5.794	-2.268	2.640
53	H	6.977	-2.908	1.531
54	C	5.011	-2.751	0.683
55	H	4.638	-3.629	1.215
56	H	5.460	-3.154	-0.227
57	C	3.802	-1.921	0.161
58	H	4.120	-1.371	-0.723
59	H	3.051	-2.639	-0.186

Mn^{III}(**2**), S = 0

1	Mn	4.835	0.156	1.544
2	N	4.591	0.787	3.373
3	C	5.929	0.922	4.077
4	H	5.719	1.082	5.138
5	H	6.410	1.827	3.712
6	C	6.862	-0.277	3.904
7	H	6.421	-1.195	4.294
8	H	7.718	-0.092	4.560
9	C	7.450	-0.476	2.507
10	H	7.928	0.444	2.172
11	H	8.228	-1.242	2.542
12	N	6.470	-0.898	1.416
13	C	7.127	-0.714	0.057
14	H	6.567	-1.302	-0.668
15	H	8.123	-1.157	0.120
16	C	7.229	0.738	-0.412
17	H	7.821	0.717	-1.333
18	H	7.822	1.346	0.272
19	C	5.913	1.421	-0.785
20	H	6.118	2.380	-1.266
21	H	5.374	0.813	-1.511
22	N	4.950	1.705	0.365
23	C	3.582	2.049	-0.200
24	H	3.740	2.778	-0.999
25	H	3.016	2.556	0.579
26	C	2.792	0.854	-0.734
27	H	1.900	1.272	-1.212
28	H	3.316	0.348	-1.546
29	C	2.273	-0.136	0.310
30	H	1.583	-0.839	-0.162

31	H	1.708	0.394	1.075
32	N	3.329	-0.971	1.026
33	C	2.706	-1.632	2.245
34	H	3.354	-2.452	2.549
35	H	1.763	-2.078	1.921
36	C	2.461	-0.692	3.426
37	H	1.906	-1.275	4.167
38	H	1.784	0.122	3.165
39	C	3.708	-0.183	4.151
40	H	3.416	0.328	5.071
41	H	4.334	-1.025	4.444
42	C	3.897	2.123	3.238
43	H	3.678	2.494	4.244
44	H	2.929	1.923	2.779
45	C	4.648	3.217	2.456
46	H	5.326	3.756	3.120
47	H	3.892	3.954	2.180
48	C	5.487	2.827	1.225
49	H	5.613	3.708	0.589
50	H	6.493	2.533	1.527
51	C	6.039	-2.331	1.633
52	H	5.646	-2.383	2.648
53	H	6.934	-2.958	1.626
54	C	5.020	-2.905	0.631
55	H	4.585	-3.779	1.120
56	H	5.535	-3.309	-0.242
57	C	3.906	-1.997	0.077
58	H	4.262	-1.445	-0.793
59	H	3.085	-2.623	-0.283

Mn^{III}(**2**), S = 1

1	Mn	4.8250	0.3310	1.5950
2	N	4.5730	0.6740	3.5270
3	C	5.8990	0.8280	4.2390
4	H	5.7030	0.8820	5.3120
5	H	6.3320	1.7850	3.9490
6	C	6.8780	-0.3060	3.9340
7	H	6.4910	-1.2680	4.2720
8	H	7.7590	-0.1310	4.5580
9	C	7.4070	-0.3780	2.4960
10	H	7.8170	0.5870	2.1990
11	H	8.2330	-1.0920	2.4580
12	N	6.4280	-0.8140	1.4010
13	C	7.0960	-0.6670	0.0430
14	H	6.5240	-1.2630	-0.6650
15	H	8.0790	-1.1360	0.1300
16	C	7.2570	0.7560	-0.4910
17	H	7.8720	0.6670	-1.3920
18	H	7.8560	1.3780	0.1760
19	C	5.9710	1.4570	-0.9300
20	H	6.2110	2.4220	-1.3850
21	H	5.4630	0.8640	-1.6890
22	N	4.9740	1.7010	0.1750
23	C	3.6160	2.0660	-0.3810
24	H	3.7660	2.7180	-1.2450
25	H	3.0870	2.6530	0.3690

26	C	2.7820	0.8450	-0.7760
27	H	1.8680	1.2310	-1.2380
28	H	3.2650	0.2720	-1.5680
29	C	2.3080	-0.0550	0.3710
30	H	1.5680	-0.7600	-0.0150
31	H	1.8030	0.5390	1.1320
32	N	3.3640	-0.9080	1.0840
33	C	2.7290	-1.5980	2.2810
34	H	3.3850	-2.4160	2.5680
35	H	1.8010	-2.0500	1.9200
36	C	2.4290	-0.7240	3.4980
37	H	1.8570	-1.3550	4.1840
38	H	1.7460	0.0920	3.2570
39	C	3.6450	-0.2390	4.2880
40	H	3.3170	0.2890	5.1870
41	H	4.2390	-1.0910	4.6180
42	C	3.8930	2.0060	3.2340
43	H	3.6020	2.4560	4.1870
44	H	2.9500	1.7630	2.7380
45	C	4.6590	3.0820	2.4160
46	H	5.3460	3.6230	3.0700
47	H	3.8960	3.8150	2.1500
48	C	5.5090	2.7310	1.1630
49	H	5.6990	3.6590	0.6170
50	H	6.4970	2.3780	1.4710
51	C	6.0300	-2.2510	1.6380
52	H	5.6430	-2.2990	2.6530
53	H	6.9400	-2.8570	1.6260
54	C	5.0160	-2.8480	0.6520
55	H	4.5890	-3.7210	1.1490
56	H	5.5250	-3.2530	-0.2240
57	C	3.9060	-1.9330	0.1190
58	H	4.2550	-1.3830	-0.7520
59	H	3.0680	-2.5470	-0.2220

Mn^{III}(**2**), S = 2

1	Mn	4.832	0.158	1.543
2	N	4.608	0.643	3.492
3	C	5.938	0.802	4.199
4	H	5.730	0.882	5.269
5	H	6.361	1.755	3.887
6	C	6.952	-0.320	3.960
7	H	6.569	-1.282	4.301
8	H	7.790	-0.112	4.631
9	C	7.568	-0.416	2.558
10	H	8.035	0.530	2.284
11	H	8.360	-1.170	2.570
12	N	6.618	-0.782	1.438
13	C	7.267	-0.629	0.078
14	H	6.744	-1.290	-0.611
15	H	8.291	-1.004	0.162
16	C	7.290	0.794	-0.487
17	H	7.894	0.745	-1.398
18	H	7.845	1.471	0.165
19	C	5.946	1.393	-0.921
20	H	6.127	2.349	-1.420

21	H	5.460	0.741	-1.648
22	N	4.944	1.646	0.185
23	C	3.580	2.015	-0.362
24	H	3.740	2.689	-1.208
25	H	3.064	2.589	0.406
26	C	2.704	0.840	-0.808
27	H	1.828	1.286	-1.285
28	H	3.181	0.269	-1.606
29	C	2.147	-0.076	0.292
30	H	1.445	-0.783	-0.159
31	H	1.586	0.508	1.022
32	N	3.168	-0.884	1.062
33	C	2.555	-1.568	2.265
34	H	3.172	-2.434	2.500
35	H	1.577	-1.950	1.961
36	C	2.394	-0.693	3.512
37	H	1.831	-1.297	4.230
38	H	1.746	0.162	3.317
39	C	3.677	-0.281	4.247
40	H	3.405	0.223	5.179
41	H	4.256	-1.164	4.520
42	C	3.930	1.985	3.253
43	H	3.711	2.423	4.232
44	H	2.961	1.765	2.807
45	C	4.662	3.056	2.407
46	H	5.362	3.609	3.037
47	H	3.886	3.784	2.161
48	C	5.477	2.709	1.137
49	H	5.611	3.629	0.561
50	H	6.480	2.391	1.421
51	C	6.075	-2.187	1.657
52	H	5.682	-2.206	2.673
53	H	6.926	-2.875	1.657
54	C	5.012	-2.743	0.680
55	H	4.609	-3.622	1.186
56	H	5.500	-3.142	-0.212
57	C	3.853	-1.875	0.132
58	H	4.202	-1.299	-0.725
59	H	3.084	-2.548	-0.260

Mo^{II}(**2**), S = 0

1	Mo	4.837	0.153	1.542
2	N	4.585	0.851	3.506
3	C	5.954	0.902	4.139
4	H	5.843	1.054	5.217
5	H	6.456	1.791	3.753
6	C	6.845	-0.341	3.898
7	H	6.333	-1.246	4.231
8	H	7.679	-0.234	4.599
9	C	7.512	-0.572	2.521
10	H	8.011	0.345	2.206
11	H	8.296	-1.328	2.634
12	N	6.594	-0.989	1.394
13	C	7.191	-0.701	0.039
14	H	6.615	-1.265	-0.696
15	H	8.209	-1.103	0.006

16	C	7.231	0.792	-0.368
17	H	7.886	0.830	-1.244
18	H	7.763	1.378	0.385
19	C	5.938	1.518	-0.809
20	H	6.213	2.450	-1.313
21	H	5.419	0.909	-1.550
22	N	4.943	1.832	0.285
23	C	3.554	2.064	-0.259
24	H	3.609	2.789	-1.078
25	H	2.973	2.539	0.533
26	C	2.812	0.801	-0.761
27	H	1.944	1.181	-1.310
28	H	3.402	0.287	-1.521
29	C	2.224	-0.216	0.249
30	H	1.524	-0.870	-0.281
31	H	1.639	0.319	0.997
32	N	3.222	-1.074	0.993
33	C	2.642	-1.641	2.265
34	H	3.303	-2.445	2.593
35	H	1.678	-2.108	2.041
36	C	2.449	-0.625	3.417
37	H	1.826	-1.144	4.153
38	H	1.829	0.211	3.089
39	C	3.668	-0.115	4.221
40	H	3.309	0.356	5.142
41	H	4.277	-0.967	4.528
42	C	3.947	2.201	3.358
43	H	3.790	2.650	4.345
44	H	2.951	2.009	2.957
45	C	4.650	3.269	2.470
46	H	5.366	3.826	3.079
47	H	3.862	3.993	2.250
48	C	5.428	2.952	1.158
49	H	5.483	3.880	0.576
50	H	6.459	2.701	1.411
51	C	6.138	-2.409	1.558
52	H	5.791	-2.485	2.589
53	H	6.995	-3.088	1.480
54	C	5.026	-2.955	0.614
55	H	4.647	-3.839	1.131
56	H	5.489	-3.349	-0.293
57	C	3.820	-2.115	0.094
58	H	4.125	-1.581	-0.806
59	H	3.044	-2.821	-0.227

Mo^{II}(**2**), S = 1

1	Mo	4.819	0.406	1.622
2	N	4.530	0.738	3.694
3	C	5.896	0.767	4.321
4	H	5.798	0.774	5.410
5	H	6.367	1.713	4.049
6	C	6.807	-0.408	3.902
7	H	6.332	-1.356	4.159
8	H	7.676	-0.350	4.563
9	C	7.410	-0.462	2.471
10	H	7.822	0.514	2.215

11	H	8.254	-1.159	2.495
12	N	6.502	-0.881	1.328
13	C	7.165	-0.641	-0.005
14	H	6.596	-1.206	-0.744
15	H	8.167	-1.082	0.024
16	C	7.291	0.824	-0.467
17	H	7.972	0.799	-1.323
18	H	7.824	1.418	0.278
19	C	6.039	1.569	-0.969
20	H	6.348	2.511	-1.435
21	H	5.554	0.978	-1.747
22	N	5.002	1.840	0.074
23	C	3.618	2.056	-0.472
24	H	3.673	2.675	-1.372
25	H	3.058	2.635	0.265
26	C	2.855	0.754	-0.800
27	H	1.961	1.073	-1.344
28	H	3.417	0.166	-1.526
29	C	2.311	-0.145	0.343
30	H	1.559	-0.812	-0.091
31	H	1.791	0.474	1.074
32	N	3.302	-1.009	1.106
33	C	2.662	-1.610	2.330
34	H	3.316	-2.417	2.663
35	H	1.716	-2.076	2.034
36	C	2.385	-0.656	3.508
37	H	1.737	-1.218	4.188
38	H	1.764	0.183	3.187
39	C	3.556	-0.168	4.382
40	H	3.154	0.332	5.270
41	H	4.128	-1.027	4.736
42	C	3.946	2.107	3.412
43	H	3.815	2.651	4.351
44	H	2.939	1.923	3.036
45	C	4.668	3.135	2.433
46	H	5.403	3.689	3.019
47	H	3.868	3.852	2.238
48	C	5.444	2.902	1.061
49	H	5.450	3.878	0.567
50	H	6.487	2.680	1.287
51	C	6.148	-2.327	1.506
52	H	5.869	-2.434	2.551
53	H	7.046	-2.938	1.362
54	C	5.020	-2.922	0.636
55	H	4.668	-3.796	1.187
56	H	5.442	-3.328	-0.285
57	C	3.818	-2.071	0.181
58	H	4.089	-1.554	-0.735
59	H	2.999	-2.752	-0.077

Mo^{II}(**2**), S = 2

1	Mo	4.9040	0.2880	1.5460
2	N	4.7740	0.6160	3.6910
3	C	6.0460	0.2360	4.4150
4	H	5.8080	0.0400	5.4630
5	H	6.7080	1.1010	4.4020

6	C	6.8050	-0.9710	3.8370
7	H	6.1670	-1.8560	3.7980
8	H	7.5670	-1.2150	4.5830
9	C	7.5770	-0.7770	2.5150
10	H	8.0870	0.1880	2.5360
11	H	8.3520	-1.5470	2.4480
12	N	6.7690	-0.8230	1.2440
13	C	7.5550	-0.2330	0.0910
14	H	7.2390	-0.7440	-0.8170
15	H	8.6120	-0.4730	0.2340
16	C	7.4070	1.2840	-0.1260
17	H	8.2400	1.5770	-0.7700
18	H	7.5740	1.8240	0.8100
19	C	6.1340	1.7830	-0.8410
20	H	6.3120	2.7920	-1.2280
21	H	5.9250	1.1440	-1.7000
22	N	4.8920	1.8040	0.0050
23	C	3.6240	1.8260	-0.8130
24	H	3.8360	2.3280	-1.7600
25	H	2.9020	2.4510	-0.2870
26	C	2.9930	0.4530	-1.0940
27	H	2.2600	0.6170	-1.8880
28	H	3.7330	-0.2210	-1.5330
29	C	2.2190	-0.2370	0.0500
30	H	1.5450	-0.9840	-0.3840
31	H	1.5880	0.4990	0.5540
32	N	3.0550	-0.9040	1.1040
33	C	2.2510	-1.1920	2.3460
34	H	2.6050	-2.1370	2.7590
35	H	1.2110	-1.3570	2.0530
36	C	2.3010	-0.1250	3.4530
37	H	1.4980	-0.3840	4.1490
38	H	2.0200	0.8570	3.0660
39	C	3.5760	-0.0480	4.3150
40	H	3.3430	0.4780	5.2470
41	H	3.8810	-1.0590	4.5880
42	C	4.6110	2.1370	3.5930
43	H	5.5850	2.5790	3.7940
44	H	3.9470	2.4500	4.4020
45	C	4.0520	2.7960	2.2810
46	H	3.8590	3.8230	2.6060
47	H	3.0600	2.4150	2.0280
48	C	4.9200	2.9640	0.9910
49	H	4.5710	3.8560	0.4650
50	H	5.9570	3.1480	1.2670
51	C	6.3190	-2.2460	0.9170
52	H	7.0360	-2.9330	1.3730
53	H	6.4140	-2.3730	-0.1600
54	C	4.8990	-2.7150	1.3240
55	H	4.7460	-2.6460	2.4020
56	H	4.9210	-3.7910	1.1230
57	C	3.6600	-2.1810	0.5660
58	H	3.9160	-2.0180	-0.4800
59	H	2.8820	-2.9510	0.5780

Fe^{IV}(**2**), S = 0

1	Fe	4.835	0.156	1.545
2	N	4.585	0.781	3.354
3	C	5.932	0.934	4.061
4	H	5.689	1.092	5.117
5	H	6.399	1.848	3.704
6	C	6.873	-0.255	3.913
7	H	6.459	-1.176	4.326
8	H	7.735	-0.041	4.556
9	C	7.443	-0.444	2.513
10	H	7.916	0.470	2.161
11	H	8.217	-1.217	2.529
12	N	6.453	-0.890	1.424
13	C	7.107	-0.720	0.051
14	H	6.553	-1.323	-0.664
15	H	8.100	-1.173	0.146
16	C	7.232	0.720	-0.430
17	H	7.805	0.677	-1.364
18	H	7.848	1.334	0.228
19	C	5.911	1.386	-0.790
20	H	6.098	2.354	-1.264
21	H	5.356	0.783	-1.506
22	N	4.956	1.690	0.378
23	C	3.578	2.050	-0.180
24	H	3.769	2.779	-0.975
25	H	3.024	2.570	0.598
26	C	2.778	0.876	-0.730
27	H	1.878	1.309	-1.182
28	H	3.275	0.378	-1.563
29	C	2.277	-0.104	0.323
30	H	1.592	-0.824	-0.137
31	H	1.718	0.412	1.100
32	N	3.346	-0.958	1.024
33	C	2.727	-1.638	2.247
34	H	3.371	-2.465	2.535
35	H	1.788	-2.075	1.890
36	C	2.460	-0.717	3.431
37	H	1.927	-1.324	4.171
38	H	1.760	0.085	3.194
39	C	3.712	-0.214	4.137
40	H	3.435	0.312	5.056
41	H	4.354	-1.044	4.428
42	C	3.876	2.114	3.198
43	H	3.637	2.463	4.210
44	H	2.914	1.908	2.729
45	C	4.648	3.214	2.455
46	H	5.313	3.749	3.136
47	H	3.905	3.959	2.163
48	C	5.510	2.800	1.254
49	H	5.659	3.667	0.601
50	H	6.511	2.494	1.561
51	C	6.002	-2.321	1.659
52	H	5.600	-2.363	2.672
53	H	6.908	-2.936	1.679
54	C	5.019	-2.902	0.632
55	H	4.564	-3.773	1.108
56	H	5.552	-3.312	-0.228
57	C	3.943	-1.968	0.061

58	H	4.309	-1.406	-0.799
59	H	3.109	-2.569	-0.318

Fe^{IV}(**2**), S = 1

1	Fe	4.825	0.334	1.595
2	N	4.618	0.710	3.530
3	C	5.943	0.857	4.240
4	H	5.735	0.918	5.313
5	H	6.387	1.807	3.944
6	C	6.909	-0.302	3.976
7	H	6.518	-1.253	4.341
8	H	7.789	-0.115	4.601
9	C	7.445	-0.406	2.547
10	H	7.882	0.535	2.217
11	H	8.257	-1.146	2.541
12	N	6.497	-0.878	1.449
13	C	7.087	-0.668	0.060
14	H	6.517	-1.280	-0.634
15	H	8.089	-1.112	0.124
16	C	7.224	0.763	-0.466
17	H	7.833	0.674	-1.373
18	H	7.828	1.391	0.189
19	C	5.928	1.443	-0.913
20	H	6.168	2.403	-1.381
21	H	5.417	0.844	-1.667
22	N	4.926	1.725	0.189
23	C	3.569	2.084	-0.369
24	H	3.730	2.742	-1.229
25	H	3.030	2.662	0.381
26	C	2.748	0.867	-0.811
27	H	1.834	1.264	-1.265
28	H	3.232	0.316	-1.619
29	C	2.271	-0.056	0.313
30	H	1.544	-0.762	-0.112
31	H	1.745	0.501	1.088
32	N	3.297	-0.943	1.007
33	C	2.737	-1.589	2.266
34	H	3.393	-2.414	2.531
35	H	1.787	-2.035	1.940
36	C	2.462	-0.702	3.481
37	H	1.896	-1.336	4.174
38	H	1.772	0.112	3.255
39	C	3.690	-0.237	4.266
40	H	3.362	0.280	5.175
41	H	4.289	-1.089	4.588
42	C	3.907	2.031	3.223
43	H	3.589	2.453	4.185
44	H	2.971	1.767	2.722
45	C	4.656	3.120	2.427
46	H	5.343	3.667	3.077
47	H	3.890	3.854	2.163
48	C	5.493	2.740	1.187
49	H	5.719	3.652	0.621
50	H	6.473	2.359	1.490
51	C	6.022	-2.286	1.663
52	H	5.647	-2.342	2.683

53	H	6.918	-2.922	1.643
54	C	5.017	-2.860	0.649
55	H	4.577	-3.734	1.135
56	H	5.536	-3.271	-0.220
57	C	3.919	-1.945	0.078
58	H	4.263	-1.395	-0.797
59	H	3.101	-2.585	-0.280

Fe^{IV}(**2**), S = 2

1	Fe	4.832	0.157	1.541
2	N	4.602	0.696	3.478
3	C	5.949	0.847	4.159
4	H	5.740	0.935	5.232
5	H	6.380	1.792	3.836
6	C	6.941	-0.303	3.948
7	H	6.552	-1.251	4.323
8	H	7.789	-0.085	4.607
9	C	7.540	-0.428	2.545
10	H	8.025	0.499	2.238
11	H	8.323	-1.197	2.571
12	N	6.594	-0.833	1.429
13	C	7.220	-0.658	0.057
14	H	6.689	-1.307	-0.635
15	H	8.244	-1.040	0.140
16	C	7.275	0.777	-0.480
17	H	7.862	0.723	-1.403
18	H	7.861	1.433	0.167
19	C	5.936	1.398	-0.888
20	H	6.135	2.362	-1.374
21	H	5.422	0.778	-1.623
22	N	4.946	1.687	0.228
23	C	3.567	2.031	-0.307
24	H	3.729	2.712	-1.151
25	H	3.043	2.592	0.465
26	C	2.717	0.848	-0.787
27	H	1.831	1.293	-1.252
28	H	3.198	0.306	-1.603
29	C	2.177	-0.088	0.298
30	H	1.485	-0.798	-0.171
31	H	1.602	0.461	1.044
32	N	3.198	-0.928	1.045
33	C	2.602	-1.598	2.270
34	H	3.224	-2.457	2.514
35	H	1.624	-1.983	1.961
36	C	2.412	-0.702	3.499
37	H	1.865	-1.313	4.226
38	H	1.738	0.132	3.296
39	C	3.688	-0.262	4.222
40	H	3.402	0.252	5.148
41	H	4.292	-1.121	4.516
42	C	3.904	2.033	3.219
43	H	3.641	2.438	4.205
44	H	2.950	1.798	2.745
45	C	4.658	3.116	2.427
46	H	5.343	3.662	3.081
47	H	3.896	3.854	2.163

48	C	5.497	2.743	1.190
49	H	5.662	3.647	0.590
50	H	6.492	2.408	1.483
51	C	6.035	-2.238	1.667
52	H	5.625	-2.238	2.678
53	H	6.901	-2.911	1.708
54	C	5.015	-2.802	0.663
55	H	4.590	-3.681	1.156
56	H	5.524	-3.208	-0.214
57	C	3.896	-1.907	0.100
58	H	4.259	-1.316	-0.743
59	H	3.109	-2.547	-0.318

Re^{III}(**2**), S = 0

1	Re	4.8340	0.1530	1.5420
2	N	4.5830	0.8330	3.4600
3	C	5.9550	0.9120	4.1240
4	H	5.7930	1.0620	5.1940
5	H	6.4460	1.8120	3.7520
6	C	6.8570	-0.3190	3.9070
7	H	6.3770	-1.2290	4.2710
8	H	7.7010	-0.1780	4.5900
9	C	7.5010	-0.5420	2.5260
10	H	8.0010	0.3680	2.1970
11	H	8.2710	-1.3130	2.6050
12	N	6.5500	-0.9620	1.4020
13	C	7.1770	-0.7050	0.0340
14	H	6.6130	-1.2850	-0.6980
15	H	8.1860	-1.1220	0.0530
16	C	7.2400	0.7760	-0.3900
17	H	7.8720	0.7910	-1.2840
18	H	7.8000	1.3690	0.3350
19	C	5.9410	1.4910	-0.8120
20	H	6.1890	2.4420	-1.2890
21	H	5.4110	0.8960	-1.5540
22	N	4.9490	1.7920	0.3140
23	C	3.5540	2.0630	-0.2430
24	H	3.6610	2.7860	-1.0560
25	H	2.9810	2.5580	0.5410
26	C	2.8000	0.8210	-0.7570
27	H	1.9230	1.2160	-1.2810
28	H	3.3640	0.3130	-1.5400
29	C	2.2280	-0.1880	0.2600
30	H	1.5450	-0.8700	-0.2500
31	H	1.6430	0.3350	1.0170
32	N	3.2580	-1.0440	1.0010
33	C	2.6570	-1.6460	2.2690
34	H	3.3100	-2.4610	2.5840
35	H	1.7010	-2.0980	1.9960
36	C	2.4450	-0.6510	3.4270
37	H	1.8480	-1.1960	4.1660
38	H	1.7980	0.1730	3.1250
39	C	3.6710	-0.1410	4.2090
40	H	3.3380	0.3600	5.1210
41	H	4.2900	-0.9820	4.5210
42	C	3.9260	2.1920	3.3230

43	H	3.7600	2.6020	4.3230
44	H	2.9340	1.9990	2.9120
45	C	4.6490	3.2680	2.4710
46	H	5.3530	3.8180	3.0980
47	H	3.8720	3.9960	2.2330
48	C	5.4510	2.9280	1.1850
49	H	5.5160	3.8310	0.5720
50	H	6.4790	2.6710	1.4460
51	C	6.1050	-2.4010	1.5790
52	H	5.7530	-2.4730	2.6090
53	H	6.9850	-3.0480	1.5170
54	C	5.0250	-2.9540	0.6120
55	H	4.6320	-3.8380	1.1190
56	H	5.5050	-3.3470	-0.2860
57	C	3.8440	-2.0950	0.0810
58	H	4.1510	-1.5600	-0.8190
59	H	3.0430	-2.7700	-0.2320

Re^{III}(**2**), S = 1

1	Re	4.8220	0.3610	1.6080
2	N	4.5280	0.7140	3.6350
3	C	5.8940	0.7850	4.2990
4	H	5.7480	0.7990	5.3810
5	H	6.3450	1.7420	4.0320
6	C	6.8290	-0.3740	3.9120
7	H	6.3990	-1.3330	4.2060
8	H	7.7080	-0.2670	4.5560
9	C	7.4110	-0.4300	2.4790
10	H	7.8240	0.5390	2.2020
11	H	8.2430	-1.1380	2.4740
12	N	6.4760	-0.8650	1.3330
13	C	7.1560	-0.6480	-0.0140
14	H	6.5900	-1.2250	-0.7450
15	H	8.1470	-1.1040	0.0540
16	C	7.3020	0.8060	-0.4860
17	H	7.9600	0.7600	-1.3590
18	H	7.8660	1.4030	0.2330
19	C	6.0430	1.5420	-0.9640
20	H	6.3220	2.5030	-1.4040
21	H	5.5460	0.9650	-1.7440
22	N	5.0120	1.7910	0.1110
23	C	3.6230	2.0600	-0.4480
24	H	3.7270	2.6830	-1.3390
25	H	3.0790	2.6540	0.2870
26	C	2.8350	0.7840	-0.7920
27	H	1.9310	1.1290	-1.3030
28	H	3.3590	0.1970	-1.5480
29	C	2.3080	-0.1100	0.3550
30	H	1.5650	-0.7970	-0.0570
31	H	1.7950	0.4970	1.1010
32	N	3.3240	-0.9910	1.1120
33	C	2.6710	-1.6200	2.3370
34	H	3.3230	-2.4330	2.6550
35	H	1.7360	-2.0750	2.0000
36	C	2.3780	-0.6840	3.5180
37	H	1.7570	-1.2700	4.2030

38	H	1.7270	0.1410	3.2210
39	C	3.5600	-0.1910	4.3630
40	H	3.1890	0.3400	5.2440
41	H	4.1430	-1.0400	4.7220
42	C	3.9160	2.0940	3.3580
43	H	3.7540	2.5950	4.3160
44	H	2.9170	1.9000	2.9600
45	C	4.6620	3.1390	2.4330
46	H	5.3790	3.6890	3.0440
47	H	3.8720	3.8580	2.2090
48	C	5.4750	2.8670	1.1020
49	H	5.5190	3.8220	0.5710
50	H	6.5100	2.6240	1.3480
51	C	6.1160	-2.3220	1.5320
52	H	5.8170	-2.4120	2.5730
53	H	7.0280	-2.9120	1.4170
54	C	5.0210	-2.9190	0.6300
55	H	4.6580	-3.7990	1.1650
56	H	5.4630	-3.3170	-0.2850
57	C	3.8360	-2.0540	0.1640
58	H	4.1060	-1.5310	-0.7490
59	H	2.9990	-2.7110	-0.0880

Re^{III}(**2**), S = 2

1	Re	4.8280	0.1600	1.5430
2	N	4.6140	0.6380	3.5910
3	C	5.9640	0.7170	4.2910
4	H	5.7720	0.7440	5.3660
5	H	6.4040	1.6770	4.0220
6	C	6.9530	-0.4180	3.9820
7	H	6.5350	-1.3860	4.2610
8	H	7.7800	-0.2770	4.6850
9	C	7.6240	-0.4670	2.5940
10	H	8.0940	0.4900	2.3660
11	H	8.4160	-1.2210	2.6140
12	N	6.7110	-0.7950	1.4230
13	C	7.3690	-0.5620	0.0710
14	H	6.8760	-1.2270	-0.6380
15	H	8.4060	-0.8940	0.1520
16	C	7.3370	0.8810	-0.4540
17	H	7.9920	0.8850	-1.3310
18	H	7.8300	1.5590	0.2450
19	C	6.0000	1.4600	-0.9590
20	H	6.1940	2.4190	-1.4470
21	H	5.5590	0.8010	-1.7060
22	N	4.9370	1.6960	0.1020
23	C	3.5620	1.9910	-0.4850
24	H	3.7130	2.6210	-1.3650
25	H	3.0280	2.5950	0.2490
26	C	2.7170	0.7680	-0.8790
27	H	1.8610	1.1750	-1.4250
28	H	3.2380	0.1630	-1.6250
29	C	2.0960	-0.1090	0.2290
30	H	1.3960	-0.8120	-0.2320
31	H	1.5250	0.5070	0.9240
32	N	3.0760	-0.9190	1.0620

33	C	2.4450	-1.5280	2.3070
34	H	3.0350	-2.4110	2.5550
35	H	1.4480	-1.8780	2.0290
36	C	2.3380	-0.6070	3.5310
37	H	1.7150	-1.1520	4.2470
38	H	1.7510	0.2840	3.2980
39	C	3.6180	-0.2540	4.3140
40	H	3.3360	0.2540	5.2410
41	H	4.1540	-1.1610	4.5930
42	C	4.0100	2.0340	3.3900
43	H	3.9670	2.5110	4.3730
44	H	2.9780	1.8710	3.0890
45	C	4.6650	3.0760	2.4150
46	H	5.4080	3.6500	2.9710
47	H	3.8480	3.7790	2.2410
48	C	5.3920	2.8140	1.0490
49	H	5.3440	3.7500	0.4860
50	H	6.4460	2.6310	1.2390
51	C	6.1910	-2.2320	1.5560
52	H	5.9190	-2.3530	2.6020
53	H	7.0400	-2.8990	1.3840
54	C	5.0190	-2.7610	0.6600
55	H	4.7100	-3.6620	1.1940
56	H	5.4380	-3.1290	-0.2790
57	C	3.7290	-1.9970	0.1900
58	H	3.9310	-1.5250	-0.7680
59	H	2.9670	-2.7570	-0.0030

Ru^{IV}(**2**), S = 0

1	Ru	4.834	0.155	1.543
2	N	4.582	0.817	3.432
3	C	5.952	0.924	4.101
4	H	5.751	1.073	5.167
5	H	6.428	1.834	3.740
6	C	6.868	-0.291	3.914
7	H	6.423	-1.207	4.307
8	H	7.722	-0.114	4.578
9	C	7.482	-0.493	2.526
10	H	7.970	0.417	2.181
11	H	8.253	-1.267	2.576
12	N	6.523	-0.940	1.410
13	C	7.150	-0.712	0.032
14	H	6.592	-1.307	-0.690
15	H	8.154	-1.144	0.090
16	C	7.242	0.752	-0.413
17	H	7.842	0.737	-1.331
18	H	7.837	1.356	0.273
19	C	5.933	1.444	-0.810
20	H	6.155	2.406	-1.282
21	H	5.387	0.851	-1.542
22	N	4.953	1.763	0.331
23	C	3.557	2.061	-0.218
24	H	3.706	2.784	-1.027
25	H	2.995	2.573	0.561

26	C	2.787	0.847	-0.749
27	H	1.897	1.262	-1.237
28	H	3.314	0.346	-1.562
29	C	2.242	-0.145	0.285
30	H	1.560	-0.847	-0.205
31	H	1.668	0.369	1.053
32	N	3.281	-1.018	1.007
33	C	2.684	-1.647	2.267
34	H	3.331	-2.470	2.565
35	H	1.732	-2.089	1.954
36	C	2.447	-0.681	3.433
37	H	1.882	-1.258	4.175
38	H	1.768	0.131	3.167
39	C	3.685	-0.180	4.183
40	H	3.377	0.335	5.098
41	H	4.318	-1.013	4.488
42	C	3.897	2.162	3.263
43	H	3.689	2.544	4.268
44	H	2.920	1.954	2.823
45	C	4.648	3.248	2.466
46	H	5.334	3.793	3.119
47	H	3.886	3.986	2.202
48	C	5.483	2.872	1.223
49	H	5.594	3.761	0.592
50	H	6.499	2.585	1.502
51	C	6.057	-2.371	1.617
52	H	5.689	-2.427	2.643
53	H	6.951	-3.005	1.593
54	C	5.022	-2.936	0.621
55	H	4.602	-3.815	1.115
56	H	5.526	-3.339	-0.261
57	C	3.892	-2.042	0.067
58	H	4.220	-1.490	-0.816
59	H	3.074	-2.684	-0.278

Ru^{IV}(**2**), S = 1

1	Ru	4.820	0.334	1.596
2	N	4.560	0.716	3.609
3	C	5.916	0.824	4.288
4	H	5.733	0.851	5.366
5	H	6.356	1.783	4.016
6	C	6.865	-0.331	3.947
7	H	6.471	-1.292	4.279
8	H	7.753	-0.180	4.572
9	C	7.410	-0.391	2.512
10	H	7.818	0.570	2.202
11	H	8.237	-1.108	2.480
12	N	6.459	-0.867	1.381
13	C	7.112	-0.663	0.007
14	H	6.542	-1.260	-0.703
15	H	8.101	-1.126	0.093
16	C	7.271	0.775	-0.492
17	H	7.899	0.695	-1.387
18	H	7.872	1.384	0.185
19	C	6.001	1.493	-0.956
20	H	6.267	2.458	-1.401

21	H	5.488	0.918	-1.726
22	N	4.982	1.778	0.129
23	C	3.599	2.085	-0.424
24	H	3.739	2.719	-1.304
25	H	3.064	2.681	0.316
26	C	2.798	0.833	-0.803
27	H	1.881	1.201	-1.278
28	H	3.289	0.259	-1.590
29	C	2.304	-0.061	0.345
30	H	1.566	-0.767	-0.051
31	H	1.798	0.522	1.113
32	N	3.336	-0.968	1.070
33	C	2.711	-1.616	2.311
34	H	3.364	-2.438	2.599
35	H	1.775	-2.061	1.957
36	C	2.414	-0.709	3.507
37	H	1.826	-1.329	4.194
38	H	1.732	0.104	3.251
39	C	3.613	-0.227	4.329
40	H	3.260	0.300	5.221
41	H	4.212	-1.071	4.673
42	C	3.900	2.061	3.292
43	H	3.661	2.536	4.252
44	H	2.925	1.828	2.854
45	C	4.656	3.125	2.428
46	H	5.355	3.677	3.060
47	H	3.878	3.850	2.179
48	C	5.496	2.800	1.148
49	H	5.640	3.745	0.609
50	H	6.507	2.483	1.419
51	C	6.058	-2.311	1.601
52	H	5.720	-2.382	2.633
53	H	6.978	-2.903	1.539
54	C	5.021	-2.905	0.636
55	H	4.615	-3.783	1.145
56	H	5.508	-3.309	-0.255
57	C	3.887	-2.007	0.115
58	H	4.191	-1.473	-0.782
59	H	3.041	-2.639	-0.177

Ru^{IV}(**2**), S = 2

1	Ru	4.820	0.334	1.596
2	N	4.560	0.716	3.609
3	C	5.916	0.824	4.288
4	H	5.733	0.851	5.366
5	H	6.356	1.783	4.016
6	C	6.865	-0.331	3.947
7	H	6.471	-1.292	4.279
8	H	7.753	-0.180	4.572
9	C	7.410	-0.391	2.512
10	H	7.818	0.570	2.202
11	H	8.237	-1.108	2.480
12	N	6.459	-0.867	1.381
13	C	7.112	-0.663	0.007
14	H	6.542	-1.260	-0.703
15	H	8.101	-1.126	0.093

16	C	7.271	0.775	-0.492
17	H	7.899	0.695	-1.387
18	H	7.872	1.384	0.185
19	C	6.001	1.493	-0.956
20	H	6.267	2.458	-1.401
21	H	5.488	0.918	-1.726
22	N	4.982	1.778	0.129
23	C	3.599	2.085	-0.424
24	H	3.739	2.719	-1.304
25	H	3.064	2.681	0.316
26	C	2.798	0.833	-0.803
27	H	1.881	1.201	-1.278
28	H	3.289	0.259	-1.590
29	C	2.304	-0.061	0.345
30	H	1.566	-0.767	-0.051
31	H	1.798	0.522	1.113
32	N	3.336	-0.968	1.070
33	C	2.711	-1.616	2.311
34	H	3.364	-2.438	2.599
35	H	1.775	-2.061	1.957
36	C	2.414	-0.709	3.507
37	H	1.826	-1.329	4.194
38	H	1.732	0.104	3.251
39	C	3.613	-0.227	4.329
40	H	3.260	0.300	5.221
41	H	4.212	-1.071	4.673
42	C	3.900	2.061	3.292
43	H	3.661	2.536	4.252
44	H	2.925	1.828	2.854
45	C	4.656	3.125	2.428
46	H	5.355	3.677	3.060
47	H	3.878	3.850	2.179
48	C	5.496	2.800	1.148
49	H	5.640	3.745	0.609
50	H	6.507	2.483	1.419
51	C	6.058	-2.311	1.601
52	H	5.720	-2.382	2.633
53	H	6.978	-2.903	1.539
54	C	5.021	-2.905	0.636
55	H	4.615	-3.783	1.145
56	H	5.508	-3.309	-0.255
57	C	3.887	-2.007	0.115
58	H	4.191	-1.473	-0.782
59	H	3.041	-2.639	-0.177

d^8 Ions

Cu^{III}(**2**), S = 0

1	Cu	4.8330	0.1600	1.5430
2	N	4.6030	0.5950	3.4920
3	C	5.9210	0.7830	4.1880
4	H	5.7100	0.8530	5.2600
5	H	6.3240	1.7440	3.8770
6	C	6.9700	-0.3080	3.9660
7	H	6.6170	-1.2810	4.3080
8	H	7.8010	-0.0680	4.6350

9	C	7.5710	-0.3740	2.5610
10	H	8.0320	0.5780	2.2940
11	H	8.3740	-1.1210	2.5640
12	N	6.6290	-0.7410	1.4590
13	C	7.2630	-0.6150	0.1020
14	H	6.7400	-1.2920	-0.5710
15	H	8.2900	-0.9820	0.1930
16	C	7.2940	0.7880	-0.5070
17	H	7.8880	0.7070	-1.4210
18	H	7.8510	1.4850	0.1190
19	C	5.9400	1.3540	-0.9380
20	H	6.1110	2.3090	-1.4480
21	H	5.4610	0.6940	-1.6640
22	N	4.9530	1.6060	0.1580
23	C	3.6000	1.9950	-0.3690
24	H	3.7660	2.6570	-1.2250
25	H	3.1040	2.5830	0.3990
26	C	2.6830	0.8490	-0.8060
27	H	1.8100	1.3220	-1.2640
28	H	3.1280	0.2640	-1.6110
29	C	2.1400	-0.0350	0.3160
30	H	1.4220	-0.7410	-0.1170
31	H	1.5890	0.5610	1.0450
32	N	3.1530	-0.8380	1.0690
33	C	2.5580	-1.5430	2.2540
34	H	3.1740	-2.4150	2.4650
35	H	1.5740	-1.9130	1.9480
36	C	2.3940	-0.7130	3.5290
37	H	1.8450	-1.3450	4.2320
38	H	1.7400	0.1450	3.3670
39	C	3.6900	-0.3230	4.2400
40	H	3.4310	0.1730	5.1830
41	H	4.2650	-1.2110	4.5050
42	C	3.9180	1.9250	3.2160
43	H	3.6710	2.3620	4.1900
44	H	2.9660	1.6940	2.7460
45	C	4.6620	2.9960	2.3880
46	H	5.3530	3.5490	3.0270
47	H	3.8930	3.7270	2.1320
48	C	5.4930	2.6390	1.1370
49	H	5.6580	3.5590	0.5660
50	H	6.4800	2.2960	1.4380
51	C	6.0520	-2.1290	1.6890
52	H	5.6390	-2.1290	2.6950
53	H	6.8980	-2.8250	1.7150
54	C	5.0080	-2.6810	0.6970
55	H	4.5920	-3.5600	1.1950
56	H	5.5050	-3.0860	-0.1870
57	C	3.8710	-1.8020	0.1370
58	H	4.2420	-1.2080	-0.6950
59	H	3.1060	-2.4630	-0.2880

Cu^{III}(**2**), S = 1

1	Cu	4.8350	0.1060	1.5260
2	N	4.5060	0.7560	3.4300
3	C	5.8790	0.8680	4.0550

4	H	5.7130	1.0000	5.1290
5	H	6.3310	1.7880	3.6940
6	C	6.8430	-0.3040	3.8450
7	H	6.4150	-1.2440	4.1960
8	H	7.6740	-0.1200	4.5330
9	C	7.4950	-0.4450	2.4640
10	H	7.9600	0.4960	2.1740
11	H	8.2980	-1.1870	2.5290
12	N	6.5980	-0.8770	1.3250
13	C	7.2440	-0.6740	-0.0040
14	H	6.7020	-1.2710	-0.7370
15	H	8.2600	-1.0810	0.0530
16	C	7.3240	0.7870	-0.4620
17	H	7.9140	0.7860	-1.3820
18	H	7.9040	1.3950	0.2330
19	C	5.9910	1.4490	-0.8210
20	H	6.2020	2.4140	-1.2950
21	H	5.4620	0.8450	-1.5570
22	N	5.0360	1.7190	0.3050
23	C	3.6380	1.9990	-0.2070
24	H	3.7550	2.7100	-1.0320
25	H	3.0980	2.5200	0.5790
26	C	2.8180	0.8030	-0.6990
27	H	1.9490	1.2390	-1.2030
28	H	3.3340	0.2590	-1.4910
29	C	2.2290	-0.1400	0.3600
30	H	1.5110	-0.8090	-0.1270
31	H	1.6720	0.4320	1.0990
32	N	3.2050	-1.0200	1.1080
33	C	2.5850	-1.6460	2.3120
34	H	3.2140	-2.4820	2.6190
35	H	1.6180	-2.0660	2.0120
36	C	2.3620	-0.6900	3.4880
37	H	1.8070	-1.2550	4.2410
38	H	1.6980	0.1330	3.2200
39	C	3.6260	-0.1890	4.1930
40	H	3.3260	0.3310	5.1100
41	H	4.2430	-1.0340	4.4990
42	C	3.8670	2.1030	3.2350
43	H	3.6590	2.5130	4.2300
44	H	2.8950	1.9230	2.7780
45	C	4.6530	3.1710	2.4430
46	H	5.3230	3.7090	3.1160
47	H	3.9070	3.9150	2.1590
48	C	5.5230	2.8110	1.2170
49	H	5.6350	3.7160	0.6100
50	H	6.5280	2.5320	1.5280
51	C	6.0950	-2.2770	1.5700
52	H	5.7380	-2.2950	2.5980
53	H	6.9660	-2.9430	1.5480
54	C	5.0200	-2.8660	0.6420
55	H	4.6500	-3.7490	1.1670
56	H	5.4760	-3.2590	-0.2690
57	C	3.8420	-2.0010	0.1570
58	H	4.1490	-1.4250	-0.7140
59	H	3.0510	-2.6720	-0.1980

Ag^{III}(**2**), S = 0

1	Ag	4.8290	0.2110	1.5630
2	N	4.6060	0.6220	3.6360
3	C	5.9540	0.7270	4.2830
4	H	5.7920	0.7500	5.3660
5	H	6.3700	1.6950	4.0050
6	C	6.9770	-0.3840	3.9840
7	H	6.5940	-1.3580	4.2890
8	H	7.8070	-0.1980	4.6720
9	C	7.6250	-0.4370	2.5870
10	H	8.0970	0.5160	2.3460
11	H	8.4280	-1.1840	2.6280
12	N	6.7340	-0.7980	1.4440
13	C	7.3290	-0.5910	0.0850
14	H	6.8180	-1.2660	-0.5990
15	H	8.3730	-0.9190	0.1350
16	C	7.3140	0.8380	-0.4870
17	H	7.9490	0.7980	-1.3770
18	H	7.8330	1.5300	0.1790
19	C	5.9750	1.4170	-0.9830
20	H	6.1940	2.3590	-1.5020
21	H	5.5190	0.7530	-1.7190
22	N	4.9430	1.7060	0.0540
23	C	3.5680	1.9970	-0.4710
24	H	3.6890	2.6270	-1.3590
25	H	3.0590	2.6010	0.2790
26	C	2.6840	0.7980	-0.8640
27	H	1.8160	1.2380	-1.3630
28	H	3.1610	0.2000	-1.6410
29	C	2.0920	-0.0850	0.2530
30	H	1.3830	-0.7760	-0.2200
31	H	1.5180	0.5190	0.9570
32	N	3.0550	-0.9040	1.0460
33	C	2.4860	-1.5370	2.2780
34	H	3.0920	-2.4140	2.5020
35	H	1.4840	-1.9000	2.0240
36	C	2.3610	-0.6560	3.5350
37	H	1.7640	-1.2440	4.2380
38	H	1.7470	0.2220	3.3350
39	C	3.6420	-0.2950	4.3130
40	H	3.3330	0.1860	5.2500
41	H	4.1910	-1.1960	4.5900
42	C	3.9790	1.9830	3.3460
43	H	3.8520	2.4830	4.3130
44	H	2.9760	1.7800	2.9830
45	C	4.6630	3.0240	2.3960
46	H	5.3930	3.5980	2.9710
47	H	3.8560	3.7330	2.2030
48	C	5.4260	2.7500	1.0570
49	H	5.4640	3.7050	0.5210
50	H	6.4580	2.4960	1.2830
51	C	6.1350	-2.1830	1.6290
52	H	5.7900	-2.2260	2.6580
53	H	6.9640	-2.8980	1.5640

54	C	5.0090	-2.7080	0.6950
55	H	4.6350	-3.5880	1.2230
56	H	5.4550	-3.1150	-0.2150
57	C	3.8080	-1.8810	0.1570
58	H	4.1310	-1.3100	-0.7080
59	H	3.0700	-2.5990	-0.2200

Ag^{III}(**2**), S = 1

1	Ag	4.8380	0.0590	1.5150
2	N	4.5030	0.8190	3.5530
3	C	5.9090	0.8510	4.0980
4	H	5.8100	0.9690	5.1840
5	H	6.3780	1.7610	3.7290
6	C	6.8230	-0.3680	3.8370
7	H	6.3250	-1.2940	4.1300
8	H	7.6290	-0.2650	4.5700
9	C	7.5590	-0.5180	2.4840
10	H	8.0540	0.4160	2.2240
11	H	8.3500	-1.2660	2.6170
12	N	6.7420	-0.9440	1.2910
13	C	7.3510	-0.6250	-0.0250
14	H	6.8360	-1.2190	-0.7810
15	H	8.3940	-0.9640	-0.0100
16	C	7.3530	0.8660	-0.4240
17	H	7.9840	0.9260	-1.3150
18	H	7.8780	1.4710	0.3170
19	C	6.0190	1.5210	-0.8390
20	H	6.2630	2.4710	-1.3320
21	H	5.5120	0.9050	-1.5810
22	N	5.0270	1.8390	0.2320
23	C	3.6070	2.0030	-0.2520
24	H	3.6540	2.7050	-1.0930
25	H	3.0530	2.5040	0.5400
26	C	2.8430	0.7460	-0.7280
27	H	2.0050	1.1440	-1.3090
28	H	3.4270	0.1930	-1.4650
29	C	2.1730	-0.1980	0.3000
30	H	1.4660	-0.8340	-0.2440
31	H	1.5870	0.3840	1.0110
32	N	3.0710	-1.1120	1.0950
33	C	2.4720	-1.6290	2.3530
34	H	3.0710	-2.4800	2.6800
35	H	1.4720	-2.0160	2.1220
36	C	2.3210	-0.6070	3.5000
37	H	1.7200	-1.1130	4.2610
38	H	1.7060	0.2410	3.1940
39	C	3.5890	-0.1390	4.2460
40	H	3.2580	0.3550	5.1690
41	H	4.1860	-0.9990	4.5490
42	C	3.9000	2.1680	3.3180
43	H	3.7410	2.6290	4.3020
44	H	2.9080	1.9890	2.9090
45	C	4.6510	3.2170	2.4550
46	H	5.3480	3.7700	3.0880
47	H	3.8790	3.9480	2.2080
48	C	5.4820	2.9030	1.1790

49	H	5.5460	3.8390	0.6100
50	H	6.5040	2.6490	1.4520
51	C	6.2180	-2.3490	1.4640
52	H	5.9790	-2.4450	2.5200
53	H	7.0580	-3.0320	1.2890
54	C	5.0240	-2.9050	0.6290
55	H	4.7330	-3.7960	1.1890
56	H	5.4010	-3.2910	-0.3200
57	C	3.7370	-2.1310	0.2030
58	H	3.9360	-1.6150	-0.7330
59	H	2.9850	-2.8930	-0.0360

Cr^{II}(**3**), S = 2

1	Cr	-0.0100	0.0710	-0.0140
2	N	0.6590	-1.7870	-0.8630
3	C	2.1240	-2.1350	-0.9270
4	H	2.2320	-2.9830	-1.6090
5	H	2.4330	-2.4910	0.0540
6	C	3.0460	-0.9930	-1.3510
7	H	2.6210	-0.4520	-2.2010
8	H	3.9510	-1.4590	-1.7430
9	C	3.4480	-0.0310	-0.2080
10	H	4.5380	0.0480	-0.1880
11	H	3.1880	-0.4720	0.7580
12	N	1.4590	1.6570	-0.1830
13	C	1.1750	2.6270	0.9250
14	H	0.1690	3.0260	0.7890
15	H	1.8590	3.4750	0.8360
16	C	1.2940	2.0010	2.3180
17	H	1.4410	2.8180	3.0290
18	H	2.2010	1.3980	2.3940
19	C	0.0680	1.2410	2.8360
20	H	0.2410	0.9760	3.8840
21	H	-0.7910	1.9130	2.8200
22	N	-0.3590	-0.0070	2.1090
23	C	-1.7010	-0.4110	2.6630
24	H	-1.7120	-0.1450	3.7240
25	H	-1.7750	-1.4960	2.6190
26	C	-2.9110	0.1930	1.9520
27	H	-3.7320	0.1650	2.6700
28	H	-2.7520	1.2560	1.7530
29	C	-3.3540	-0.5650	0.6780
30	H	-4.4210	-0.7850	0.7590
31	H	-2.8740	-1.5470	0.6450
32	N	-1.8040	0.4870	-1.1420
33	C	-1.5840	-0.0770	-2.5150
34	H	-0.7250	0.4220	-2.9640
35	H	-2.4480	0.1700	-3.1400
36	C	-1.3540	-1.5910	-2.5140
37	H	-1.5740	-1.9530	-3.5220
38	H	-2.0820	-2.0930	-1.8730
39	C	0.0740	-2.0670	-2.2240
40	H	0.1220	-3.1480	-2.3940
41	H	0.7480	-1.6050	-2.9470
42	C	-0.0310	-2.6290	0.1780
43	H	0.0880	-3.6860	-0.0850

44	H	-1.0980	-2.4210	0.0930
45	C	0.4070	-2.4780	1.6570
46	H	1.3360	-3.0280	1.8200
47	H	-0.3400	-3.0380	2.2230
48	C	0.6470	-1.1050	2.3370
49	H	0.7290	-1.2910	3.4140
50	H	1.6160	-0.7130	2.0300
51	C	1.0120	2.1940	-1.5200
52	H	1.2390	1.4080	-2.2430
53	H	1.6550	3.0380	-1.7890
54	C	-0.4390	2.6840	-1.7160
55	H	-0.5500	2.7620	-2.8000
56	H	-0.5160	3.7140	-1.3600
57	C	-1.6900	1.9920	-1.1340
58	H	-1.8280	2.2910	-0.0930
59	H	-2.5440	2.4080	-1.6780
60	C	2.9590	1.4100	-0.2690
61	H	3.3180	1.8740	-1.1890
62	H	3.4270	1.9610	0.5460
63	C	-3.2060	0.1330	-0.6680
64	H	-3.7940	1.0530	-0.6610
65	H	-3.6560	-0.5030	-1.4290

Cr^{II}(**4**), S = 2

C3	-3.44589	0.22323	0.53819
C6	-3.46729	1.70227	0.86285
C9	-2.69046	2.60572	-0.11149
C13	0.36055	2.78536	-1.15280
C16	1.59171	2.01825	-1.69028
C19	1.37852	1.17445	-2.96646
C23	0.45346	-2.47424	-1.97782
C26	1.82035	-3.03346	-1.59765
C29	2.29465	-3.01543	-0.14582
C33	1.38160	-0.99879	2.29111
C36	0.29579	-2.07793	2.14902
C39	-2.37944	-1.88163	0.10025
C42	-2.86092	-1.90387	-1.36938
C45	-2.38853	-0.78255	-2.31001
C48	2.29802	2.94124	1.35224
C51	2.80255	1.70850	2.10657
C54	3.09001	0.44035	1.31284
C57	-1.39973	3.17782	0.45608
C60	2.84820	-1.70952	0.42689
C63	1.37919	-0.34238	-2.76656
C66	-1.07044	-1.73252	2.73888
C69	-1.80497	-0.52829	2.15032
C72	0.79257	3.14410	1.27152
C75	-1.00013	-0.79220	-2.93515
Cr1	-0.04152	0.14634	-0.08252
H4	-4.14802	-0.30355	1.19123
H5	-3.81867	0.09666	-0.46982
H7	-3.15058	1.89067	1.89156
H8	-4.52365	1.97976	0.83696
H10	-2.52916	2.11089	-1.07251
H11	-3.31737	3.46777	-0.34931
H14	-0.49385	2.60940	-1.80765

H15	0.54978	3.86316	-1.18763
H17	2.01486	1.38133	-0.90999
H18	2.37736	2.74695	-1.89018
H20	0.49976	1.52040	-3.51255
H21	2.21362	1.35942	-3.64593
H24	0.25165	-2.84626	-2.98452
H25	-0.31213	-2.90298	-1.33568
H27	1.74606	-4.08723	-1.88205
H28	2.60139	-2.63486	-2.24795
H30	3.16456	-3.67881	-0.11721
H31	1.57188	-3.49889	0.50547
H34	0.96330	-0.10765	2.75962
H35	2.17962	-1.34467	2.95796
H37	0.63977	-3.00571	2.60838
H38	0.17045	-2.31710	1.09636
H40	-3.13552	-2.38104	0.71374
H41	-1.47010	-2.46374	0.20847
H43	-3.95091	-1.88043	-1.37187
H44	-2.60441	-2.88119	-1.78596
H46	-3.07122	-0.77453	-3.16409
H47	-2.53603	0.18519	-1.83512
H49	2.63780	3.81157	1.91903
H50	2.78807	3.03886	0.38397
H52	2.17524	1.51850	2.98007
H53	3.77551	1.97481	2.52575
H55	3.55871	0.71304	0.36650
H56	3.84702	-0.11542	1.87308
H58	-1.52762	3.29571	1.53068
H59	-1.24203	4.18325	0.05794
H61	3.47943	-1.25692	-0.33930
H62	3.52112	-1.98675	1.24439
H64	1.45099	-0.82893	-3.74463
H65	2.28159	-0.60519	-2.21927
H67	-1.70852	-2.61586	2.68173
H68	-0.96862	-1.52092	3.80766
H70	-1.25394	0.39442	2.36177
H71	-2.74637	-0.43665	2.69646
H73	0.36441	2.90355	2.24667
H74	0.62116	4.21365	1.11257
H76	-0.89166	0.16076	-3.44655
H77	-0.94208	-1.55901	-3.71021
N2	-2.12588	-0.50976	0.65881
N12	-0.08323	2.44191	0.24819
N22	0.21010	-0.96833	-2.03729
N32	1.99910	-0.57138	0.99010