Supporting Information: Magnetic Properties of Mononuclear Co(II) Complexes with Carborane Ligands

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Table 1: DFT(B3LYP) Optimized geometry for $S = \frac{3}{2}$ ground state of complex I with the def2-TZVP basis set. Cartesian coordinates in Å.

	X	Y	Z
B	2.430608	5.825065	-8.060517
H	2.730192	4.698222	-8.273849
B	1.103443	6.427456	-7.061817
H	0.309832	5.688931	-6.586149
B	1.824418	8.483999	-8.973371
H	1.541905	9.210223	-9.863055
B	2.732770	6.454902	-6.426948
H	3.257122	5.843670	-5.557842
C	3.270692	8.060396	-6.688275
H	4.048890	8.407074	-6.027450
C	3.705422	6.906494	-7.760964
H	4.732616	6.581118	-7.716139
B	2.872485	7.083300	-9.231809
H	3.459132	6.783900	-10.216767
B	2.109710	9.109141	-7.343264
H	2.165042	10.241047	-6.996931
B	1.665459	7.849983	-6.169736
H	1.416680	8.153094	-5.051595
B	3.451081	8.500928	-8.333468
H	4.410403	9.131653	-8.626733
B	-7.873115	8.121475	-10.788931
H	-9.040638	7.940803	-10.637345
B	-6.764504	8.050886	-9.408819
⋮	⋮	⋮	⋮

⋮	⋮	⋮	⋮
H	-7.046159	7.796648	-8.287895
B	-5.353788	7.111353	-11.705985
H	-4.654473	6.270135	-12.141115
B	-6.994931	7.529861	-12.221542
H	-7.520565	6.932650	-13.106183
B	-7.211069	9.277850	-11.967691
H	-7.897902	9.942677	-12.677681
B	-6.728881	6.776674	-10.638470
H	-6.986696	5.657377	-10.351995
B	-5.657054	8.645398	-12.541200
H	-5.157414	8.841140	-13.596521
B	-5.693661	9.917842	-11.311930
H	-5.216882	10.979109	-11.528717
B	-7.053455	9.597928	-10.224937
H	-7.619826	10.486985	-9.673469
B	-5.411364	9.143814	-9.742667
H	-4.747318	9.625559	-8.899511
C	-5.287592	7.436177	-10.007083
C	-4.625943	8.591732	-11.182823
B	1.124904	6.809572	-8.843256
B	0.642570	8.089025	-7.637379
Co	-2.013434	7.506466	-9.446340
S	-0.113472	6.176516	-10.019175
S	-1.071617	8.689731	-7.603763
S	-4.154143	6.513098	-9.008139
S	-2.868606	8.752223	-11.293459

Table 2: DFT(PBE) Optimized geometry for $S = \frac{3}{2}$ ground state of complex I with the def2-TZVP basis set. Cartesian coordinates in Å.

	X	Y	Z
B	2.063086	5.788340	-7.969280
H	1.821298	4.645027	-8.178424
B	0.886324	6.741145	-7.069627
H	-0.138661	6.303762	-6.677418
B	1.929837	8.383832	-9.126554
H	1.576108	9.014556	-10.060340
B	2.509735	6.505265	-6.412280
H	2.673973	5.827726	-5.444938
B	3.439392	7.980502	-6.734040
H	4.283844	8.377627	-5.990393
B	3.650456	6.551263	-7.766798
H	4.650804	5.901992	-7.775092
B	2.718545	6.811634	-9.248317
H	2.946926	6.364190	-10.323691
B	2.378489	9.109233	-7.582062
H	2.359799	10.291154	-7.472254
B	1.726411	8.085529	-6.301157
H	1.257538	8.568695	-5.323995
B	3.563708	8.167381	-8.492597
H	4.486470	8.697113	-9.030638
B	-7.711638	7.743322	-10.940996
H	-8.822745	7.308565	-10.956137
B	-6.776959	7.802741	-9.438803
H	-7.108589	7.402464	-8.371806
⋮	⋮	⋮	⋮

⋮	⋮	⋮	⋮
B	-4.958217	7.355800	-11.584552
H	-4.035660	6.721264	-11.959562
B	-6.578872	7.463081	-12.273447
H	-6.865117	6.835153	-13.245901
B	-7.189490	9.098052	-11.959111
H	-7.920764	9.661145	-12.714882
B	-6.327796	6.668347	-10.712623
H	-6.353300	5.500408	-10.502671
B	-5.484887	8.849519	-12.358182
H	-4.906520	9.229752	-13.321979
B	-5.933005	9.983640	-11.083021
H	-5.655439	11.133469	-11.181721
B	-7.308885	9.306010	-10.202237
H	-8.114907	10.010861	-9.676827
B	-5.678305	9.178225	-9.534926
H	-5.215501	9.713381	-8.588947
C	-5.144908	7.580826	-9.891766
C	-4.640987	8.890809	-10.876685
C	1.082470	6.930868	-8.767897
C	0.883274	8.313468	-7.766498
Co	-1.960990	7.943447	-9.295054
S	-0.253204	6.446917	-9.816457
S	-0.632024	9.204459	-7.857027
S	-3.962361	6.826997	-8.826227
S	-2.967886	9.432342	-10.774868

Table 3: DFT(BP86) Optimized geometry for $S = \frac{3}{2}$ ground state of complex I with the def2-TZVP basis set. Cartesian coordinates in Å.

	X	Y	Z
B	2.208243	5.794162	-8.146470
H	2.090988	4.648826	-8.459382
B	0.969236	6.532536	-7.105202
H	0.006556	5.946942	-6.730200
B	1.758470	8.494658	-8.979719
H	1.313390	9.195137	-9.828996
B	2.640009	6.378295	-6.522652
H	2.910050	5.608052	-5.645023
B	3.419826	7.974597	-6.695610
H	4.263794	8.358672	-5.935304
B	3.724166	6.696749	-7.905262
H	4.787653	6.155106	-8.020619
B	2.704881	7.030104	-9.326391
H	2.932605	6.747146	-10.462846
B	2.213348	9.096461	-7.369494
H	2.098688	10.260773	-7.135251
B	1.716123	7.860439	-6.189007
H	1.254347	8.162649	-5.131430
B	3.443729	8.377926	-8.433976
H	4.294642	9.056198	-8.936397
B	-7.749139	7.889158	-10.894127
H	-8.901644	7.560283	-10.860960
B	-6.789916	8.017941	-9.400038
H	-7.146655	7.775501	-8.287665
⋮	⋮	⋮	⋮

⋮	⋮	⋮	⋮
B	-5.024531	7.212366	-11.504762
H	-4.162933	6.459846	-11.821430
B	-6.647965	7.379635	-12.203303
H	-6.993771	6.680964	-13.113716
B	-7.124218	9.092690	-12.055458
H	-7.824021	9.635927	-12.863664
B	-6.450802	6.716300	-10.566047
H	-6.572631	5.567668	-10.267177
B	-5.441492	8.662216	-12.444521
H	-4.857729	8.879450	-13.462408
B	-5.780569	9.964155	-11.278418
H	-5.432497	11.086888	-11.482607
B	-7.197328	9.485567	-10.316286
H	-7.939813	10.309643	-9.861723
B	-5.563001	9.279842	-9.652574
H	-5.055547	9.876208	-8.760004
C	-5.189319	7.593994	-9.820787
C	-4.563217	8.804005	-10.987614
C	1.086078	6.905152	-8.796085
C	0.780512	8.191085	-7.579376
Co	-1.998527	7.841044	-9.233411
S	-0.290001	6.477291	-9.830475
S	-0.857037	8.873784	-7.570598
S	-3.993680	6.899460	-8.707006
S	-2.828479	9.157812	-10.879226

Table 4: DFT(BP86) Optimized geometry for $S = \frac{3}{2}$ ground state of complex II with the def2-TZVP basis set. Cartesian coordinates in Å.

	X	Y	Z
B	2.258140	5.788269	-8.128160
H	2.442312	4.632044	-8.366912
B	1.039059	6.489915	-7.045529
H	0.203949	5.806758	-6.535716
B	1.829037	8.512383	-8.971093
H	1.557147	9.280657	-9.841742
B	2.703509	6.361947	-6.502419
H	3.225757	5.686852	-5.666102
C	3.365142	7.926812	-6.769328
H	4.212917	8.191224	-6.142755
C	3.641913	6.753197	-7.889750
H	4.648369	6.343207	-7.905816
B	2.742484	7.030945	-9.310234
H	3.251666	6.707099	-10.341216
B	2.258871	9.085913	-7.348336
H	2.427620	10.214128	-6.992920
B	1.774817	7.843282	-6.165505
H	1.617818	8.137487	-5.017998
B	3.490453	8.380750	-8.423650
H	4.493211	8.937051	-8.758923
B	-7.831085	7.901059	-10.935693
H	-8.985082	7.573195	-10.909430
B	-6.882591	8.034904	-9.434090
⋮	⋮	⋮	⋮

⋮	⋮	⋮	⋮
H	-7.256281	7.806587	-8.323502
B	-5.098199	7.228429	-11.513902
H	-4.240902	6.469972	-11.829285
B	-6.718531	7.385089	-12.232498
H	-7.057609	6.680485	-13.142055
B	-7.199610	9.097578	-12.098255
H	-7.896426	9.636256	-12.913432
B	-6.537153	6.727340	-10.592150
H	-6.667535	5.577266	-10.299520
B	-5.513837	8.667372	-12.477094
H	-4.931863	8.872412	-13.499346
B	-5.860354	9.975116	-11.319241
H	-5.522975	11.101906	-11.523422
B	-7.279013	9.497926	-10.361010
H	-8.023781	10.325385	-9.913991
B	-5.643624	9.286948	-9.691571
H	-5.148071	9.892327	-8.797930
C	-5.285983	7.592324	-9.827116
C	-4.634442	8.831234	-11.028842
B	1.000715	6.895310	-8.821897
B	0.694285	8.197870	-7.578507
Co	-2.070332	7.849234	-9.236789
S	-0.378481	6.412884	-9.909776
S	-0.969834	8.936079	-7.509228
S	-4.097438	6.910825	-8.710985
S	-2.907291	9.178070	-10.906040

Table 5: DFT(BP86) Optimized geometry for $S = \frac{3}{2}$ ground state of complex III with the def2-TZVP basis set. Cartesian coordinates in Å.

	X	Y	Z
B	2.273564	5.782372	-8.120894
H	2.471239	4.627934	-8.361659
B	1.071425	6.466913	-7.011958
H	0.261765	5.770862	-6.478094
B	1.783153	8.497895	-8.960087
H	1.481701	9.261799	-9.825300
B	2.748296	6.365594	-6.510794
H	3.303179	5.700426	-5.686022
C	3.380708	7.942106	-6.794634
H	4.238395	8.221964	-6.188652
C	3.648888	6.767525	-7.922156
H	4.660144	6.371672	-7.963224
B	2.708258	7.032326	-9.319704
H	3.198028	6.714324	-10.362676
B	2.242519	9.081316	-7.352134
H	2.403518	10.213642	-7.003798
B	1.807763	7.830974	-6.152664
H	1.675469	8.125452	-5.001277
B	3.457899	8.391182	-8.452449
H	4.444178	8.963317	-8.812940
C	-7.657747	7.936411	-10.945033
H	-8.719717	7.722355	-11.033947
B	-6.869090	8.045488	-9.438927
H	-7.532682	7.821807	-8.469836
⋮	⋮	⋮	⋮

⋮	⋮	⋮	⋮
B	-5.076333	7.197944	-11.533812
H	-4.336776	6.370746	-11.973632
B	-6.670085	7.382252	-12.240182
H	-7.221537	6.817323	-13.138535
C	-7.055469	9.042842	-12.011415
H	-7.771020	9.462631	-12.713773
B	-6.503262	6.733345	-10.593529
H	-6.920653	5.630498	-10.396252
B	-5.454574	8.662348	-12.453826
H	-5.130566	8.925133	-13.574029
B	-5.820425	9.975240	-11.299079
H	-5.743446	11.116438	-11.646658
B	-7.261225	9.508935	-10.368086
H	-8.173837	10.242083	-10.122959
B	-5.669974	9.330223	-9.655258
H	-5.356307	10.037068	-8.746165
B	-5.137477	7.582065	-9.744370
B	-4.466844	8.818230	-10.936254
B	0.975871	6.861661	-8.795798
B	0.677732	8.174765	-7.535675
Co	-2.023964	7.827131	-9.166494
S	-0.377150	6.302134	-9.868162
S	-0.970479	8.916538	-7.366823
S	-4.041798	6.806938	-8.521490
S	-2.710384	9.271134	-10.889584

Table 6: g-values and tensor from CASSCF calculation on complex I with DFT(BP86) optimized geometry.

	g-values	g-tensor		
g_1	2.018455	0.1291430	0.9913830	0.0219527
g_2	2.023477	-0.3620697	0.0265324	0.9317733
g_3	3.257789	0.9231617	-0.1282804	0.3623763

Table 7: g-values and tensor from CASSCF/NEVPT2 calculation on complex I with DFT(BP86) optimized geometry.

	g-values	g-tensor		
g_1	2.071610	0.1255654	0.9915390	0.0329214
g_2	2.074431	-0.3639097	0.0151627	0.9313108
g_3	2.910551	0.9229318	-0.1289208	0.3627346

Table 8: D-values and tensor from CASSCF calculation on complex I with DFT(BP86) optimized geometry. D in cm^{-1}.

	D-values	D-tensor		
D_{xx}	36.396873	-0.365550	0.000320	0.930791
D_{yy}	36.661112	0.120059	0.991663	0.046810
D_{zz}	-73.057984	0.923016	-0.128861	0.362541
D	-109.586977			
E/D	0.001206			

Table 9: D-values and tensor from CASSCF/NEVPT2 calculation on complex I with DFT(BP86) optimized geometry. D in cm^{-1}.

	D-values	D-tensor		
D_{xx}	24.167314	-0.346829	0.133276	0.928411
D_{yy}	24.396612	0.169616	0.982445	-0.077669
D_{zz}	-48.563926	0.922464	-0.130535	0.363346
D	-72.845889			
E/D	0.001574			

Table 10: Calculated δ excitation energies (in cm^{-1}) and individual contributions to D and E parameters arising from the CASSCF method on complex I with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten $S = \frac{3}{2}$ and forty $S = \frac{1}{2}$ ($'$) configurations.

Root	Mult	δ	D	E
0	4	0.0	0.000	0.000
1	4	474.2	-135.738	0.000
2	4	5138.2	10.603	-10.574
3	4	5168.8	9.506	9.485
4	4	5669.9	1.218	1.209
5	4	5753.4	0.290	-0.261
6	4	7474.4	0.008	-0.003
$0'$	2	18323.4	-0.742	-0.763
$1'$	2	18427.4	-0.744	0.749
$2'$	2	18704.7	-0.010	-0.007
$3'$	2	19012.2	-0.006	0.004
$4'$	2	19405.6	0.000	0.000
$5'$	2	19744.7	0.000	0.000
7	4	20102.3	0.000	0.000
8	4	21277.1	0.002	0.002
9	4	22213.7	0.001	-0.001
$6'$	2	22302.8	7.077	0.000
$7'$	2	22969.3	-1.760	1.207
$8'$	2	22992.7	-1.806	-1.210
$9'$	2	23481.6	-0.068	0.037
$10'$	2	24760.3	1.104	0.000
$11'$	2	25191.3	-0.002	0.001
$12'$	2	25632.9	-0.006	0.007
$13'$	2	25647.8	0.000	-0.005
$14'$	2	27970.5	-0.004	-0.005
$15'$	2	27972.6	-0.002	0.003
$16'$	2	28494.0	0.000	0.000
$\vdots$			$\vdots$	

Root	Mult	δ	D	E
⋮			⋮	
$17'$	2	28615.5	-0.001	0.001
$18'$	2	28699.3	-0.005	0.005
$19'$	2	28810.3	-0.123	0.123
$20'$	2	28846.8	-0.115	-0.115
$21'$	2	30469.1	-1.071	1.071
$22'$	2	30487.7	-1.103	-1.102
$23'$	2	31761.4	0.000	0.000
$24'$	2	31875.3	0.000	0.000
$25'$	2	32050.0	0.000	0.000
$26'$	2	33019.8	0.206	0.000
$27'$	2	33509.2	0.000	0.000
$28'$	2	43466.5	0.336	0.000
$29'$	2	43786.5	0.000	0.000
$30'$	2	44819.3	-0.076	-0.076
$31'$	2	44867.5	-0.075	0.075
$32'$	2	45713.5	-0.044	-0.044
$33'$	2	45717.3	-0.044	0.044
$34'$	2	46489.3	0.000	0.000
$35'$	2	66172.3	0.000	0.000
$36'$	2	68315.2	-0.026	0.026
$37'$	2	68395.4	-0.026	-0.026
$38'$	2	69824.9	0.038	0.000
$39'$	2	70112.4	0.000	0.000

Table 11: Calculated δ excitation energies (in cm^{-1}) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on complex I with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten $S = \frac{3}{2}$ and forty $S = \frac{1}{2}$ ($'$) configurations.

Root	Mult	δ	D	E
0	4	0.0	0.000	0.000
1	4	1049.0	-90.444	0.001
2	4	8130.4	6.742	-6.620
3	4	8137.8	6.069	5.972
4	4	9333.4	0.740	0.733
5	4	9419.1	0.177	-0.174
6	4	11053.0	0.005	0.000
$0'$	2	15669.8	-0.868	-0.872
$1'$	2	15862.1	-0.864	0.848
$2'$	2	17417.0	-0.011	-0.003
$3'$	2	17864.3	-0.007	0.003
$5'$	2	18484.8	0.000	0.000
$4'$	2	18623.1	0.000	0.000
$6'$	2	19311.2	7.367	0.000
$9'$	2	21275.6	-0.075	0.022
7	4	21324.0	0.000	0.000
8	4	21601.7	0.002	0.002
9	4	21726.0	0.001	-0.001
$10'$	2	23021.0	1.188	0.000
$11'$	2	23662.2	-0.002	0.002
$7'$	2	24538.3	-1.648	0.771
$8'$	2	24719.8	-1.680	-0.754
$12'$	2	26009.4	-0.006	0.007
$13'$	2	26066.8	0.000	-0.005
$19'$	2	28062.2	-0.127	0.125
$\vdots$			$\vdots$	

Root	Mult	δ	D	E
⋮			⋮	
$16'$	2	28153.4	0.000	0.000
$20'$	2	28179.2	-0.117	-0.116
$14'$	2	28263.7	-0.004	-0.005
$15'$	2	28264.3	-0.002	0.003
$18'$	2	29270.6	-0.005	0.005
$17'$	2	29853.7	-0.001	0.000
$21'$	2	30523.3	-1.069	1.037
$22'$	2	30559.8	-1.100	-1.067
$23'$	2	33516.9	0.000	0.000
$25'$	2	34392.4	0.000	0.000
$24'$	2	35309.0	0.000	0.000
$26'$	2	35802.1	0.190	0.000
$27'$	2	36714.6	0.000	0.000
$28'$	2	39223.2	0.372	0.000
$29'$	2	39557.0	0.000	0.000
$30'$	2	41363.9	-0.082	-0.081
$31'$	2	41431.1	-0.081	0.080
$32'$	2	42599.9	-0.048	-0.043
$33'$	2	42610.0	-0.048	0.043
$34'$	2	44691.7	0.000	0.000
$35'$	2	57518.4	0.000	0.000
$36'$	2	61074.0	-0.029	0.028
$37'$	2	61189.9	-0.029	-0.028
$38'$	2	62972.8	0.042	0.000
$39'$	2	62989.7	0.000	0.000

Table 12: Calculated Δ excitation energies (in cm^{-1}) arising from the CASSCF method on complex I with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Δ	State	Δ	State	Δ	State	Δ	State	Δ
1	0.0	26	8054.3	51	22527.5	76	28890.9	101	45073.4
2	219.2	27	8054.3	52	22816.8	77	28890.9	102	45344.0
3	219.2	28	18298.2	53	22816.8	78	29252.5	103	45344.0
4	796.0	29	18298.2	54	23111.3	79	29252.5	104	45987.8
5	796.0	30	18803.3	55	23111.3	80	29611.0	105	45987.8
6	1102.9	31	18803.3	56	23535.1	81	29611.0	106	46220.2
7	1102.9	32	18950.9	57	23535.1	82	30832.9	107	46220.2
8	5120.4	33	18950.9	58	23999.1	83	30832.9	108	46880.9
9	5120.4	34	19545.1	59	23999.1	84	31014.9	109	46880.9
10	5352.8	35	19545.1	60	25094.5	85	31014.9	110	66560.8
11	5352.8	36	20016.5	61	25094.5	86	32258.9	111	66560.8
12	5398.0	37	20016.5	62	25580.5	87	32258.9	112	68716.1
13	5398.0	38	20074.6	63	25580.5	88	32325.0	113	68716.1
14	5430.7	39	20074.6	64	25977.4	89	32325.0	114	68806.9
15	5430.7	40	20419.4	65	25977.4	90	32615.6	115	68806.9
16	5781.9	41	20419.4	66	26390.4	91	32615.6	116	70099.6
17	5781.9	42	21538.7	67	26390.4	92	33233.3	117	70099.6
18	5930.2	43	21538.7	68	28100.6	93	33233.3	118	70636.5
19	5930.2	44	21549.2	69	28100.6	94	34218.0	119	70636.5
20	6306.6	45	21549.2	70	28560.3	95	34218.0		
21	6306.6	46	22338.2	71	28560.3	96	43825.5		
22	6758.9	47	22338.2	72	28747.6	97	43825.5		
23	6758.9	48	22456.0	73	28747.6	98	44143.1		
24	7916.3	49	22456.0	74	28825.1	99	44143.1		
25	7916.3	50	22527.5	75	28825.1	100	45073.4		

Table 13: Calculated Δ excitation energies (in cm^{-1}) arising from the CASSCF/NEVPT2 method on complex I with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Δ	State	Δ	State	Δ	State	Δ	State	Δ
1	0.0	26	11459.0	51	21791.8	76	28799.6	101	41504.4
2	145.7	27	11459.0	52	22088.0	77	28799.6	102	41777.7
3	145.7	28	15702.2	53	22088.0	78	29471.6	103	41777.7
4	1243.0	29	15702.2	54	22379.1	79	29471.6	104	42738.4
5	1243.0	30	16233.9	55	22379.1	80	30182.4	105	42738.4
6	1449.3	31	16233.9	56	23260.5	81	30182.4	106	42986.5
7	1449.3	32	17493.1	57	23260.5	82	30790.4	107	42986.5
8	8159.3	33	17493.1	58	24023.7	83	30790.4	108	44946.1
9	8159.3	34	18222.3	59	24023.7	84	31033.0	109	44946.1
10	8215.8	35	18222.3	60	24614.3	85	31033.0	110	57797.4
11	8215.8	36	18694.3	61	24614.3	86	33856.5	111	57797.4
12	8255.9	37	18694.3	62	25083.8	87	33856.5	112	61351.2
13	8255.9	38	19012.4	63	25083.8	88	34726.5	113	61351.2
14	8341.4	39	19012.4	64	26099.0	89	34726.5	114	61477.3
15	8341.4	40	19512.3	65	26099.0	90	35600.9	115	61477.3
16	9104.7	41	19512.3	66	26614.4	91	35600.9	116	63030.1
17	9104.7	42	21200.2	67	26614.4	92	35952.4	117	63030.1
18	9396.7	43	21200.2	68	28038.4	93	35952.4	118	63486.9
19	9396.7	44	21396.7	69	28038.4	94	37158.4	119	63486.9
20	9811.8	45	21396.7	70	28266.5	95	37158.4		
21	9811.8	46	21426.2	71	28266.5	96	39462.8		
22	10250.5	47	21426.2	72	28334.9	97	39462.8		
23	10250.5	48	21609.5	73	28334.9	98	39796.4		
24	11327.5	49	21609.5	74	28747.7	99	39796.4		
25	11327.5	50	21791.8	75	28747.7	100	41504.4		

Table 14: g-values and tensor from CASSCF calculation on complex II with DFT(BP86) optimized geometry.

	g-values	g-tensor		
g_1	1.787492	0.2987310	0.8416805	-0.4498151
g_2	1.817162	-0.2434029	0.5229466	0.8168732
g_3	3.459621	0.9227756	-0.1345391	0.3610879

Table 15: g-values and tensor from CASSCF/NEVPT2 calculation on complex II with DFT(BP86) optimized geometry.

	g-values	g-tensor		
g_1	1.474341	0.2955210	0.8478174	-0.4403102
g_2	1.488862	-0.2471627	0.5130551	0.8220006
g_3	3.521237	0.9228098	-0.1340901	0.3611674

Table 16: D-values and tensor from CASSCF calculation on complex II with DFT(BP86) optimized geometry. D in cm^{-1}.

	D-values	D-tensor		
D_{xx}	43.265461	-0.280067	0.407359	0.869265
D_{yy}	43.667557	0.265004	0.903124	-0.337845
D_{zz}	-86.933018	0.922678	-0.135739	0.360887
D	-130.399528			
E/D	0.001542			

Table 17: D-values and tensor from CASSCF/NEVPT2 calculation on complex II with DFT(BP86) optimized geometry. D in cm^{-1}.

	D-values	D-tensor		
D_{xx}	48.948456	-0.385047	-0.380174	0.840955
D_{yy}	49.198941	-0.023353	0.914935	0.402926
D_{zz}	-98.147397	0.922601	-0.135507	0.361171
D	-147.221096			
E/D	0.000851			

Table 18: Calculated δ excitation energies (in cm^{-1}) and individual contributions to D and E parameters arising from the CASSCF method on complex II with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten $S = \frac{3}{2}$ and forty $S = \frac{1}{2}$ ($'$) configurations.

Root	Mult	δ	D	E
0	4	0.0	0.000	0.000
1	4	189.2	-162.634	0.000
2	4	3635.4	7.454	-6.819
3	4	4310.1	10.379	5.697
4	4	4612.1	8.494	-3.324
5	4	4982.0	0.814	0.783
6	4	6263.0	0.019	-0.001
$0'$	2	18592.8	-0.548	0.437
$1'$	2	18720.7	-0.552	-0.533
$2'$	2	18867.3	0.023	-0.005
$3'$	2	18941.5	0.008	-0.009
$4'$	2	19067.6	0.015	0.000
$5'$	2	19671.6	-0.001	0.001
$6'$	2	19849.2	6.945	-0.001
7	4	20497.7	0.000	0.000
8	4	20848.5	0.000	0.000
$7'$	2	21975.3	-2.356	-1.445
$8'$	2	22008.3	-1.686	0.991
9	4	22105.0	0.002	-0.001
$9'$	2	23466.9	-0.002	-0.001
$10'$	2	24942.8	0.072	-0.003
$11'$	2	24980.1	0.253	-0.015
$12'$	2	25056.4	0.637	0.000
$13'$	2	25095.3	0.133	0.001
$14'$	2	27186.9	-0.072	0.063
$15'$	2	27221.0	-0.014	-0.011
$16'$	2	27521.4	-0.004	0.001
$\vdots$			$\vdots$	

Root	Mult	δ	D	E
⋮			⋮	
17′	2	27552.9	0.000	-0.001
18′	2	27873.1	-0.001	0.001
19′	2	28268.1	-0.150	0.091
20′	2	28292.2	-0.047	0.047
21′	2	29274.9	-1.263	-1.007
22′	2	29967.4	0.075	0.004
23′	2	30157.7	-0.038	0.029
24′	2	30230.3	-0.939	0.715
25′	2	30843.7	0.065	0.000
26′	2	31907.3	0.013	0.000
27′	2	31956.2	0.242	0.000
28′	2	43249.1	0.000	0.000
29′	2	43583.3	0.316	0.000
30′	2	44170.2	-0.073	-0.046
31′	2	44577.4	-0.061	0.040
32′	2	45083.1	-0.074	0.051
33′	2	45120.7	-0.026	-0.016
34′	2	45538.3	0.000	0.000
35′	2	66072.0	0.001	0.000
36′	2	67455.3	-0.014	0.010
37′	2	68692.7	-0.034	-0.024
38′	2	69046.6	-0.001	0.000
39′	2	69544.1	0.043	0.000

Table 19: Calculated δ excitation energies (in cm^{-1}) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on complex II with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten $S = \frac{3}{2}$ and forty $S = \frac{1}{2}$ ($'$) configurations.

Root	Mult	δ	D	E
0	4	0.0	0.000	0.000
1	4	68.5	-169.406	0.000
2	4	5690.6	4.791	2.215
3	4	6867.0	6.562	-5.706
4	4	7334.4	5.371	5.069
5	4	7458.4	0.544	0.118
6	4	9195.4	0.013	0.013
$0'$	2	16275.0	-0.626	0.348
$1'$	2	16445.4	-0.628	-0.173
$3'$	2	17523.0	0.009	-0.007
$2'$	2	17537.4	0.024	0.020
$4'$	2	17794.1	0.016	0.000
$5'$	2	18424.8	-0.001	-0.001
$6'$	2	18567.6	7.423	0.000
8	4	19308.1	0.000	0.000
7	4	19472.5	0.000	0.000
$9'$	2	20769.2	-0.002	-0.002
9	4	20943.7	0.002	0.001
$7'$	2	22783.9	-2.273	1.881
$8'$	2	22838.1	-1.625	-1.373
$10'$	2	23437.5	0.077	0.004
$12'$	2	23597.5	0.677	0.001
$13'$	2	23772.2	0.141	0.000
$11'$	2	24052.1	0.263	0.012
$18'$	2	26397.6	-0.002	-0.001
$14'$	2	26722.7	-0.073	-0.041
$\vdots$			$\vdots$	

Root	Mult	δ	D	E
⋮			⋮	
$15'$	2	26810.7	-0.014	-0.008
$16'$	2	27275.7	-0.004	-0.004
$17'$	2	27408.7	0.000	0.001
$19'$	2	27504.6	-0.154	-0.128
$20'$	2	27569.8	-0.048	0.002
$21'$	2	27982.6	-1.321	0.865
$24'$	2	29876.1	-0.950	-0.663
$25'$	2	31065.1	0.064	0.000
$22'$	2	31509.6	0.071	-0.003
$23'$	2	32070.9	-0.035	-0.024
$26'$	2	33575.1	0.012	0.000
$27'$	2	33607.9	0.230	0.000
$28'$	2	38495.4	0.000	0.000
$29'$	2	38824.3	0.355	0.000
$30'$	2	39949.1	-0.081	0.067
$31'$	2	40611.7	-0.067	-0.053
$32'$	2	41209.5	-0.081	-0.062
$33'$	2	41250.7	-0.028	0.022
$34'$	2	42559.7	0.000	0.000
$35'$	2	56895.6	0.001	0.000
$36'$	2	59284.9	-0.016	-0.013
$37'$	2	61024.1	-0.038	0.029
$38'$	2	61205.3	-0.001	0.001
$39'$	2	61681.7	0.048	0.000

Table 20: Calculated Δ excitation energies (in cm^{-1}) arising from the CASSCF method on complex II with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Δ	State	Δ	State	Δ	State	Δ	State	Δ
1	0.0	26	7008.4	51	22213.3	76	28337.6	101	44606.3
2	260.8	27	7008.4	52	22428.0	77	28337.6	102	45078.4
3	260.8	28	18624.1	53	22428.0	78	28489.1	103	45078.4
4	640.1	29	18624.1	54	22586.9	79	28489.1	104	45469.3
5	640.1	30	18938.1	55	22586.9	80	29090.0	105	45469.3
6	1008.0	31	18938.1	56	22670.4	81	29090.0	106	45716.9
7	1008.0	32	19245.2	57	22670.4	82	29844.7	107	45716.9
8	3923.3	33	19245.2	58	23978.4	83	29844.7	108	46044.9
9	3923.3	34	19688.5	59	23978.4	84	30530.1	109	46044.9
10	4056.3	35	19688.5	60	25215.1	85	30530.1	110	66561.5
11	4056.3	36	19885.8	61	25215.1	86	30716.2	111	66561.5
12	4355.5	37	19885.8	62	25325.8	87	30716.2	112	67968.9
13	4355.5	38	20117.9	63	25325.8	88	30753.1	113	67968.9
14	4669.7	39	20117.9	64	25769.7	89	30753.1	114	69192.3
15	4669.7	40	20284.7	65	25769.7	90	31601.6	115	69192.3
16	5047.1	41	20284.7	66	26002.9	91	31601.6	116	69480.7
17	5047.1	42	20816.6	67	26002.9	92	32094.9	117	69480.7
18	5139.2	43	20816.6	68	27447.5	93	32094.9	118	70131.2
19	5139.2	44	20879.1	69	27447.5	94	32959.8	119	70131.2
20	5467.6	45	20879.1	70	27786.4	95	32959.8		
21	5467.6	46	21205.9	71	27786.4	96	43709.5		
22	5867.0	47	21205.9	72	27883.3	97	43709.5		
23	5867.0	48	21337.8	73	27883.3	98	44041.6		
24	6825.4	49	21337.8	74	28142.3	99	44041.6		
25	6825.4	50	22213.3	75	28142.3	100	44606.3		

Table 21: Calculated Δ excitation energies (in cm^{-1}) arising from the CASSCF/NEVPT2 method on complex II with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Δ	State	Δ	State	Δ	State	Δ	State	Δ
1	0.0	26	9914.0	51	21041.0	76	27771.9	101	40443.4
2	294.4	27	9914.0	52	21448.5	77	27771.9	102	41146.4
3	294.4	28	16533.5	53	21448.5	78	28140.3	103	41146.4
4	635.5	29	16533.5	54	21704.8	79	28140.3	104	41628.7
5	635.5	30	17023.9	55	21704.8	80	28329.2	105	41628.7
6	1002.6	31	17023.9	56	23070.3	81	28329.2	106	41889.4
7	1002.6	32	17654.3	57	23070.3	82	28787.3	107	41889.4
8	6074.5	33	17654.3	58	23481.1	83	28787.3	108	43092.7
9	6074.5	34	18274.8	59	23481.1	84	30439.5	109	43092.7
10	6156.4	35	18274.8	60	23839.6	85	30439.5	110	57443.1
11	6156.4	36	18576.7	61	23839.6	86	31735.5	111	57443.1
12	6936.9	37	18576.7	62	24116.7	87	31735.5	112	59841.6
13	6936.9	38	18914.4	63	24116.7	88	32111.0	113	59841.6
14	7269.9	39	18914.4	64	24494.4	89	32111.0	114	61554.2
15	7269.9	40	19043.4	65	24494.4	90	32650.7	115	61554.2
16	7651.4	41	19043.4	66	24824.3	91	32650.7	116	61693.8
17	7651.4	42	19624.7	67	24824.3	92	33789.4	117	61693.8
18	7747.7	43	19624.7	68	26812.2	93	33789.4	118	62319.7
19	7747.7	44	19652.8	69	26812.2	94	34581.7	119	62319.7
20	8067.7	45	19652.8	70	27051.5	95	34581.7		
21	8067.7	46	19912.5	71	27051.5	96	39002.9		
22	8497.0	47	19912.5	72	27498.8	97	39002.9		
23	8497.0	48	20050.6	73	27498.8	98	39334.9		
24	9760.5	49	20050.6	74	27622.7	99	39334.9		
25	9760.5	50	21041.0	75	27622.7	100	40443.4		

Table 22: g-values and tensor from CASSCF calculation on complex III with DFT(BP86) optimized geometry.

	g-values	g-tensor		
g_1	2.274593	0.2040732	0.9788956	-0.0108461
g_2	2.291874	-0.3718304	0.0877560	0.9241434
g_3	2.878946	0.9055917	-0.1845600	0.3818918

Table 23: g-values and tensor from CASSCF/NEVPT2 calculation on complex III with DFT(BP86) optimized geometry.

	g-values	g-tensor		
g_1	2.187228	0.2020261	0.9792843	-0.0137039
g_2	2.198058	-0.3704863	0.0893689	0.9245286
g_3	2.705761	0.9066010	-0.1817018	0.3808663

Table 24: D-values and tensor from CASSCF calculation on complex III with DFT(BP86) optimized geometry. D in cm^{-1}.

	D-values	D-tensor		
D_{xx}	16.300864	-0.371378	0.093078	0.923804
D_{yy}	17.491067	0.208088	0.977997	-0.014885
D_{zz}	-33.791931	0.904863	-0.186705	0.382575
D	-50.687896			
E/D	0.011741			

Table 25: D-values and tensor from CASSCF/NEVPT2 calculation on complex III with DFT(BP86) optimized geometry. D in cm^{-1}.

	D-values	D-tensor		
D_{xx}	14.099932	-0.368912	0.101443	0.923912
D_{yy}	14.919405	0.209408	0.977541	-0.023716
D_{zz}	-29.019337	0.905567	-0.184725	0.381869
D	-43.529006			
E/D	0.009413			

Table 26: Calculated δ excitation energies (in cm^{-1}) and individual contributions to D and E parameters arising from the CASSCF method on complex III with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten $S = \frac{3}{2}$ and forty $S = \frac{1}{2}$ ($'$) configurations.

Root	Mult	δ	D	E
0	4	0.0	0.000	0.000
1	4	1090.2	-89.405	0.009
2	4	3241.2	17.193	-17.145
3	4	3378.8	16.154	16.140
4	4	4235.5	0.598	0.598
5	4	4316.5	0.352	-0.349
6	4	5220.7	0.003	0.003
$0'$	2	19288.2	0.000	0.000
$1'$	2	19313.1	0.010	0.000
$2'$	2	19389.4	-0.288	0.287
$3'$	2	19458.6	-0.249	-0.249
$4'$	2	19553.7	-0.006	0.005
$5'$	2	19640.5	-0.004	0.003
$6'$	2	20452.9	6.630	-0.003
7	4	20523.5	0.000	0.000
8	4	20793.8	0.001	-0.001
9	4	20963.9	0.001	0.001
$7'$	2	21524.2	-2.472	2.433
$8'$	2	21545.9	-2.464	-2.427
$9'$	2	24373.1	0.005	0.000
$10'$	2	25222.6	-0.022	0.024
$11'$	2	25313.8	0.046	-0.019
$12'$	2	25429.6	0.903	-0.006
$13'$	2	25764.3	-0.005	0.004
$14'$	2	26139.6	-0.089	-0.081
$15'$	2	26143.9	-0.097	0.090
$\vdots$			$\vdots$	

Root	Mult	δ	D	E
⋮			⋮	
$16'$	2	27391.5	-0.006	-0.008
$17'$	2	27414.4	-0.012	0.012
$18'$	2	27746.9	-0.084	-0.084
$19'$	2	27789.0	-0.072	0.072
$20'$	2	27867.8	-0.002	-0.001
$21'$	2	28117.3	-0.004	0.003
$22'$	2	28666.0	-0.001	-0.001
$23'$	2	29360.6	-1.002	-0.959
$24'$	2	29379.3	-0.964	0.915
$25'$	2	30381.1	0.000	0.000
$26'$	2	30643.1	0.732	0.000
$27'$	2	31162.8	0.000	0.000
$28'$	2	43413.1	0.000	0.000
$29'$	2	43817.8	0.278	-0.003
$30'$	2	44258.8	-0.116	0.115
$31'$	2	44320.8	-0.106	-0.111
$32'$	2	44749.0	-0.011	-0.011
$33'$	2	44753.9	-0.013	0.012
$34'$	2	45047.2	0.000	0.000
$35'$	2	66990.1	0.000	0.000
$36'$	2	67951.9	-0.001	0.001
$37'$	2	68330.1	-0.012	-0.020
$38'$	2	68502.8	-0.021	0.022
$39'$	2	68707.1	0.037	-0.003

Table 27: Calculated δ excitation energies (in cm^{-1}) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on complex III with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten $S = \frac{3}{2}$ and forty $S = \frac{1}{2}$ ($'$) configurations.

Root	Mult	δ	D	E
0	4	0.0	0.000	0.000
1	4	1548.0	-68.607	0.005
2	4	5153.8	10.984	-10.937
3	4	5364.7	10.324	10.296
4	4	6717.3	0.378	0.376
5	4	6813.5	0.223	-0.221
6	4	8088.0	0.002	0.002
$2'$	2	18061.8	-0.309	0.308
$0'$	2	18104.4	0.000	0.000
$3'$	2	18214.9	-0.266	-0.266
$1'$	2	18237.7	0.011	0.000
$5'$	2	18540.7	-0.004	0.003
$4'$	2	18959.7	-0.006	0.006
7	4	19077.0	0.000	0.000
8	4	19265.8	0.001	-0.001
9	4	19537.2	0.001	0.001
$6'$	2	19856.8	6.831	-0.003
$9'$	2	21917.6	0.005	0.000
$7'$	2	22114.2	-2.406	2.360
$8'$	2	22149.0	-2.397	-2.354
$12'$	2	23793.0	0.966	-0.006
$10'$	2	23986.9	-0.023	0.025
$11'$	2	24066.8	0.048	-0.020
$13'$	2	24273.3	-0.005	0.005
$14'$	2	25169.3	-0.092	-0.084
$\vdots$			$\vdots$	

Root	Mult	δ	D	E
⋮			⋮	
$15'$	2	25177.3	-0.101	0.092
$18'$	2	26621.4	-0.088	-0.088
$20'$	2	26730.5	-0.002	-0.001
$19'$	2	26829.6	-0.075	0.075
$17'$	2	27263.8	-0.012	0.012
$16'$	2	27382.7	-0.006	-0.008
$23'$	2	28452.4	-1.035	-0.995
$21'$	2	28509.8	-0.004	0.003
$24'$	2	28522.3	-0.993	0.947
$22'$	2	29910.6	-0.001	-0.001
$25'$	2	30527.1	0.000	0.000
$26'$	2	31321.4	0.716	0.000
$27'$	2	32373.2	0.000	0.000
$28'$	2	38769.6	0.000	0.000
$29'$	2	39203.1	0.312	-0.003
$30'$	2	39980.5	-0.128	0.127
$31'$	2	40075.3	-0.117	-0.122
$32'$	2	40819.2	-0.012	-0.012
$33'$	2	40836.5	-0.014	0.014
$34'$	2	41568.9	0.000	0.000
$35'$	2	58047.0	0.000	0.000
$36'$	2	59492.7	-0.001	0.001
$37'$	2	60368.8	-0.014	-0.022
$38'$	2	60632.7	-0.024	0.025
$39'$	2	60661.1	0.042	-0.004

Table 28: Calculated Δ excitation energies (in cm^{-1}) arising from the CASSCF method on complex III with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Δ	State	Δ	State	Δ	State	Δ	State	Δ
1	0.0	26	5792.8	51	21171.9	76	27869.1	101	44421.9
2	101.4	27	5792.8	52	21438.6	77	27869.1	102	44654.6
3	101.4	28	19121.1	53	21438.6	78	28034.2	103	44654.6
4	1222.9	29	19121.1	54	21558.8	79	28034.2	104	44960.0
5	1222.9	30	19152.1	55	21558.8	80	28439.7	105	44960.0
6	1460.8	31	19152.1	56	22012.2	81	28439.7	106	45136.9
7	1460.8	32	19551.9	57	22012.2	82	28557.2	107	45136.9
8	3247.8	33	19551.9	58	24570.7	83	28557.2	108	45356.8
9	3247.8	34	19977.6	59	24570.7	84	29040.3	109	45356.8
10	3442.6	35	19977.6	60	25273.8	85	29040.3	110	67260.5
11	3442.6	36	20042.1	61	25273.8	86	29593.6	111	67260.5
12	3493.5	37	20042.1	62	25636.7	87	29593.6	112	68190.6
13	3493.5	38	20168.5	63	25636.7	88	29754.5	113	68190.6
14	3569.0	39	20168.5	64	25922.4	89	29754.5	114	68651.7
15	3569.0	40	20588.9	65	25922.4	90	30793.2	115	68651.7
16	4103.7	41	20588.9	66	26133.1	91	30793.2	116	68814.3
17	4103.7	42	20617.7	67	26133.1	92	30985.1	117	68814.3
18	4372.7	43	20617.7	68	26312.1	93	30985.1	118	69056.6
19	4372.7	44	20699.0	69	26312.1	94	31837.9	119	69056.6
20	4744.3	45	20699.0	70	26658.9	95	31837.9		
21	4744.3	46	20863.5	71	26658.9	96	43658.7		
22	5200.1	47	20863.5	72	27525.2	97	43658.7		
23	5200.1	48	21014.1	73	27525.2	98	44065.4		
24	5614.6	49	21014.1	74	27591.2	99	44065.4		
25	5614.6	50	21171.9	75	27591.2	100	44421.9		

Table 29: Calculated Δ excitation energies (in cm^{-1}) arising from the CASSCF/NEVPT2 method on complex III with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Δ	State	Δ	State	Δ	State	Δ	State	Δ
1	0.0	26	8501.6	51	19919.9	76	27208.9	101	40107.8
2	87.1	27	8501.6	52	20015.7	77	27208.9	102	40339.6
3	87.1	28	17883.0	53	20015.7	78	27515.1	103	40339.6
4	1661.2	29	17883.0	54	22083.1	79	27515.1	104	40949.8
5	1661.2	30	18014.5	55	22083.1	80	27758.8	105	40949.8
6	1840.2	31	18014.5	56	22193.7	81	27758.8	106	41151.9
7	1840.2	32	18295.8	57	22193.7	82	28671.7	107	41151.9
8	5179.4	33	18295.8	58	22511.0	83	28671.7	108	41796.9
9	5179.4	34	18745.8	59	22511.0	84	28733.7	109	41796.9
10	5302.6	35	18745.8	60	23841.1	85	28733.7	110	58273.5
11	5302.6	36	18833.9	61	23841.1	86	29012.6	111	58273.5
12	5416.3	37	18833.9	62	24078.7	87	29012.6	112	59698.5
13	5416.3	38	19082.5	63	24078.7	88	30174.8	113	59698.5
14	5507.3	39	19082.5	64	24534.2	89	30174.8	114	60618.0
15	5507.3	40	19137.2	65	24534.2	90	30944.0	115	60618.0
16	6463.0	41	19137.2	66	24800.9	91	30944.0	116	60845.7
17	6463.0	42	19293.7	67	24800.9	92	31485.4	117	60845.7
18	6760.2	43	19293.7	68	25102.5	93	31485.4	118	60971.3
19	6760.2	44	19337.8	69	25102.5	94	32809.1	119	60971.3
20	7149.6	45	19337.8	70	25671.2	95	32809.1		
21	7149.6	46	19462.6	71	25671.2	96	38956.9		
22	7587.4	47	19462.6	72	26600.3	97	38956.9		
23	7587.4	48	19668.7	73	26600.3	98	39402.9		
24	8368.9	49	19668.7	74	26764.0	99	39402.9		
25	8368.9	50	19919.9	75	26764.0	100	40107.8		