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

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Part 1: Summary of structural parameters of all complexes.

Table S1: Bond distances (in Å) and bond angles (in degrees) for the complexes with 1,2- dicarba-closo-dodecaborane ligands from DFT (BP86) geometry optimization

No. S atoms substituted	bond distances					bond angles				
		A	B		C		A	B		C
0	CoX_1	2.2661	2.3191		2.3516	$\widehat{X_1CoX_2}$	95.04	99.22		102.41
	CoX_2	2.2659	2.3188		2.3528	$\widehat{X_1CoX_3}$	118.33	117.23		113.67
	CoX_3	2.2681	2.2948		2.3513	$\widehat{X_1CoX_4}$	115.76	114.47		112.59
	CoX_4	2.2653	2.2919		2.3506	$\widehat{X_2CoX_3}$	117.52	116.12		112.05
						$\widehat{X_2CoX_4}$	116.92	116.37		114.02
						$\widehat{X_3CoX_4}$	95.03	94.67		102.53
2	CoX_1	2.0140	2.3063	1.9764	2.0066	$\widehat{X_1CoX_2}$	87.17	100.81	96.88	96.32
	CoX_2	2.0157	2.3064	1.9828	2.0093	$\widehat{X_1CoX_3}$	120.14	118.74	119.00	115.40
	CoX_3	2.2587	2.0475	2.3143	2.3507	$\widehat{X_1CoX_4}$	117.17	115.87	114.51	113.95
	CoX_4	2.2561	2.0420	2.3180	2.3514	$\widehat{X_2CoX_3}$	119.38	117.49	113.89	114.50
						$\widehat{X_2CoX_4}$	119.10	118.43	117.35	114.90
						$\widehat{X_3CoX_4}$	96.14	86.62	96.64	102.46
4	CoX_1	1.9994	1.9783		2.0185	$\widehat{X_1CoX_2}$	90.73	97.82		96.32
	CoX_2	2.0007	1.9795		2.0182	$\widehat{X_1CoX_3}$	120.33	119.13		116.58
	CoX_3	2.0028	2.0399		2.0194	$\widehat{X_1CoX_4}$	119.22	116.87		116.02
	CoX_4	1.9969	2.0377		2.0176	$\widehat{X_2CoX_3}$	117.61	117.25		116.71
						$\widehat{X_2CoX_4}$	121.23	118.39		116.41
						$\widehat{X_3CoX_4}$	90.67	89.19		96.28

Table S2: Bond distances (in Å) and bond angles (in degrees) for the complexes with 1,2-dicarba-closo-hexaboran ligands from DFT (BP86) geometry optimization

No. S atoms substituted	bond distances					bond angles				
		A	B		C		A	B		C
0	CoX_1	2.3232	2.4086		2.4179	$\widehat{X_1CoX_2}$	94.50	109.01		108.49
	CoX_2	2.3209	2.4075		2.4165	$\widehat{X_1CoX_3}$	118.40	113.68		109.57
	CoX_3	2.3231	2.3521		2.4179	$\widehat{X_1CoX_4}$	116.73	111.64		110.13
	CoX_4	2.3215	2.3502		2.4173	$\widehat{X_2CoX_3}$	116.49	111.45		110.37
						$\widehat{X_2CoX_4}$	118.14	114.03		109.71
						$\widehat{X_3CoX_4}$	94.50	96.70		108.56
2	CoX_1	2.0314	2.4034	2.0683	2.0822	$\widehat{X_1CoX_2}$	91.00	109.82	104.55	104.18
	CoX_2	2.0309	2.4022	2.0650	2.0676	$\widehat{X_1CoX_3}$	121.56	114.17	114.75	110.80
	CoX_3	2.3419	2.0410	2.3528	2.4183	$\widehat{X_1CoX_4}$	113.83	113.41	113.15	111.19
	CoX_4	2.3390	2.0380	2.3512	2.4197	$\widehat{X_2CoX_3}$	113.95	113.49	113.04	111.34
						$\widehat{X_2CoX_4}$	121.25	114.21	114.96	110.59
						$\widehat{X_3CoX_4}$	97.31	90.73	96.78	108.73
4	CoX_1	2.0321	2.0682		2.0867	$\widehat{X_1CoX_2}$	91.00	105.58		104.34
	CoX_2	2.0324	2.0667		2.0760	$\widehat{X_1CoX_3}$	121.51	115.66		112.03
	CoX_3	2.0310	2.0450		2.0814	$\widehat{X_1CoX_4}$	117.33	114.78		112.08
	CoX_4	2.0307	2.0437		2.0787	$\widehat{X_2CoX_3}$	117.35	114.87		112.50
						$\widehat{X_2CoX_4}$	121.53	115.59		111.56
						$\widehat{X_3CoX_4}$	91.05	90.40		104.55

Part 2: Optimized structures, g-tensors, excitation energies, temperature-dependent magnetic susceptibility, and field-dependent molar magnetization for Co(II) 1,2-dicarba-closo-dodecaborane complexes (Figure 2 in the main text).

Table S3. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex A0 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	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 S4. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex B0 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	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 S5. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex C0 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	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 S6. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex A2 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
B	1.962956	5.812532	-8.243246
H	1.858089	4.664932	-8.560363
B	0.757104	6.552372	-7.181661
H	-0.228839	5.985215	-6.828893
B	1.550431	8.525656	-9.057431
H	1.068731	9.218604	-9.898140
B	2.409085	6.395561	-6.615410
H	2.695506	5.624770	-5.741693
B	3.184291	7.993658	-6.785043
H	4.038544	8.365711	-6.028890
B	3.481965	6.714072	-8.005840
H	4.547460	6.174062	-8.119559
B	2.463815	7.058604	-9.426638
H	2.702050	6.772416	-10.562353
B	1.982841	9.126868	-7.451951
H	1.884688	10.291812	-7.203296
B	1.482176	7.880876	-6.268003
H	1.038882	8.184001	-5.200425
B	3.214447	8.400683	-8.521764
H	4.078188	9.072029	-9.014471
B	-7.551468	7.861708	-10.819194
H	-8.702241	7.527799	-10.784778
B	-6.594027	8.001355	-9.325293
H	-6.949040	7.760741	-8.212206
B	-4.824657	7.189921	-11.426183
H	-3.959158	6.439940	-11.737245
B	-6.448021	7.350204	-12.125331
H	-6.789843	6.646000	-13.032629
B	-6.930215	9.061762	-11.985293
H	-7.630071	9.598937	-12.797097
B	-6.249095	6.695840	-10.484791
H	-6.365648	5.548953	-10.178116
B	-5.245700	8.635723	-12.370058
H	-4.659579	8.852177	-13.386461
B	-5.591061	9.941462	-11.210412
H	-5.244530	11.063388	-11.420193
B	-7.007477	9.462857	-10.248404
H	-7.753492	10.286007	-9.798691
B	-5.374086	9.268453	-9.580185
H	-4.867877	9.869212	-8.690150
C	-4.990546	7.584701	-9.745734
C	-4.371698	8.783893	-10.909756
C	0.833844	6.928282	-8.898080
C	0.531817	8.229600	-7.655639
Co	-1.826694	7.842259	-9.165483
O	-0.236486	6.688008	-9.607137
O	-0.695990	8.672560	-7.717955
S	-3.801611	6.891416	-8.620384
S	-2.636889	9.153708	-10.812752

Table S7. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex B2 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
B	2.062664	5.811584	-8.208383
H	2.247770	4.656361	-8.450327
B	0.840037	6.509218	-7.126827
H	0.003441	5.825033	-6.621241
B	1.633415	8.538354	-9.044555
H	1.362250	9.308436	-9.913610
B	2.503571	6.380599	-6.579794
H	3.024410	5.703557	-5.744376
C	3.165258	7.946628	-6.841246
H	4.010877	8.209546	-6.211150
C	3.444822	6.776966	-7.963303
H	4.451473	6.367436	-7.978885
B	2.548768	7.058257	-9.385428
H	3.060027	6.737488	-10.416170
B	2.059770	9.107033	-7.418845
H	2.225984	10.234346	-7.059991
B	1.573450	7.860735	-6.241210
H	1.412982	8.151754	-5.093532
B	3.294197	8.405872	-8.493333
H	4.297316	8.963565	-8.824683
B	-7.593776	7.875431	-10.836280
H	-8.751207	7.555655	-10.814308
B	-6.646296	8.013723	-9.333388
H	-7.032161	7.780459	-8.225614
B	-4.893560	7.192030	-11.441628
H	-4.014755	6.441952	-11.730099
B	-6.493183	7.356818	-12.141754
H	-6.851727	6.658577	-13.050703
B	-6.956777	9.073762	-12.007712
H	-7.659890	9.609469	-12.820986
B	-6.302977	6.695845	-10.495213
H	-6.451050	5.547353	-10.195386
B	-5.273700	8.634365	-12.391699
H	-4.700699	8.847055	-13.419915
B	-5.616306	9.952562	-11.229361
H	-5.282199	11.079613	-11.449833
B	-7.045944	9.477124	-10.272191
H	-7.801359	10.303905	-9.838037
B	-5.435664	9.273076	-9.606515
H	-4.905017	9.860476	-8.716327
C	-5.033985	7.563117	-9.725968
C	-4.380213	8.797670	-10.932789
B	0.806128	6.919579	-8.901567
B	0.496345	8.219399	-7.655660
Co	-2.229788	7.870456	-9.310051
S	-0.564323	6.432864	-10.001725
S	-1.167112	8.962213	-7.578523
O	-4.096347	7.112072	-8.945033
O	-3.104071	8.991915	-10.775546

Table S8. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex B'2 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
B	1.982407	5.815085	-8.264421
H	2.180971	4.659375	-8.506421
B	0.781365	6.491803	-7.149371
H	-0.055917	5.799784	-6.648368
B	1.554185	8.557616	-9.056574
H	1.261265	9.336854	-9.914304
B	2.432273	6.367208	-6.627965
H	2.977804	5.687375	-5.808639
C	3.086265	7.941423	-6.876598
H	3.940253	8.194734	-6.254614
C	3.360608	6.786563	-8.017478
H	4.369915	6.385244	-8.041400
B	2.453994	7.079290	-9.429993
H	2.973398	6.784159	-10.467490
B	1.973485	9.108144	-7.426097
H	2.156694	10.233685	-7.061302
B	1.501856	7.845052	-6.259082
H	1.364098	8.106895	-5.098658
B	3.200747	8.423714	-8.526151
H	4.208218	8.981664	-8.849042
B	-7.582467	7.868384	-10.846540
H	-8.735009	7.534633	-10.822450
B	-6.646999	8.037875	-9.340207
H	-7.031760	7.830635	-8.229029
B	-4.841049	7.203002	-11.387290
H	-3.976787	6.443746	-11.682932
B	-6.457062	7.336324	-12.124206
H	-6.783111	6.611991	-13.023167
B	-6.947518	9.047703	-12.027719
H	-7.639927	9.567274	-12.859189
B	-6.285007	6.708394	-10.472891
H	-6.413429	5.562634	-10.162650
B	-5.256030	8.617868	-12.384362
H	-4.669216	8.804250	-13.407464
B	-5.621711	9.948225	-11.253423
H	-5.292560	11.074169	-11.475820
B	-7.042931	9.479017	-10.298579
H	-7.796455	10.310323	-9.873340
B	-5.411581	9.289430	-9.613964
H	-4.928453	9.915003	-8.726895
C	-5.046865	7.587968	-9.704128
C	-4.384331	8.823867	-10.938183
B	0.677762	6.926367	-8.948166
B	0.370076	8.222910	-7.667014
Co	-1.860280	7.838407	-9.153609
O	-0.398835	6.630311	-9.711180
O	-0.891460	8.709228	-7.658819
S	-3.898799	6.927329	-8.545036
S	-2.671224	9.208369	-10.838481

Table S9. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex C2 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
B	2.028602	5.806800	-8.211771
H	2.215326	4.643457	-8.431555

B	0.825464	6.519355	-7.121025
H	-0.022815	5.845361	-6.613220
B	1.650596	8.541797	-9.054712
H	1.388079	9.313810	-9.929059
B	2.468482	6.377730	-6.579794
H	2.996392	5.702773	-5.743124
C	3.152705	7.936751	-6.846769
H	4.004492	8.186612	-6.220160
C	3.420096	6.759879	-7.964708
H	4.423230	6.342158	-7.971232
B	2.531024	7.042743	-9.391732
H	3.060169	6.721399	-10.417803
B	2.062681	9.110358	-7.427655
H	2.262831	10.239127	-7.078134
B	1.558741	7.875721	-6.246290
H	1.415860	8.159094	-5.090374
B	3.289212	8.389986	-8.503788
H	4.310276	8.927232	-8.824111
C	-7.475108	7.890750	-10.842295
H	-8.535910	7.663940	-10.911912
B	-6.659403	8.005908	-9.351149
H	-7.301681	7.770732	-8.370271
B	-4.895781	7.185526	-11.481729
H	-4.154583	6.368733	-11.938245
B	-6.505148	7.352104	-12.157324
H	-7.067303	6.783427	-13.046873
C	-6.906833	9.007351	-11.916921
H	-7.640954	9.419653	-12.604464
B	-6.299384	6.701083	-10.516265
H	-6.700170	5.592749	-10.314835
B	-5.309851	8.647659	-12.390533
H	-5.011545	8.917785	-13.516269
B	-5.669656	9.953101	-11.225254
H	-5.613897	11.096175	-11.571023
B	-7.087027	9.466704	-10.268868
H	-8.004292	10.187745	-10.005072
B	-5.480021	9.305413	-9.586837
H	-5.158472	10.013946	-8.681536
B	-4.927823	7.564009	-9.689692
B	-4.294417	8.812470	-10.892409
B	0.738596	6.923597	-8.932953
B	0.437767	8.251937	-7.672467
Co	-1.807776	7.855455	-9.160057
O	-0.321627	6.622524	-9.705523
O	-0.806591	8.765192	-7.674294
S	-3.798883	6.800356	-8.490783
S	-2.542798	9.283130	-10.877830

Table S10. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex A4 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
B	1.753979	5.831743	-8.332115
H	1.667561	4.683137	-8.650551
B	0.546088	6.547732	-7.256747
H	-0.424847	5.961301	-6.893483
B	1.278900	8.538230	-9.131731

H	0.772466	9.223438	-9.965170
B	2.207642	6.418858	-6.709822
H	2.517371	5.650802	-5.841921
B	2.951430	8.031680	-6.882591
H	3.806637	8.417838	-6.134923
B	3.258390	6.761524	-8.111698
H	4.331689	6.241185	-8.240988
B	2.218622	7.093191	-9.519076
H	2.448537	6.816864	-10.658741
B	1.723584	9.145107	-7.532477
H	1.607461	10.307451	-7.280536
B	1.258713	7.884247	-6.344890
H	0.822873	8.174737	-5.270951
B	2.953734	8.444250	-8.617713
H	3.797764	9.133167	-9.119593
B	-7.276356	7.843328	-10.718714
H	-8.431418	7.520073	-10.694042
B	-6.329956	7.992410	-9.216550
H	-6.709916	7.760235	-8.107617
B	-4.575627	7.162689	-11.322460
H	-3.689942	6.417144	-11.602818
B	-6.175595	7.322790	-12.022710
H	-6.529785	6.620168	-12.928239
B	-6.641489	9.039186	-11.895447
H	-7.342997	9.570028	-12.711366
B	-5.983423	6.668377	-10.375172
H	-6.123435	5.522297	-10.066480
B	-4.957943	8.600403	-12.276487
H	-4.379703	8.811490	-13.300905
B	-5.306141	9.925093	-11.118436
H	-4.968641	11.049249	-11.342954
B	-6.734318	9.449355	-10.161860
H	-7.490567	10.275103	-9.730810
B	-5.124784	9.255034	-9.492899
H	-4.590546	9.843047	-8.605205
C	-4.721372	7.544142	-9.610484
C	-4.072361	8.773560	-10.818072
C	0.599938	6.921175	-8.977570
C	0.285038	8.227989	-7.713582
Co	-1.992403	7.851599	-9.240288
O	-0.462710	6.644019	-9.686674
O	-0.948038	8.661762	-7.738423
O	-3.793144	7.086816	-8.811824
O	-2.790089	8.986253	-10.676897

Table S11. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex B4 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
B	1.787220	5.835164	-8.312605
H	1.981550	4.675227	-8.537587
B	0.577879	6.534217	-7.220871
H	-0.267490	5.852899	-6.718480
B	1.382743	8.568921	-9.148280
H	1.106200	9.338736	-10.020043
B	2.222047	6.407110	-6.679666
H	2.754141	5.735195	-5.845001

C	2.888152	7.974157	-6.942970
H	3.736825	8.231556	-6.315441
C	3.167687	6.801837	-8.064909
H	4.174735	6.394171	-8.073028
B	2.278225	7.080523	-9.490721
H	2.806869	6.767150	-10.518212
B	1.788797	9.138905	-7.520888
H	1.974029	10.268198	-7.168762
B	1.296913	7.894629	-6.341396
H	1.147966	8.174591	-5.186584
B	3.022624	8.432616	-8.598153
H	4.036466	8.980776	-8.918236
B	-7.352983	7.841426	-10.743637
H	-8.508729	7.515365	-10.720158
B	-6.404996	7.985883	-9.241566
H	-6.791222	7.750679	-8.134095
B	-4.648866	7.174230	-11.350126
H	-3.766020	6.428954	-11.640743
B	-6.250875	7.330070	-12.050462
H	-6.607166	6.630856	-12.959740
B	-6.723365	9.044285	-11.915608
H	-7.429799	9.576671	-12.728337
B	-6.056048	6.668151	-10.406639
H	-6.199738	5.518353	-10.108787
B	-5.038607	8.612460	-12.301657
H	-4.470061	8.828533	-13.331902
B	-5.388736	9.930833	-11.136949
H	-5.063707	11.060704	-11.357911
B	-6.812965	9.445886	-10.179662
H	-7.573462	10.267854	-9.744825
B	-5.199653	9.249487	-9.516283
H	-4.672307	9.839674	-8.625418
C	-4.794383	7.534982	-9.629268
C	-4.140528	8.789778	-10.849998
B	0.495771	6.942328	-9.027538
B	0.182289	8.262056	-7.765328
Co	-2.026795	7.855013	-9.250734
O	-0.569552	6.635677	-9.801669
O	-1.074334	8.761568	-7.771026
O	-3.868306	7.079704	-8.839737
O	-2.867563	9.003261	-10.709067

Table S12. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex C4 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
B	1.846997	5.827361	-8.269196
H	2.032302	4.661653	-8.478975
B	0.633339	6.551112	-7.198133
H	-0.222241	5.882375	-6.695020
B	1.487570	8.557675	-9.136304
H	1.239997	9.325150	-10.019549
B	2.269912	6.408065	-6.636255
H	2.786155	5.737233	-5.788680
C	2.962519	7.963077	-6.905634
H	3.807720	8.214835	-6.270869
C	3.239152	6.777303	-8.012625

H	4.241101	6.356581	-8.004736
B	2.367217	7.053425	-9.451718
H	2.908207	6.723412	-10.469204
B	1.882323	9.135569	-7.508236
H	2.082145	10.266236	-7.163667
B	1.360747	7.910754	-6.324303
H	1.205017	8.202966	-5.172009
B	3.119337	8.404381	-8.564402
H	4.146558	8.935518	-8.876196
C	-7.260486	7.870918	-10.746573
H	-8.323346	7.653805	-10.813534
B	-6.431914	7.963556	-9.259805
H	-7.080614	7.736155	-8.277558
B	-4.705816	7.156881	-11.429349
H	-3.965439	6.341714	-11.897719
B	-6.305686	7.334767	-12.077439
H	-6.893998	6.784320	-12.963781
C	-6.701931	8.990946	-11.815127
H	-7.448265	9.405894	-12.487439
B	-6.090971	6.670834	-10.436668
H	-6.505369	5.560382	-10.257116
B	-5.111006	8.637951	-12.312967
H	-4.840394	8.906559	-13.449348
B	-5.451754	9.931008	-11.136426
H	-5.415227	11.082056	-11.468578
B	-6.862134	9.441201	-10.160537
H	-7.784267	10.157210	-9.892506
B	-5.264889	9.273717	-9.501314
H	-4.926073	9.973907	-8.591933
B	-4.664948	7.515197	-9.601590
B	-4.036151	8.781638	-10.809789
B	0.567141	6.941492	-9.016378
B	0.255303	8.283203	-7.764768
Co	-1.982654	7.871542	-9.265552
O	-0.480249	6.634449	-9.800888
O	-0.984609	8.803184	-7.779309
O	-3.737720	7.001796	-8.774294
O	-2.721734	9.050341	-10.726706

Table S13. g-values and tensor from CASSCF calculation on Complex A0 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.018455	2.023477	3.257789
		g-tensor	
X	0.1291430	-0.3620697	0.9231617
Y	0.9913830	0.0265324	-0.1282804
Z	0.0219527	0.9317733	0.3623763

Table S14. g-values and tensor from CASSCF/NEVPT2 calculation on Complex A0 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.071610	2.074431	2.910551
		g-tensor	

X	0.1255654	-0.3639097	0.9229318
Y	0.9915390	0.0151627	-0.1289208
Z	0.0329214	0.9313108	0.3627346

Table S15. g-values and tensor from CASSCF calculation on Complex B0 with DFT(BP86) optimized geometry.

		g-values	
	1.787492	1.817162	3.459621
		g-tensor	
X	0.2987310	-0.2434029	0.9227756
Y	0.8416805	0.5229466	-0.1345391
Z	-0.4498151	0.8168732	0.3610879

Table S16. g-values and tensor from CASSCF/NEVPT2 calculation on Complex B0 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	1.474341	1.488862	3.521237
		g-tensor	
X	0.2955210	-0.2471627	0.9228098
Y	0.8478174	0.5130551	-0.1340901
Z	-0.4403102	0.8220006	0.3611674

Table S17. g-values and tensor from CASSCF calculation on Complex C0 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.274593	2.291874	2.878946
		g-tensor	
X	0.2040732	-0.3718304	0.9055917
Y	0.9788956	0.0877560	-0.1845600
Z	-0.0108461	0.9241434	0.3818918

Table S18. g-values and tensor from CASSCF/NEVPT2 calculation on Complex C0 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.187228	2.198058	2.705761
		g-tensor	
X	0.2020261	-0.3704863	0.9066010
Y	0.9792843	0.0893689	-0.1817018
Z	-0.0137039	0.9245286	0.3808663

Table S19. g-values and tensor from CASSCF calculation on Complex A2 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	1.671169	1.713031	3.498957
		g-tensor	

X	0.3060795	-0.2094605	0.9286774
Y	0.7871174	0.6043936	-0.1231040
Z	-0.5355012	0.7686577	0.3498625

Table S20. g-values and tensor from CASSCF/NEVPT2 calculation on Complex A2 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	1.674447	1.691807	3.486312
		g-tensor	
X	0.3016243	-0.2164827	0.9285246
Y	0.8000015	0.5872645	-0.1229556
Z	-0.5186718	0.7799075	0.3503198

Table S21. g-values and tensor from CASSCF calculation on Complex B2 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.148042	2.173564	3.174428
		g-tensor	
X	0.0273727	-0.3951767	0.9181972
Y	0.9591524	-0.2483407	-0.1354753
Z	0.2815624	0.8843994	0.3722369

Table S22. g-values and tensor from CASSCF/NEVPT2 calculation on Complex B2 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.067862	2.078891	3.184920
		g-tensor	
X	0.2795102	-0.2795209	0.9185544
Y	0.8865449	0.4424700	-0.1351239
Z	-0.3686628	0.8521082	0.3714827

Table S23. g-values and tensor from CASSCF calculation on Complex B2' with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.110784	2.310122	2.904887
		g-tensor	
X	-0.3370423	-0.1646453	-0.926981
Y	-0.7508293	0.6410388	0.159137
Z	0.5680298	0.7496407	-0.339677

Table S24. g-values and tensor from CASSCF/NEVPT2 calculation on Complex B2' with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.075016	2.208211	2.868764
		g-tensor	

X	-0.3384092	-0.1656893	-0.926297
Y	-0.7456357	0.6477030	0.156550
Z	0.5740266	0.7436584	-0.342732

Table S25. g-values and tensor from CASSCF calculation on Complex C2 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.199898	2.364370	2.771566
		g-tensor	
X	-0.3389365	0.1504250	0.9287057
Y	-0.7026213	-0.6969357	-0.1435411
Z	0.6256560	-0.7011797	0.3419088

Table S26. g-values and tensor from CASSCF/NEVPT2 calculation on Complex C2 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.152657	2.250117	2.673557
		g-tensor	
X	-0.3396444	0.1515818	0.9282590
Y	-0.6996211	-0.7003377	-0.1416242
Z	0.6286271	-0.6975314	0.3439156

Table S27. g-values and tensor from CASSCF calculation on Complex A4 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.160402	2.185068	3.062497
		g-tensor	
X	0.1707271	-0.3732705	0.9118779
Y	0.9853098	0.0608262	-0.1595767
Z	0.0040992	0.9257264	0.3781718

Table S28. g-values and tensor from CASSCF/NEVPT2 calculation on Complex A4 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.102377	2.123458	3.100670
		g-tensor	
X	0.1682119	-0.3727653	0.9125518
Y	0.9857354	0.0584298	-0.1578342
Z	0.0055148	0.9260842	0.3772766

Table S29. g-values and tensor from CASSCF calculation on Complex B4 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.170244	2.319370	2.835496

		g-tensor	
X	-0.3395891	0.1757972	0.9239992
Y	-0.7234903	-0.6765682	-0.1371761
Z	0.6010333	-0.7150880	0.3569428

Table S30. g-values and tensor from CASSCF/NEVPT2 calculation on Complex B4 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.132819	2.257354	2.802094
		g-tensor	
X	-0.3395007	0.1768687	0.9238272
Y	-0.7239662	-0.6761760	-0.1365977
Z	0.6005099	-0.7151947	0.3576092

Table S31. g-values and tensor from CASSCF calculation on Complex C4 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.263915	2.265288	2.733296
		g-tensor	
X	0.1732607	-0.3384989	0.9248780
Y	0.9780479	0.1695246	-0.1211764
Z	-0.1157715	0.9255700	0.3604401

Table S32. g-values and tensor from CASSCF/NEVPT2 calculation on Complex C4 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.212315	2.213415	2.669779
		g-tensor	
X	0.1725989	-0.3387507	0.9249095
Y	0.9783822	0.1675620	-0.1212074
Z	-0.1139206	0.9258353	0.3603487

Table S33. D-values and tensor from CASSCF calculation on Complex A0 with DFT(BP86) optimized geometry. D in cm-1.

	Dxx	Dyy	Dzz
		D-values	
	36.396873	36.661112	-73.057984
		D-tensor	
	-0.365550	0.120059	0.923016
	0.000320	0.991663	-0.128861
	0.930791	0.046810	0.362541

D = -109.586977
E/D = 0.001206

Table S34. D-values and tensor from CASSCF/NEVPT2 calculation on Complex A0 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
D-values		
24.167314	24.396612	-48.563926
D-tensor		
-0.346829	0.169616	0.922464
0.133276	0.982445	-0.130535
0.928411	-0.077669	0.363346

D = -72.845889
E/D = 0.001574

Table S35. D-values and tensor from CASSCF calculation on Complex B0 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
D-values		
43.265461	43.667557	-86.933018
D-tensor		
-0.280067	0.265004	0.922678
0.407359	0.903124	-0.135739
0.869265	-0.337845	0.360887

D = -130.399528
E/D = 0.001542

Table S36. D-values and tensor from CASSCF/NEVPT2 calculation on Complex B0 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
D-values		
48.948456	49.198941	-98.147397
D-tensor		
-0.385047	-0.023353	0.922601
-0.380174	0.914935	-0.135507
0.840955	0.402926	0.361171

D = -147.221096
E/D = 0.000851

Table S37. D-values and tensor from CASSCF calculation on Complex C0 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
D-values		
16.300864	17.491067	-33.791931
D-tensor		
-0.371378	0.208088	0.904863
0.093078	0.977997	-0.186705
0.923804	-0.014885	0.382575

D = -50.687896
E/D = 0.011741

Table S38. D-values and tensor from CASSCF/NEVPT2 calculation on Complex C0 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz

```
                D-values
   14.099932    14.919405   -29.019337
                D-tensor
   -0.368912     0.209408     0.905567
    0.101443     0.977541    -0.184725
    0.923912    -0.023716     0.381869

D   =  -43.529006
E/D =    0.009413
```

Table S39. D-values and tensor from CASSCF calculation on Complex A2 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
   45.527362    46.195819   -91.723181
                D-tensor
   -0.201272     0.310889     0.928891
    0.622485     0.772784    -0.123762
    0.756308    -0.553311     0.349063

D   = -137.584771
E/D =    0.002429
```

Table S40. D-values and tensor from CASSCF/NEVPT2 calculation on Complex A2 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
   47.048641    48.033216   -95.081858
                D-tensor
   -0.151841     0.338297     0.928708
    0.734697     0.667169    -0.122906
    0.661184    -0.663657     0.349850

D   = -142.622787
E/D =    0.003452
```

Table S41. D-values and tensor from CASSCF calculation on Complex B2 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
   29.106255    30.741389   -59.847644
                D-tensor
   -0.396168    -0.015214     0.918052
   -0.350675     0.926574    -0.135972
    0.848574     0.375805     0.372414

D   =  -89.771466
E/D =    0.009107
```

Table S42. D-values and tensor from CASSCF/NEVPT2 calculation on Complex B2 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
```

```
   32.928185    33.405122   -66.333307
                D-tensor
   -0.303348     0.254009     0.918401
    0.362072     0.922252    -0.135482
    0.881410    -0.291429     0.371733

D   =  -99.499960
E/D =    0.002397
```

Table S43. D-values and tensor from CASSCF calculation on Complex B2' with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
   12.860666    27.464511   -40.325177
                D-tensor
   -0.159847    -0.338715    -0.927211
    0.648424    -0.744255     0.160095
    0.744309     0.575635    -0.338598

D   =  -60.487765
E/D =    0.120717
```

Table S44. D-values and tensor from CASSCF/NEVPT2 calculation on Complex B2' with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
   15.656270    26.649133   -42.305403
                D-tensor
   -0.159750    -0.340246    -0.926668
    0.656521    -0.737647     0.157664
    0.737198     0.583189    -0.341217

D   =  -63.458104
E/D =    0.086615
```

Table S45. D-values and tensor from CASSCF calculation on Complex C2 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
    7.266241    20.435506   -27.701748
                D-tensor
   -0.148424    -0.339394    -0.928860
    0.698284    -0.701067     0.144581
    0.700264     0.627149    -0.341049

D   =  -41.552621
E/D =    0.158465
```

Table S46. D-values and tensor from CASSCF/NEVPT2 calculation on Complex C2 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
    8.907413    17.739129   -26.646542
```

D-tensor
0.148947 -0.340109 -0.928515
-0.702330 -0.697385 0.142784
-0.696095 0.630857 -0.342742

D = -39.969813
E/D = 0.110480

Table S47. D-values and tensor from CASSCF calculation on Complex A4 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
D-values		
25.537761	27.118845	-52.656606
D-tensor		
-0.373457	0.172887	0.911394
0.063177	0.984938	-0.160950
0.925494	0.002529	0.378755

D = -78.984908
E/D = 0.010009

Table S48. D-values and tensor from CASSCF/NEVPT2 calculation on Complex A4 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
D-values		
28.688900	30.104019	-58.792918
D-tensor		
-0.373058	0.170355	0.912035
0.060546	0.985374	-0.159288
0.925830	0.004203	0.377916

D = -88.189378
E/D = 0.008023

Table S49. D-values and tensor from CASSCF calculation on Complex B4 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
D-values		
11.241619	22.755504	-33.997124
D-tensor		
0.174224	-0.339997	-0.924147
-0.678418	-0.721674	0.137607
-0.713719	0.602984	-0.356393

D = -50.995685
E/D = 0.112891

Table S50. D-values and tensor from CASSCF/NEVPT2 calculation on Complex B4 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
D-values		
12.306359	22.588089	-34.894447
D-tensor		

0.174756	-0.340033	-0.924034
-0.678879	-0.721346	0.137054
-0.713150	0.603356	-0.356901

D = -52.341671
E/D = 0.098217

Table S51. D-values and tensor from CASSCF calculation on Complex C4 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
	D-values	
13.224577	13.331862	-26.556439
	D-tensor	
-0.336891	0.176715	0.924812
0.179190	0.976310	-0.121280
0.924335	-0.124859	0.360575

D = -39.834659
E/D = 0.001347

Table S52. D-values and tensor from CASSCF/NEVPT2 calculation on Complex C4 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
	D-values	
12.867456	12.950834	-25.818289
	D-tensor	
-0.321624	0.202997	0.924851
0.256618	0.958880	-0.121225
0.911430	-0.198345	0.360492

D = -38.727434
E/D = 0.001076

Table S53. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex A0 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	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
7	4	21277.1	0.000	-0.000
8	4	22213.7	0.002	0.002
9	4	22302.8	0.001	-0.001
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
6'	2	20102.3	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
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 S54. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex A0 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	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
7	4	21324.0	0.000	-0.000
8	4	21601.7	0.002	0.002
9	4	21726.0	0.001	-0.001
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

4'	2	18623.1	0.000	-0.000
5'	2	18484.8	-0.000	0.000
6'	2	19311.2	7.367	0.000
7'	2	24538.3	-1.648	0.771
8'	2	24719.8	-1.680	-0.754
9'	2	21275.6	-0.075	0.022
10'	2	23021.0	1.188	-0.000
11'	2	23662.2	-0.002	0.002
12'	2	26009.4	-0.006	0.007
13'	2	26066.8	-0.000	-0.005
14'	2	28263.7	-0.004	-0.005
15'	2	28264.3	-0.002	0.003
16'	2	28153.4	-0.000	0.000
17'	2	29853.7	-0.001	0.000
18'	2	29270.6	-0.005	0.005
19'	2	28062.2	-0.127	0.125
20'	2	28179.2	-0.117	-0.116
21'	2	30523.3	-1.069	1.037
22'	2	30559.8	-1.100	-1.067
23'	2	33516.9	-0.000	-0.000
24'	2	35309.0	-0.000	0.000
25'	2	34392.4	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 S55. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex B0 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	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
7	4	20497.7	0.000	-0.000
8	4	20848.5	0.000	0.000
9	4	22105.0	0.002	-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'	2	21975.3	-2.356	-1.445
8'	2	22008.3	-1.686	0.991
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
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 S56. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex B0 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	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
7	4	19472.5	0.000	0.000
8	4	19308.1	0.000	-0.000
9	4	20943.7	0.002	0.001
0'	2	16275.0	-0.626	0.348
1'	2	16445.4	-0.628	-0.173
2'	2	17537.4	0.024	0.020

3'	2	17523.0	0.009	-0.007
4'	2	17794.1	0.016	0.000
5'	2	18424.8	-0.001	-0.001
6'	2	18567.6	7.423	-0.000
7'	2	22783.9	-2.273	1.881
8'	2	22838.1	-1.625	-1.373
9'	2	20769.2	-0.002	-0.002
10'	2	23437.5	0.077	0.004
11'	2	24052.1	0.263	0.012
12'	2	23597.5	0.677	0.001
13'	2	23772.2	0.141	0.000
14'	2	26722.7	-0.073	-0.041
15'	2	26810.7	-0.014	-0.008
16'	2	27275.7	-0.004	-0.004
17'	2	27408.7	0.000	0.001
18'	2	26397.6	-0.002	-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
22'	2	31509.6	0.071	-0.003
23'	2	32070.9	-0.035	-0.024
24'	2	29876.1	-0.950	-0.663
25'	2	31065.1	0.064	0.000
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 S57. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex C0 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	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
7	4	20523.5	0.000	0.000
8	4	20793.8	0.001	-0.001
9	4	20963.9	0.001	0.001
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'	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
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 S58. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex C0 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	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
7	4	19077.0	0.000	0.000
8	4	19265.8	0.001	-0.001
9	4	19537.2	0.001	0.001
0'	2	18104.4	-0.000	-0.000
1'	2	18237.7	0.011	-0.000

2'	2	18061.8	-0.309	0.308
3'	2	18214.9	-0.266	-0.266
4'	2	18959.7	-0.006	0.006
5'	2	18540.7	-0.004	0.003
6'	2	19856.8	6.831	-0.003
7'	2	22114.2	-2.406	2.360
8'	2	22149.0	-2.397	-2.354
9'	2	21917.6	0.005	-0.000
10'	2	23986.9	-0.023	0.025
11'	2	24066.8	0.048	-0.020
12'	2	23793.0	0.966	-0.006
13'	2	24273.3	-0.005	0.005
14'	2	25169.3	-0.092	-0.084
15'	2	25177.3	-0.101	0.092
16'	2	27382.7	-0.006	-0.008
17'	2	27263.8	-0.012	0.012
18'	2	26621.4	-0.088	-0.088
19'	2	26829.6	-0.075	0.075
20'	2	26730.5	-0.002	-0.001
21'	2	28509.8	-0.004	0.003
22'	2	29910.6	-0.001	-0.001
23'	2	28452.4	-1.035	-0.995
24'	2	28522.3	-0.993	0.947
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 S59. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex A2 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	-0.000
1	4	138.3	-167.133	-0.000
2	4	4344.5	11.604	-11.171
3	4	4678.8	3.318	-2.623
4	4	4730.4	3.734	3.582
5	4	4997.6	6.648	6.251
6	4	6583.1	0.016	-0.000
7	4	20743.8	0.000	-0.000
8	4	21342.2	0.001	0.001
9	4	23227.3	0.000	-0.000
0'	2	18646.7	-0.796	-0.521
1'	2	18806.3	-0.538	0.184

2'	2	19186.0	0.009	-0.001
3'	2	19365.4	0.051	0.002
4'	2	19443.6	0.235	-0.003
5'	2	20048.8	0.005	0.000
6'	2	20165.3	6.713	0.000
7'	2	22580.6	-2.097	-2.051
8'	2	22587.7	-1.757	1.651
9'	2	23530.9	-0.015	0.004
10'	2	25220.2	0.683	-0.002
11'	2	25275.7	0.287	-0.000
12'	2	25351.5	0.170	0.001
13'	2	25405.7	0.046	0.001
14'	2	27922.2	-0.035	0.035
15'	2	27956.3	-0.048	-0.047
16'	2	28168.0	-0.002	0.002
17'	2	28395.3	-0.025	-0.026
18'	2	28456.8	-0.007	0.004
19'	2	28799.4	-0.027	0.004
20'	2	28839.9	-0.111	0.104
21'	2	30184.2	-1.291	-1.291
22'	2	30579.1	-1.005	1.005
23'	2	31161.2	0.101	0.000
24'	2	31289.0	0.000	0.000
25'	2	31725.8	0.028	-0.000
26'	2	32368.2	0.028	0.000
27'	2	32413.1	0.194	0.000
28'	2	44023.1	0.002	0.000
29'	2	44358.1	0.356	0.000
30'	2	44896.8	-0.076	-0.074
31'	2	45466.2	-0.036	0.036
32'	2	46124.8	-0.092	0.088
33'	2	46146.1	-0.027	-0.024
34'	2	46468.2	0.000	-0.000
35'	2	66911.4	0.001	0.000
36'	2	67972.6	-0.015	0.015
37'	2	69587.5	-0.039	-0.039
38'	2	70918.9	0.000	-0.000
39'	2	71266.7	0.044	-0.000

Table S60. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex A2 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	167.6	-165.234	-0.000
1	4	0.0	0.000	0.000
2	4	5854.4	4.788	4.788
3	4	6770.2	4.327	1.739
4	4	6678.7	4.248	-0.963
5	4	6981.1	4.406	-4.406
6	4	8574.5	-0.063	0.007
7	4	19526.5	-0.004	0.000
8	4	19689.7	0.000	-0.000
9	4	21219.8	0.002	0.002
0'	2	16468.2	-0.911	0.725

1'	2	16501.4	-0.850	-0.583
2'	2	17824.2	0.015	0.002
3'	2	18027.9	0.100	-0.004
4'	2	18227.2	0.033	0.004
5'	2	18777.2	7.237	-0.000
6'	2	18679.6	0.006	0.000
7'	2	22826.8	-1.549	1.247
8'	2	22850.4	-1.865	-1.626
9'	2	21434.5	0.374	-0.007
10'	2	23911.7	-0.001	0.000
11'	2	23885.0	0.267	-0.002
12'	2	24115.1	0.091	-0.008
13'	2	23671.1	0.640	-0.001
14'	2	27151.9	-0.008	-0.010
15'	2	27129.9	-0.018	0.019
16'	2	25936.3	0.002	-0.003
17'	2	27299.3	-0.065	0.065
18'	2	27305.5	-0.028	-0.028
19'	2	28104.4	-0.022	-0.009
20'	2	27926.3	-0.099	-0.100
21'	2	27986.8	-1.427	1.374
22'	2	29415.0	-1.198	-1.142
23'	2	31838.0	0.000	-0.000
24'	2	32216.1	0.047	-0.000
25'	2	31007.9	0.000	0.000
26'	2	32969.0	0.230	-0.000
27'	2	33154.7	0.029	0.000
28'	2	39147.0	0.425	-0.000
29'	2	39446.8	0.002	0.000
30'	2	40658.7	-0.063	0.063
31'	2	40978.0	-0.085	-0.085
32'	2	41817.5	-0.027	-0.027
33'	2	41816.1	-0.103	0.104
34'	2	42932.6	0.008	0.000
35'	2	57999.1	-0.000	-0.000
36'	2	59965.1	-0.035	-0.034
37'	2	61272.0	-0.035	0.034
38'	2	62848.4	0.053	0.000
39'	2	62972.8	0.000	0.000

Table S61. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex B2 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	-0.000
1	4	611.1	-125.155	-0.000
2	4	3530.1	14.761	-14.759
3	4	3745.5	5.442	4.904
4	4	4009.6	10.371	9.551
5	4	4607.2	0.722	-0.226
6	4	5616.8	0.013	0.013
7	4	20224.8	0.000	0.000
8	4	21477.8	0.001	0.001
9	4	21980.2	0.002	-0.002
0'	2	19162.4	-0.581	0.173

1'	2	19304.6	-0.470	-0.176
2'	2	19387.1	0.106	0.000
3'	2	19572.1	0.019	-0.003
4'	2	19608.0	-0.002	0.001
5'	2	19994.4	0.000	-0.000
6'	2	20408.9	6.708	0.000
7'	2	21958.5	-2.272	2.025
8'	2	22007.6	-2.026	-1.832
9'	2	24110.4	0.008	-0.001
10'	2	25029.0	-0.027	0.027
11'	2	25112.8	-0.020	-0.004
12'	2	25381.8	1.039	0.000
13'	2	25484.8	0.000	-0.000
14'	2	27589.2	-0.020	0.008
15'	2	27663.5	-0.028	-0.019
16'	2	27822.6	-0.014	-0.003
17'	2	27877.2	0.000	-0.001
18'	2	27949.4	-0.000	-0.000
19'	2	28174.0	-0.000	-0.000
20'	2	28231.8	-0.026	-0.016
21'	2	29673.8	-1.156	0.706
22'	2	29808.2	0.008	0.000
23'	2	29982.8	-1.234	-0.820
24'	2	30093.7	-0.004	-0.003
25'	2	30871.0	0.542	-0.000
26'	2	31146.8	0.000	-0.000
27'	2	31169.8	0.048	0.000
28'	2	44013.0	0.000	0.000
29'	2	44263.1	0.364	0.000
30'	2	44818.0	-0.086	-0.021
31'	2	44983.8	-0.062	0.005
32'	2	45692.5	-0.053	0.029
33'	2	45695.6	-0.043	-0.018
34'	2	45764.9	-0.000	-0.001
35'	2	67128.7	0.000	0.000
36'	2	68525.9	-0.028	0.004
37'	2	68827.1	-0.028	-0.004
38'	2	70261.2	-0.000	-0.000
39'	2	70678.6	0.049	0.000

Table S62. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex B2 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	0.000
1	4	606.3	-125.587	0.000
2	4	5234.6	10.067	-0.748
3	4	5466.7	3.743	1.948
4	4	5494.9	7.613	-2.261
5	4	5666.0	0.587	0.538
6	4	7334.6	0.010	-0.001
7	4	18493.4	0.000	0.000
8	4	19636.0	0.001	-0.000
9	4	19584.3	0.003	0.001

0'	2	17357.0	-0.641	0.628
1'	2	17472.4	-0.519	-0.509
2'	2	18243.8	0.112	-0.005
3'	2	18207.2	0.020	-0.002
4'	2	18301.5	-0.002	0.002
5'	2	18734.1	0.000	0.001
6'	2	19196.1	7.132	-0.000
7'	2	22007.0	-2.267	-0.823
8'	2	22005.8	-2.026	0.681
9'	2	21830.3	0.008	-0.001
10'	2	23646.2	-0.029	0.007
11'	2	23715.5	-0.021	-0.024
12'	2	23341.6	1.130	-0.001
13'	2	23458.0	0.001	0.000
14'	2	26391.1	-0.021	-0.019
15'	2	26803.1	-0.029	0.020
16'	2	26401.4	-0.015	0.014
17'	2	26765.2	0.000	0.000
18'	2	25649.0	-0.000	-0.000
19'	2	26673.4	-0.000	0.001
20'	2	26659.3	-0.028	0.021
21'	2	27619.6	-1.242	-0.904
22'	2	29747.6	0.008	0.000
23'	2	27859.8	-1.329	0.901
24'	2	30513.9	-0.004	0.003
25'	2	30583.3	0.548	-0.000
26'	2	31036.0	0.000	0.000
27'	2	30145.4	0.050	0.000
28'	2	38956.1	0.000	0.000
29'	2	39197.6	0.412	-0.000
30'	2	40342.6	-0.095	0.090
31'	2	40207.1	-0.070	-0.069
32'	2	41135.1	-0.059	-0.047
33'	2	41144.7	-0.048	0.042
34'	2	41756.3	-0.000	0.000
35'	2	58049.6	0.000	-0.000
36'	2	60388.6	-0.032	-0.031
37'	2	60196.3	-0.032	0.031
38'	2	61719.4	-0.000	0.000
39'	2	62201.7	0.056	-0.000

Table S63. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex B2' with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	0.000
1	4	1026.6	-91.794	-0.008
2	4	3758.2	18.585	-18.311
3	4	4905.7	4.397	3.802
4	4	5142.3	3.436	3.391
5	4	5357.2	1.353	1.195
6	4	6829.2	0.004	0.000
7	4	20366.7	0.009	0.009
8	4	21350.0	0.000	0.000

9	4	24378.2	0.001	-0.001
0'	2	18944.3	-0.746	-0.701
1'	2	19352.4	0.596	0.000
2'	2	19426.8	0.416	-0.003
3'	2	19833.4	-0.231	0.226
4'	2	19865.7	-0.011	0.049
5'	2	20339.9	-0.001	0.001
6'	2	21041.8	5.583	0.000
7'	2	22619.0	-2.641	-2.000
8'	2	22682.8	-1.854	1.095
9'	2	23320.0	-0.004	-0.001
10'	2	25442.1	-0.002	0.001
11'	2	25729.5	0.011	-0.001
12'	2	25903.1	1.091	0.001
13'	2	27132.5	-0.090	0.090
14'	2	27144.9	-0.053	0.056
15'	2	27381.7	-0.055	-0.053
16'	2	28400.3	-0.075	-0.074
17'	2	28447.8	-0.150	-0.132
18'	2	28563.0	-0.082	0.040
19'	2	29337.3	-0.299	0.286
20'	2	29383.9	-0.010	-0.007
21'	2	30065.4	0.215	-0.065
22'	2	30195.0	-0.906	-0.923
23'	2	30839.0	-0.005	-0.005
24'	2	31387.7	-0.481	0.484
25'	2	31726.7	0.043	0.001
26'	2	32642.1	0.249	0.000
27'	2	33212.8	-0.000	-0.000
28'	2	44362.7	-0.000	-0.000
29'	2	44870.0	-0.083	-0.085
30'	2	45008.2	0.267	-0.000
31'	2	46253.0	-0.002	0.002
32'	2	46426.9	-0.131	0.129
33'	2	46451.6	-0.009	-0.001
34'	2	46790.5	0.000	0.000
35'	2	67303.8	0.005	0.000
36'	2	67829.3	-0.008	0.008
37'	2	70430.5	-0.001	-0.001
38'	2	71416.7	-0.042	-0.042
39'	2	71645.8	0.038	-0.000

Table S64. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex B2' with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	-0.000
1	4	1115.0	-86.729	-0.004
2	4	5425.4	13.046	-12.797
3	4	6852.3	3.155	2.695
4	4	6722.2	2.632	2.589
5	4	7204.2	1.007	0.880
6	4	8952.7	0.003	0.000
7	4	18446.4	0.010	0.010

8	4	19884.6	0.000	0.000
9	4	22628.0	0.001	-0.001
0'	2	16754.3	-0.843	-0.799
1'	2	17996.0	0.642	0.000
2'	2	18076.2	0.447	-0.003
3'	2	18365.9	-0.249	0.246
4'	2	18678.6	-0.012	0.053
5'	2	18960.6	-0.001	0.001
6'	2	19850.0	5.918	0.000
7'	2	22616.9	-2.642	-2.035
8'	2	22829.2	-1.842	1.118
9'	2	20888.8	-0.005	-0.001
10'	2	25066.5	-0.002	0.001
11'	2	24227.0	0.012	-0.001
12'	2	23994.2	1.178	0.001
13'	2	25563.7	-0.096	0.095
14'	2	25498.6	-0.057	0.061
15'	2	26316.5	-0.058	-0.055
16'	2	26899.6	-0.079	-0.078
17'	2	27001.1	-0.158	-0.141
18'	2	27054.5	-0.087	0.044
19'	2	28438.6	-0.309	0.297
20'	2	28564.8	-0.010	-0.008
21'	2	29791.7	0.218	-0.065
22'	2	28173.8	-0.971	-0.990
23'	2	31246.6	-0.005	-0.005
24'	2	30522.0	-0.495	0.498
25'	2	31165.1	0.044	0.001
26'	2	33069.5	0.246	0.000
27'	2	33619.8	-0.000	-0.000
28'	2	39651.3	-0.000	-0.000
29'	2	40375.5	-0.092	-0.094
30'	2	40270.3	0.299	-0.000
31'	2	42037.1	-0.002	0.002
32'	2	41966.0	-0.145	0.143
33'	2	42116.1	-0.010	-0.002
34'	2	42906.1	0.000	0.000
35'	2	58539.3	0.006	0.000
36'	2	59549.9	-0.009	0.009
37'	2	62055.0	-0.001	-0.001
39'	2	63174.9	-0.048	-0.047
38'	2	63465.8	0.043	-0.000

Table S65. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex C2 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	-0.000
1	4	1348.9	-76.969	-0.004
2	4	3200.9	19.835	-19.835
3	4	4080.0	7.873	7.853
4	4	4446.1	4.631	4.629
5	4	5196.9	0.114	-0.109
6	4	5881.8	0.001	0.001
7	4	20526.6	0.008	0.008

8	4	20986.5	0.000	0.000
9	4	22960.1	0.002	-0.002
0'	2	19374.9	0.493	-0.069
1'	2	19432.9	-0.351	-0.416
2'	2	19602.4	-0.003	-0.003
3'	2	19964.4	-0.237	0.236
4'	2	20065.2	0.056	0.001
5'	2	20179.4	-0.000	0.001
6'	2	21078.8	5.948	0.000
7'	2	22110.8	-2.313	2.309
8'	2	22230.7	-2.536	-2.532
9'	2	24090.1	0.000	0.000
10'	2	25509.8	-0.014	-0.009
11'	2	25617.5	-0.029	0.027
12'	2	26013.3	0.980	0.000
13'	2	26826.9	-0.089	0.090
14'	2	26901.9	-0.003	0.000
15'	2	26984.4	-0.030	-0.030
16'	2	28214.7	-0.135	-0.133
17'	2	28360.1	-0.090	0.089
18'	2	28384.0	-0.012	0.010
19'	2	28586.1	-0.030	-0.030
20'	2	28803.6	-0.111	0.109
21'	2	29120.3	0.085	0.001
22'	2	29854.8	-0.034	-0.034
23'	2	29992.6	-1.055	-1.054
24'	2	30370.3	-0.676	0.677
25'	2	31330.1	0.545	0.000
26'	2	31406.1	0.104	0.000
27'	2	32072.5	0.000	0.000
28'	2	44267.6	-0.000	-0.000
29'	2	44729.5	0.293	-0.002
30'	2	44799.3	-0.099	-0.104
31'	2	45706.0	-0.105	0.105
32'	2	45849.5	-0.029	0.029
33'	2	45924.0	-0.011	-0.011
34'	2	46128.2	0.000	0.000
35'	2	67719.5	0.004	0.000
36'	2	68412.8	-0.017	0.017
37'	2	69680.1	-0.000	-0.000
38'	2	70431.6	-0.033	-0.033
39'	2	70664.6	0.045	-0.000

Table S66. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex C2 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	0.000
1	4	1657.8	-65.259	-0.002
2	4	4809.4	13.429	-13.420
3	4	5570.6	5.792	5.772
4	4	6330.7	3.261	3.259
5	4	6782.6	0.087	-0.084
6	4	7910.8	0.001	0.001

7	4	18640.3	0.009	0.009
8	4	19315.0	0.000	0.000
9	4	20948.1	0.002	-0.002
1'	2	17818.4	0.530	-0.075
0'	2	18050.5	-0.382	-0.455
2'	2	18379.5	-0.003	-0.003
3'	2	18691.2	-0.253	0.252
4'	2	19210.3	0.059	0.001
5'	2	18861.5	-0.000	0.001
6'	2	20160.2	6.219	0.000
7'	2	22195.5	-2.305	2.298
8'	2	22251.9	-2.533	-2.528
9'	2	21826.3	0.000	0.000
10'	2	24541.6	-0.015	-0.009
11'	2	24022.2	-0.031	0.029
12'	2	24172.6	1.054	0.000
13'	2	25344.5	-0.095	0.095
14'	2	25200.6	-0.003	0.000
15'	2	25868.7	-0.032	-0.032
16'	2	27539.8	-0.139	-0.137
17'	2	26641.6	-0.096	0.095
18'	2	26543.4	-0.013	0.011
19'	2	26701.1	-0.032	-0.033
20'	2	28237.7	-0.113	0.112
21'	2	28688.6	0.087	0.001
22'	2	30093.6	-0.034	-0.034
23'	2	28318.8	-1.117	-1.117
24'	2	29004.7	-0.709	0.709
25'	2	30953.4	0.552	0.000
26'	2	31036.7	0.105	0.000
27'	2	32256.4	0.000	0.000
28'	2	39490.9	-0.000	-0.000
29'	2	39900.8	0.328	-0.003
30'	2	40288.9	-0.110	-0.116
31'	2	41105.1	-0.116	0.116
32'	2	41507.5	-0.032	0.032
33'	2	41554.5	-0.012	-0.012
34'	2	42102.9	0.000	0.000
35'	2	58987.6	0.004	0.000
36'	2	60298.6	-0.019	0.019
37'	2	61064.5	-0.000	-0.000
39'	2	62127.2	-0.038	-0.038
38'	2	62229.0	0.051	-0.000

Table S67. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex A4 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	-0.000
1	4	804.4	-110.105	0.003
2	4	4126.1	14.063	-14.048
3	4	4447.1	11.808	11.812
4	4	4771.1	1.521	1.518
5	4	4990.0	0.307	-0.300
6	4	6314.6	0.002	0.002

7	4	20851.7	0.000	0.000
8	4	22505.4	0.001	-0.001
9	4	22853.3	0.000	0.000
0'	2	19398.9	-0.642	0.641
1'	2	19608.8	-0.545	-0.546
2'	2	19856.3	-0.002	0.000
3'	2	20073.5	0.078	-0.000
4'	2	20142.8	-0.000	-0.000
5'	2	20466.9	-0.000	0.000
6'	2	20951.8	6.791	-0.001
7'	2	22794.2	-2.144	2.127
8'	2	22825.2	-2.121	-2.106
9'	2	24483.5	0.017	-0.000
10'	2	25624.4	-0.011	0.018
11'	2	25723.9	0.171	-0.010
12'	2	25839.8	0.866	-0.005
13'	2	26010.9	-0.005	0.004
14'	2	28552.6	-0.018	-0.018
15'	2	28636.9	0.000	-0.001
16'	2	28660.4	-0.010	0.010
17'	2	28809.9	-0.000	-0.001
18'	2	28812.3	-0.005	-0.007
19'	2	29068.9	-0.030	-0.030
20'	2	29084.2	-0.054	0.054
21'	2	30779.1	-1.183	-1.184
22'	2	30847.7	-1.075	1.075
23'	2	31126.4	-0.002	0.001
24'	2	31565.1	0.004	-0.000
25'	2	31855.7	0.498	-0.000
26'	2	32235.9	-0.000	0.000
27'	2	32475.9	-0.000	0.000
28'	2	44992.4	-0.000	0.000
29'	2	45197.5	0.382	-0.001
30'	2	45890.0	-0.067	0.067
31'	2	46043.5	-0.059	-0.062
32'	2	46897.3	-0.055	0.035
33'	2	46898.2	-0.050	-0.030
34'	2	47023.5	0.001	0.000
35'	2	68282.0	-0.000	0.000
36'	2	69663.3	-0.028	-0.028
37'	2	69966.9	-0.028	0.028
38'	2	72159.9	-0.000	0.000
39'	2	72548.1	0.047	-0.000

Table S68. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex A4 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	0.000
1	4	747.5	-114.602	0.002
2	4	5092.4	11.461	-11.452
3	4	5525.1	9.552	9.556
4	4	5641.3	1.287	1.285
5	4	5920.4	0.259	-0.253

6	4	7270.7	0.002	0.002
7	4	18843.6	0.000	0.000
8	4	20019.8	0.001	-0.001
9	4	20377.1	0.000	0.000
0'	2	17400.1	-0.715	0.715
1'	2	17709.3	-0.603	-0.604
2'	2	18439.6	-0.002	0.000
3'	2	18592.4	0.084	-0.000
4'	2	18704.4	-0.000	-0.000
5'	2	19006.8	-0.000	0.000
6'	2	19511.1	7.292	-0.001
7'	2	22237.2	-2.197	2.182
8'	2	22271.4	-2.174	-2.160
9'	2	22203.2	0.019	-0.000
10'	2	24058.6	-0.012	0.019
11'	2	24065.8	0.182	-0.011
12'	2	23877.0	0.938	-0.005
13'	2	23928.4	-0.006	0.004
14'	2	26463.0	-0.020	-0.019
15'	2	25524.1	0.001	-0.001
16'	2	26528.1	-0.011	0.011
17'	2	27502.2	-0.000	-0.001
18'	2	27473.6	-0.006	-0.007
19'	2	27402.8	-0.032	-0.032
20'	2	27458.6	-0.057	0.057
21'	2	28139.9	-1.295	-1.295
22'	2	28206.1	-1.176	1.176
23'	2	30105.1	-0.002	0.001
24'	2	31130.2	0.004	-0.000
25'	2	30805.5	0.515	-0.000
26'	2	31273.4	-0.000	0.000
27'	2	30845.5	-0.000	0.000
28'	2	39813.7	-0.000	0.000
29'	2	39991.9	0.432	-0.001
30'	2	40993.4	-0.075	0.075
31'	2	41159.9	-0.067	-0.069
32'	2	41985.5	-0.061	0.039
33'	2	41985.2	-0.056	-0.033
34'	2	42556.3	0.001	0.000
35'	2	59336.5	-0.000	0.000
36'	2	61147.1	-0.032	-0.032
37'	2	61452.8	-0.032	0.032
38'	2	63372.0	-0.000	0.000
39'	2	63790.5	0.053	-0.000

Table S69. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex B4 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	-0.000
1	4	1215.3	-83.514	-0.001
2	4	3705.1	18.440	-18.243
3	4	4409.6	10.091	9.728
4	4	4881.0	0.366	0.302
5	4	5089.4	0.909	0.907

6	4	6300.0	0.002	-0.001
7	4	21003.9	0.000	-0.000
8	4	21422.3	0.000	0.000
9	4	23663.2	0.001	-0.001
0'	2	19478.7	-0.614	-0.588
1'	2	19856.9	0.361	-0.001
2'	2	19946.8	-0.001	-0.000
3'	2	20065.5	-0.381	0.367
4'	2	20317.2	0.306	0.000
5'	2	20613.5	-0.000	0.001
6'	2	21294.4	6.012	0.000
7'	2	22678.0	-2.517	-1.623
8'	2	22710.7	-2.086	0.977
9'	2	24314.6	0.003	0.000
10'	2	25655.7	-0.012	-0.006
11'	2	25824.7	-0.017	0.014
12'	2	26035.7	1.002	0.000
13'	2	26846.5	0.001	0.000
14'	2	27922.5	-0.131	0.126
15'	2	28100.8	-0.035	-0.035
16'	2	28599.8	-0.001	-0.000
17'	2	28740.1	-0.165	-0.156
18'	2	28979.0	-0.006	0.005
19'	2	29057.1	-0.008	-0.006
20'	2	29310.8	-0.079	0.069
21'	2	30277.3	0.225	-0.005
22'	2	30619.2	-1.012	-1.013
23'	2	30982.7	-0.004	0.002
24'	2	31060.1	-0.839	0.838
25'	2	31897.6	0.437	-0.000
26'	2	32254.3	0.017	0.000
27'	2	32525.1	0.000	0.000
28'	2	44975.2	0.000	-0.000
29'	2	45351.2	0.339	-0.001
30'	2	45543.5	-0.076	-0.075
31'	2	46404.7	-0.051	0.050
32'	2	46777.9	-0.087	0.086
33'	2	46853.6	-0.022	-0.021
34'	2	46967.8	0.000	0.000
35'	2	68334.5	0.002	0.000
36'	2	69038.9	-0.016	0.016
37'	2	71022.4	-0.039	-0.038
38'	2	71644.8	-0.000	-0.000
39'	2	72381.5	0.045	-0.000

Table S70. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex B4 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	0.000
1	4	1305.4	-79.186	-0.001
2	4	4617.9	14.924	-14.762
3	4	5595.5	7.986	7.697
4	4	6035.6	0.296	0.244

5	4	6044.1	0.766	0.764
6	4	7473.5	0.002	-0.001
7	4	19031.6	0.000	-0.000
8	4	18896.6	0.000	0.000
9	4	21493.6	0.001	-0.001
0'	2	17459.4	-0.686	-0.656
1'	2	18337.6	0.391	-0.001
2'	2	18448.6	-0.001	-0.000
3'	2	18534.9	-0.413	0.398
4'	2	19063.8	0.326	0.000
5'	2	19231.6	-0.000	0.001
6'	2	20071.2	6.378	0.000
7'	2	22173.4	-2.574	-1.662
8'	2	22228.9	-2.132	1.000
9'	2	21828.8	0.004	0.001
10'	2	24307.5	-0.013	-0.006
11'	2	23984.3	-0.018	0.015
12'	2	24130.8	1.081	-0.000
13'	2	25082.7	0.002	0.000
14'	2	25804.1	-0.141	0.137
16'	2	25863.5	-0.037	-0.037
15'	2	26375.3	-0.001	-0.000
17'	2	27242.8	-0.174	-0.164
18'	2	27362.6	-0.006	0.005
19'	2	27444.4	-0.008	-0.006
20'	2	27995.4	-0.083	0.072
21'	2	29149.4	0.234	-0.005
22'	2	28003.1	-1.107	-1.107
23'	2	30477.6	-0.004	0.002
24'	2	28897.7	-0.902	0.901
25'	2	30980.7	0.449	-0.000
26'	2	30742.5	0.018	0.000
27'	2	31749.5	0.000	0.000
28'	2	39934.0	0.000	-0.000
29'	2	40280.0	0.382	-0.001
30'	2	40629.6	-0.085	-0.085
31'	2	41753.5	-0.057	0.056
32'	2	41983.8	-0.097	0.096
33'	2	42085.2	-0.024	-0.023
34'	2	42562.5	0.000	0.000
35'	2	59476.0	0.003	0.000
36'	2	60442.5	-0.019	0.018
37'	2	62837.6	-0.044	-0.044
38'	2	62893.3	-0.000	-0.000
39'	2	63774.7	0.051	-0.000

Table S71. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex C4 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	0.000
1	4	1488.8	-72.313	-0.000
2	4	3965.4	15.009	-14.782
3	4	3981.4	14.951	14.723
4	4	5076.8	0.013	0.013

5	4	5089.6	0.014	-0.013
6	4	6197.9	0.001	0.001
7	4	21169.7	0.000	0.000
8	4	22314.5	0.000	-0.000
9	4	22334.7	0.000	0.000
0'	2	19997.5	-0.076	0.063
1'	2	20017.1	-0.322	0.322
2'	2	20022.5	-0.378	-0.379
3'	2	20220.2	-0.001	-0.001
4'	2	20401.9	-0.000	0.000
5'	2	20540.1	-0.000	0.000
6'	2	21378.9	6.715	-0.000
7'	2	22666.3	-2.423	2.367
8'	2	22668.4	-2.424	-2.368
9'	2	25128.1	-0.000	-0.000
10'	2	26013.4	-0.036	0.035
11'	2	26024.4	-0.029	-0.035
12'	2	26139.6	0.930	-0.000
13'	2	26652.1	-0.000	0.000
14'	2	27950.2	-0.095	-0.084
15'	2	27953.5	-0.095	0.084
16'	2	28785.0	-0.001	-0.001
17'	2	28797.3	-0.001	0.001
18'	2	28862.7	-0.000	-0.000
19'	2	29105.6	-0.002	-0.002
20'	2	29110.6	-0.002	0.002
21'	2	29985.4	-0.000	0.000
22'	2	30743.0	-0.827	-0.688
23'	2	30745.7	-0.962	0.705
24'	2	30756.6	-0.198	-0.022
25'	2	31686.1	0.683	-0.000
26'	2	32399.2	-0.000	0.000
27'	2	32464.2	-0.000	0.000
28'	2	45042.6	-0.000	0.000
29'	2	45357.0	0.341	-0.000
30'	2	45936.2	-0.091	0.079
31'	2	45944.9	-0.091	-0.078
32'	2	46659.3	-0.032	0.006
33'	2	46659.7	-0.032	-0.006
34'	2	46802.4	-0.000	-0.000
35'	2	68785.8	-0.000	0.000
36'	2	70149.3	-0.026	-0.022
37'	2	70169.1	-0.026	0.022
38'	2	71169.6	-0.000	0.000
39'	2	71755.0	0.049	-0.000

Table S72. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex C4 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	0.000
1	4	1699.2	-64.913	-0.000
2	4	5036.8	11.900	-11.242
3	4	5057.1	11.853	11.195

4	4	6347.7	0.010	0.009
5	4	6362.4	0.011	-0.009
6	4	7550.2	0.001	0.000
7	4	19248.0	0.000	0.000
8	4	20056.2	0.000	-0.000
9	4	20077.6	0.000	0.000
0'	2	18533.0	-0.082	0.060
1'	2	18414.6	-0.350	0.347
2'	2	18383.1	-0.412	-0.402
3'	2	18852.4	-0.001	-0.001
4'	2	18974.1	-0.000	0.000
5'	2	19466.5	-0.000	0.000
6'	2	20255.8	7.087	-0.000
7'	2	22270.5	-2.466	2.294
8'	2	22273.0	-2.466	-2.295
9'	2	22837.6	-0.000	-0.000
10'	2	24395.4	-0.039	0.035
11'	2	24401.1	-0.031	-0.035
12'	2	24223.3	1.003	-0.000
13'	2	24762.7	-0.000	0.000
14'	2	26157.5	-0.102	-0.081
15'	2	26165.4	-0.102	0.081
16'	2	27620.4	-0.001	-0.001
17'	2	27857.7	-0.001	0.001
18'	2	26464.5	-0.000	-0.000
19'	2	27222.7	-0.002	-0.002
20'	2	27254.9	-0.003	0.003
21'	2	28988.1	-0.000	0.000
22'	2	28912.0	-0.879	-0.645
23'	2	28639.3	-1.033	0.636
24'	2	30182.7	-0.202	0.010
25'	2	30744.4	0.704	-0.000
26'	2	31241.0	-0.000	0.000
27'	2	31894.4	-0.000	0.000
28'	2	40055.1	-0.000	0.000
29'	2	40335.1	0.384	-0.000
30'	2	41181.5	-0.102	0.078
31'	2	41191.8	-0.102	-0.078
32'	2	41992.0	-0.035	0.013
33'	2	41992.2	-0.035	-0.012
34'	2	42498.1	-0.000	-0.000
35'	2	59978.6	-0.000	0.000
36'	2	61860.6	-0.030	-0.022
37'	2	61882.1	-0.030	0.022
38'	2	62462.6	-0.000	0.000
39'	2	63254.1	0.055	-0.000

Table S73. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex A0 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	219.2
3	219.2
4	796.0
5	796.0

6	1102.9
7	1102.9
8	5120.4
9	5120.4
10	5352.8
11	5352.8
12	5398.0
13	5398.0
14	5430.7
15	5430.7
16	5781.9
17	5781.9
18	5930.2
19	5930.2
20	6306.6
21	6306.6
22	6758.9
23	6758.9
24	7916.3
25	7916.3
26	8054.3
27	8054.3
28	18298.2
29	18298.2
30	18803.3
31	18803.3
32	18950.9
33	18950.9
34	19545.1
35	19545.1
36	20016.5
37	20016.5
38	20074.6
39	20074.6
40	20419.4
41	20419.4
42	21538.7
43	21538.7
44	21549.2
45	21549.2
46	22338.2
47	22338.2
48	22456.0
49	22456.0
50	22527.5
51	22527.5
52	22816.8
53	22816.8
54	23111.3
55	23111.3
56	23535.1
57	23535.1
58	23999.1
59	23999.1
60	25094.5
61	25094.5
62	25580.5

63 25580.5
64 25977.4
65 25977.4
66 26390.4
67 26390.4
68 28100.6
69 28100.6
70 28560.3
71 28560.3
72 28747.6
73 28747.6
74 28825.1
75 28825.1
76 28890.9
77 28890.9
78 29252.5
79 29252.5
80 29611.0
81 29611.0
82 30832.9
83 30832.9
84 31014.9
85 31014.9
86 32258.9
87 32258.9
88 32325.0
89 32325.0
90 32615.6
91 32615.6
92 33233.3
93 33233.3
94 34218.0
95 34218.0
96 43825.5
97 43825.5
98 44143.1
99 44143.1
100 45073.4
101 45073.4
102 45344.0
103 45344.0
104 45987.8
105 45987.8
106 46220.2
107 46220.2
108 46880.9
109 46880.9
110 66560.8
111 66560.8
112 68716.1
113 68716.1
114 68806.9
115 68806.9
116 70099.6
117 70099.6
118 70636.5
119 70636.5

Table S74. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex A0 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	145.7
3	145.7
4	1243.0
5	1243.0
6	1449.3
7	1449.3
8	8159.3
9	8159.3
10	8215.8
11	8215.8
12	8255.9
13	8255.9
14	8341.4
15	8341.4
16	9104.7
17	9104.7
18	9396.7
19	9396.7
20	9811.8
21	9811.8
22	10250.5
23	10250.5
24	11327.5
25	11327.5
26	11459.0
27	11459.0
28	15702.2
29	15702.2
30	16233.9
31	16233.9
32	17493.1
33	17493.1
34	18222.3
35	18222.3
36	18694.3
37	18694.3
38	19012.4
39	19012.4
40	19512.3
41	19512.3
42	21200.2
43	21200.2
44	21396.7
45	21396.7
46	21426.2
47	21426.2
48	21609.5
49	21609.5
50	21791.8
51	21791.8

52 22088.0
53 22088.0
54 22379.1
55 22379.1
56 23260.5
57 23260.5
58 24023.7
59 24023.7
60 24614.3
61 24614.3
62 25083.8
63 25083.8
64 26099.0
65 26099.0
66 26614.4
67 26614.4
68 28038.4
69 28038.4
70 28266.5
71 28266.5
72 28334.9
73 28334.9
74 28747.7
75 28747.7
76 28799.6
77 28799.6
78 29471.6
79 29471.6
80 30182.4
81 30182.4
82 30790.4
83 30790.4
84 31033.0
85 31033.0
86 33856.5
87 33856.5
88 34726.5
89 34726.5
90 35600.9
91 35600.9
92 35952.4
93 35952.4
94 37158.4
95 37158.4
96 39462.8
97 39462.8
98 39796.4
99 39796.4
100 41504.4
101 41504.4
102 41777.7
103 41777.7
104 42738.4
105 42738.4
106 42986.5
107 42986.5
108 44946.1

109	44946.1
110	57797.4
111	57797.4
112	61351.2
113	61351.2
114	61477.3
115	61477.3
116	63030.1
117	63030.1
118	63486.9
119	63486.9

Table S75. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex B0 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	260.8
3	260.8
4	640.1
5	640.1
6	1008.0
7	1008.0
8	3923.3
9	3923.3
10	4056.3
11	4056.3
12	4355.5
13	4355.5
14	4669.7
15	4669.7
16	5047.1
17	5047.1
18	5139.2
19	5139.2
20	5467.6
21	5467.6
22	5867.0
23	5867.0
24	6825.4
25	6825.4
26	7008.4
27	7008.4
28	18624.1
29	18624.1
30	18938.1
31	18938.1
32	19245.2
33	19245.2
34	19688.5
35	19688.5
36	19885.8
37	19885.8
38	20117.9
39	20117.9
40	20284.7

41 20284.7
42 20816.6
43 20816.6
44 20879.1
45 20879.1
46 21205.9
47 21205.9
48 21337.8
49 21337.8
50 22213.3
51 22213.3
52 22428.0
53 22428.0
54 22586.9
55 22586.9
56 22670.4
57 22670.4
58 23978.4
59 23978.4
60 25215.1
61 25215.1
62 25325.8
63 25325.8
64 25769.7
65 25769.7
66 26002.9
67 26002.9
68 27447.5
69 27447.5
70 27786.4
71 27786.4
72 27883.3
73 27883.3
74 28142.3
75 28142.3
76 28337.6
77 28337.6
78 28489.1
79 28489.1
80 29090.0
81 29090.0
82 29844.7
83 29844.7
84 30530.1
85 30530.1
86 30716.2
87 30716.2
88 30753.1
89 30753.1
90 31601.6
91 31601.6
92 32094.9
93 32094.9
94 32959.8
95 32959.8
96 43709.5
97 43709.5

98	44041.6
99	44041.6
100	44606.3
101	44606.3
102	45078.4
103	45078.4
104	45469.3
105	45469.3
106	45716.9
107	45716.9
108	46044.9
109	46044.9
110	66561.5
111	66561.5
112	67968.9
113	67968.9
114	69192.3
115	69192.3
116	69480.7
117	69480.7
118	70131.2
119	70131.2

Table S76. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex B0 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	294.4
3	294.4
4	635.5
5	635.5
6	1002.6
7	1002.6
8	6074.5
9	6074.5
10	6156.4
11	6156.4
12	6936.9
13	6936.9
14	7269.9
15	7269.9
16	7651.4
17	7651.4
18	7747.7
19	7747.7
20	8067.7
21	8067.7
22	8497.0
23	8497.0
24	9760.5
25	9760.5
26	9914.0
27	9914.0
28	16533.5
29	16533.5

30	17023.9
31	17023.9
32	17654.3
33	17654.3
34	18274.8
35	18274.8
36	18576.7
37	18576.7
38	18914.4
39	18914.4
40	19043.4
41	19043.4
42	19624.7
43	19624.7
44	19652.8
45	19652.8
46	19912.5
47	19912.5
48	20050.6
49	20050.6
50	21041.0
51	21041.0
52	21448.5
53	21448.5
54	21704.8
55	21704.8
56	23070.3
57	23070.3
58	23481.1
59	23481.1
60	23839.6
61	23839.6
62	24116.7
63	24116.7
64	24494.4
65	24494.4
66	24824.3
67	24824.3
68	26812.2
69	26812.2
70	27051.5
71	27051.5
72	27498.8
73	27498.8
74	27622.7
75	27622.7
76	27771.9
77	27771.9
78	28140.3
79	28140.3
80	28329.2
81	28329.2
82	28787.3
83	28787.3
84	30439.5
85	30439.5
86	31735.5

87	31735.5
88	32111.0
89	32111.0
90	32650.7
91	32650.7
92	33789.4
93	33789.4
94	34581.7
95	34581.7
96	39002.9
97	39002.9
98	39334.9
99	39334.9
100	40443.4
101	40443.4
102	41146.4
103	41146.4
104	41628.7
105	41628.7
106	41889.4
107	41889.4
108	43092.7
109	43092.7
110	57443.1
111	57443.1
112	59841.6
113	59841.6
114	61554.2
115	61554.2
116	61693.8
117	61693.8
118	62319.7
119	62319.7

Table S77. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex C0 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	101.4
3	101.4
4	1222.9
5	1222.9
6	1460.8
7	1460.8
8	3247.8
9	3247.8
10	3442.6
11	3442.6
12	3493.5
13	3493.5
14	3569.0
15	3569.0
16	4103.7
17	4103.7
18	4372.7

19	4372.7
20	4744.3
21	4744.3
22	5200.1
23	5200.1
24	5614.6
25	5614.6
26	5792.8
27	5792.8
28	19121.1
29	19121.1
30	19152.1
31	19152.1
32	19551.9
33	19551.9
34	19977.6
35	19977.6
36	20042.1
37	20042.1
38	20168.5
39	20168.5
40	20588.9
41	20588.9
42	20617.7
43	20617.7
44	20699.0
45	20699.0
46	20863.5
47	20863.5
48	21014.1
49	21014.1
50	21171.9
51	21171.9
52	21438.6
53	21438.6
54	21558.8
55	21558.8
56	22012.2
57	22012.2
58	24570.7
59	24570.7
60	25273.8
61	25273.8
62	25636.7
63	25636.7
64	25922.4
65	25922.4
66	26133.1
67	26133.1
68	26312.1
69	26312.1
70	26658.9
71	26658.9
72	27525.2
73	27525.2
74	27591.2
75	27591.2

76	27869.1
77	27869.1
78	28034.2
79	28034.2
80	28439.7
81	28439.7
82	28557.2
83	28557.2
84	29040.3
85	29040.3
86	29593.6
87	29593.6
88	29754.5
89	29754.5
90	30793.2
91	30793.2
92	30985.1
93	30985.1
94	31837.9
95	31837.9
96	43658.7
97	43658.7
98	44065.4
99	44065.4
100	44421.9
101	44421.9
102	44654.6
103	44654.6
104	44960.0
105	44960.0
106	45136.9
107	45136.9
108	45356.8
109	45356.8
110	67260.5
111	67260.5
112	68190.6
113	68190.6
114	68651.7
115	68651.7
116	68814.3
117	68814.3
118	69056.6
119	69056.6

Table S78. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex C0 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	87.1
3	87.1
4	1661.2
5	1661.2
6	1840.2
7	1840.2

8	5179.4
9	5179.4
10	5302.6
11	5302.6
12	5416.3
13	5416.3
14	5507.3
15	5507.3
16	6463.0
17	6463.0
18	6760.2
19	6760.2
20	7149.6
21	7149.6
22	7587.4
23	7587.4
24	8368.9
25	8368.9
26	8501.6
27	8501.6
28	17883.0
29	17883.0
30	18014.5
31	18014.5
32	18295.8
33	18295.8
34	18745.8
35	18745.8
36	18833.9
37	18833.9
38	19082.5
39	19082.5
40	19137.2
41	19137.2
42	19293.7
43	19293.7
44	19337.8
45	19337.8
46	19462.6
47	19462.6
48	19668.7
49	19668.7
50	19919.9
51	19919.9
52	20015.7
53	20015.7
54	22083.1
55	22083.1
56	22193.7
57	22193.7
58	22511.0
59	22511.0
60	23841.1
61	23841.1
62	24078.7
63	24078.7
64	24534.2

65 24534.2
66 24800.9
67 24800.9
68 25102.5
69 25102.5
70 25671.2
71 25671.2
72 26600.3
73 26600.3
74 26764.0
75 26764.0
76 27208.9
77 27208.9
78 27515.1
79 27515.1
80 27758.8
81 27758.8
82 28671.7
83 28671.7
84 28733.7
85 28733.7
86 29012.6
87 29012.6
88 30174.8
89 30174.8
90 30944.0
91 30944.0
92 31485.4
93 31485.4
94 32809.1
95 32809.1
96 38956.9
97 38956.9
98 39402.9
99 39402.9
100 40107.8
101 40107.8
102 40339.6
103 40339.6
104 40949.8
105 40949.8
106 41151.9
107 41151.9
108 41796.9
109 41796.9
110 58273.5
111 58273.5
112 59698.5
113 59698.5
114 60618.0
115 60618.0
116 60845.7
117 60845.7
118 60971.3
119 60971.3

Table S79. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex A2 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	275.2
3	275.2
4	636.9
5	636.9
6	1011.1
7	1011.1
8	4378.3
9	4378.3
10	4731.8
11	4731.8
12	4803.5
13	4803.5
14	4970.5
15	4970.5
16	5253.5
17	5253.5
18	5464.8
19	5464.8
20	5546.9
21	5546.9
22	5960.7
23	5960.7
24	7171.2
25	7171.2
26	7348.7
27	7348.7
28	18752.3
29	18752.3
30	19313.9
31	19313.9
32	19420.7
33	19420.7
34	19960.8
35	19960.8
36	20330.8
37	20330.8
38	20502.1
39	20502.1
40	20629.1
41	20629.1
42	21117.2
43	21117.2
44	21161.2
45	21161.2
46	21715.3
47	21715.3
48	21839.5
49	21839.5
50	22807.8
51	22807.8
52	23291.7

53 23291.7
54 23490.6
55 23490.6
56 23698.9
57 23698.9
58 24169.7
59 24169.7
60 25532.8
61 25532.8
62 25658.1
63 25658.1
64 26029.2
65 26029.2
66 26359.2
67 26359.2
68 28266.6
69 28266.6
70 28422.3
71 28422.3
72 28693.0
73 28693.0
74 28790.8
75 28790.8
76 29101.6
77 29101.6
78 29157.3
79 29157.3
80 29577.7
81 29577.7
82 30684.0
83 30684.0
84 31155.6
85 31155.6
86 31758.9
87 31758.9
88 31891.3
89 31891.3
90 32487.5
91 32487.5
92 32615.8
93 32615.8
94 33415.8
95 33415.8
96 44508.6
97 44508.6
98 44840.1
99 44840.1
100 45373.0
101 45373.0
102 45978.3
103 45978.3
104 46519.2
105 46519.2
106 46778.4
107 46778.4
108 46996.9
109 46996.9

110	67424.5
111	67424.5
112	68512.3
113	68512.3
114	70120.0
115	70120.0
116	71330.1
117	71330.1
118	71911.9
119	71911.9

Table S80. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex A2 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	285.3
3	285.3
4	659.2
5	659.2
6	1019.8
7	1019.8
8	6161.6
9	6161.6
10	6254.3
11	6254.3
12	6486.7
13	6486.7
14	6944.9
15	6944.9
16	7198.0
17	7198.0
18	7430.1
19	7430.1
20	7496.0
21	7496.0
22	7940.4
23	7940.4
24	9119.7
25	9119.7
26	9298.8
27	9298.8
28	16618.3
29	16618.3
30	17126.2
31	17126.2
32	18045.3
33	18045.3
34	18518.8
35	18518.8
36	19015.2
37	19015.2
38	19123.9
39	19123.9
40	19227.6
41	19227.6

42	19798.6
43	19798.6
44	19887.2
45	19887.2
46	20052.1
47	20052.1
48	20237.1
49	20237.1
50	21454.4
51	21454.4
52	21688.9
53	21688.9
54	22106.0
55	22106.0
56	23038.1
57	23038.1
58	23494.8
59	23494.8
60	24046.1
61	24046.1
62	24246.0
63	24246.0
64	24596.9
65	24596.9
66	24947.3
67	24947.3
68	26356.3
69	26356.3
70	27437.9
71	27437.9
72	27562.2
73	27562.2
74	27808.8
75	27808.8
76	27990.5
77	27990.5
78	28154.0
79	28154.0
80	28656.9
81	28656.9
82	28881.6
83	28881.6
84	29978.4
85	29978.4
86	31650.1
87	31650.1
88	32385.0
89	32385.0
90	32752.4
91	32752.4
92	33249.7
93	33249.7
94	34016.5
95	34016.5
96	39616.8
97	39616.8
98	39915.1

99	39915.1
100	41102.8
101	41102.8
102	41486.0
103	41486.0
104	42175.8
105	42175.8
106	42441.4
107	42441.4
108	43427.6
109	43427.6
110	58506.4
111	58506.4
112	60483.4
113	60483.4
114	61788.2
115	61788.2
116	63179.7
117	63179.7
118	63665.0
119	63665.0

Table S81. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex B2 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	179.6
3	179.6
4	869.7
5	869.7
6	1170.3
7	1170.3
8	3374.1
9	3374.1
10	3769.4
11	3769.4
12	3946.5
13	3946.5
14	4092.4
15	4092.4
16	4374.7
17	4374.7
18	4465.7
19	4465.7
20	4918.0
21	4918.0
22	5287.6
23	5287.6
24	6091.8
25	6091.8
26	6291.6
27	6291.6
28	19049.7
29	19049.7
30	19447.3

31 19447.3
32 19632.4
33 19632.4
34 20041.5
35 20041.5
36 20298.3
37 20298.3
38 20424.3
39 20424.3
40 20486.3
41 20486.3
42 20495.7
43 20495.7
44 20741.3
45 20741.3
46 21677.1
47 21677.1
48 21755.0
49 21755.0
50 22054.0
51 22054.0
52 22214.3
53 22214.3
54 22388.0
55 22388.0
56 22571.3
57 22571.3
58 24419.2
59 24419.2
60 25183.1
61 25183.1
62 25596.6
63 25596.6
64 25855.2
65 25855.2
66 26161.4
67 26161.4
68 27720.4
69 27720.4
70 27975.1
71 27975.1
72 28050.6
73 28050.6
74 28258.5
75 28258.5
76 28385.7
77 28385.7
78 28520.3
79 28520.3
80 28800.0
81 28800.0
82 29932.2
83 29932.2
84 30203.3
85 30203.3
86 30537.0
87 30537.0

88	30596.3
89	30596.3
90	31035.8
91	31035.8
92	31798.0
93	31798.0
94	32016.9
95	32016.9
96	44348.9
97	44348.9
98	44597.4
99	44597.4
100	45110.6
101	45110.6
102	45382.1
103	45382.1
104	45945.9
105	45945.9
106	46147.8
107	46147.8
108	46192.9
109	46192.9
110	67493.5
111	67493.5
112	68914.6
113	68914.6
114	69223.7
115	69223.7
116	70552.0
117	70552.0
118	71157.4
119	71157.4

Table S82. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex B2 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	199.0
3	199.0
4	887.3
5	887.3
6	1176.6
7	1176.6
8	4956.1
9	4956.1
10	5423.1
11	5423.1
12	5574.8
13	5574.8
14	5630.1
15	5630.1
16	5732.0
17	5732.0
18	5993.7
19	5993.7

20	6136.6
21	6136.6
22	6583.0
23	6583.0
24	7772.4
25	7772.4
26	7943.2
27	7943.2
28	17371.2
29	17371.2
30	17833.0
31	17833.0
32	18127.9
33	18127.9
34	18710.5
35	18710.5
36	18728.3
37	18728.3
38	18747.9
39	18747.9
40	19019.5
41	19019.5
42	19108.2
43	19108.2
44	19479.7
45	19479.7
46	19695.4
47	19695.4
48	19809.5
49	19809.5
50	19911.5
51	19911.5
52	20166.2
53	20166.2
54	22063.1
55	22063.1
56	22208.4
57	22208.4
58	22547.1
59	22547.1
60	23575.2
61	23575.2
62	23659.4
63	23659.4
64	24241.2
65	24241.2
66	24408.2
67	24408.2
68	25892.0
69	25892.0
70	26552.6
71	26552.6
72	26706.6
73	26706.6
74	26839.6
75	26839.6
76	27157.9

77	27157.9
78	27253.7
79	27253.7
80	27301.9
81	27301.9
82	27936.6
83	27936.6
84	28502.2
85	28502.2
86	30194.2
87	30194.2
88	30617.9
89	30617.9
90	30847.2
91	30847.2
92	30942.1
93	30942.1
94	31732.8
95	31732.8
96	39287.5
97	39287.5
98	39531.4
99	39531.4
100	40491.2
101	40491.2
102	40738.2
103	40738.2
104	41372.3
105	41372.3
106	41628.6
107	41628.6
108	42121.6
109	42121.6
110	58419.1
111	58419.1
112	60572.0
113	60572.0
114	60782.4
115	60782.4
116	62014.3
117	62014.3
118	62667.5
119	62667.5

Table S83. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex B2' with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	123.6
3	123.6
4	1194.6
5	1194.6
6	1425.1
7	1425.1
8	3844.7

9	3844.7
10	4011.4
11	4011.4
12	4719.6
13	4719.6
14	5066.3
15	5066.3
16	5265.3
17	5265.3
18	5496.6
19	5496.6
20	5663.9
21	5663.9
22	6048.9
23	6048.9
24	7184.1
25	7184.1
26	7374.4
27	7374.4
28	18957.8
29	18957.8
30	19256.6
31	19256.6
32	19767.6
33	19767.6
34	20167.5
35	20167.5
36	20268.9
37	20268.9
38	20508.2
39	20508.2
40	20551.8
41	20551.8
42	20723.2
43	20723.2
44	21270.1
45	21270.1
46	21546.5
47	21546.5
48	21603.3
49	21603.3
50	22657.6
51	22657.6
52	23108.8
53	23108.8
54	23598.0
55	23598.0
56	24554.6
57	24554.6
58	24625.4
59	24625.4
60	25635.6
61	25635.6
62	26057.5
63	26057.5
64	26294.3
65	26294.3

66 27288.6
67 27288.6
68 27520.8
69 27520.8
70 27788.0
71 27788.0
72 28440.3
73 28440.3
74 28746.1
75 28746.1
76 28914.3
77 28914.3
78 29394.6
79 29394.6
80 29964.5
81 29964.5
82 30354.4
83 30354.4
84 30753.9
85 30753.9
86 31169.8
87 31169.8
88 31599.1
89 31599.1
90 32276.8
91 32276.8
92 32818.7
93 32818.7
94 33819.9
95 33819.9
96 44615.8
97 44615.8
98 45122.4
99 45122.4
100 45271.2
101 45271.2
102 46514.5
103 46514.5
104 46577.0
105 46577.0
106 46842.2
107 46842.2
108 47118.8
109 47118.8
110 67582.8
111 67582.8
112 68138.6
113 68138.6
114 70700.8
115 70700.8
116 71666.2
117 71666.2
118 72025.2
119 72025.2

Table S84. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex B2' with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	128.3
3	128.3
4	1287.0
5	1287.0
6	1495.5
7	1495.5
8	5504.9
9	5504.9
10	5634.3
11	5634.3
12	6463.4
13	6463.4
14	6788.5
15	6788.5
16	7043.5
17	7043.5
18	7199.8
19	7199.8
20	7463.5
21	7463.5
22	7858.6
23	7858.6
24	9257.2
25	9257.2
26	9420.6
27	9420.6
28	16870.7
29	16870.7
30	17885.8
31	17885.8
32	18301.0
33	18301.0
34	18528.9
35	18528.9
36	18593.4
37	18593.4
38	18784.2
39	18784.2
40	18999.4
41	18999.4
42	19333.5
43	19333.5
44	20010.4
45	20010.4
46	20097.9
47	20097.9
48	20108.9
49	20108.9
50	21199.1
51	21199.1
52	22680.6

53 22680.6
54 22779.0
55 22779.0
56 22852.3
57 22852.3
58 23185.6
59 23185.6
60 24152.7
61 24152.7
62 24558.5
63 24558.5
64 25355.6
65 25355.6
66 25740.4
67 25740.4
68 25955.5
69 25955.5
70 26599.7
71 26599.7
72 26957.3
73 26957.3
74 27229.7
75 27229.7
76 27468.1
77 27468.1
78 28401.4
79 28401.4
80 28684.9
81 28684.9
82 29123.1
83 29123.1
84 30188.5
85 30188.5
86 30740.6
87 30740.6
88 31427.5
89 31427.5
90 31737.3
91 31737.3
92 33205.9
93 33205.9
94 34148.1
95 34148.1
96 39886.2
97 39886.2
98 40492.8
99 40492.8
100 40631.9
101 40631.9
102 42131.3
103 42131.3
104 42282.4
105 42282.4
106 42459.9
107 42459.9
108 43185.8
109 43185.8

110	58810.8
111	58810.8
112	59836.3
113	59836.3
114	62305.5
115	62305.5
116	63434.6
117	63434.6
118	63801.6
119	63801.6

Table S85. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex C2 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	86.2
3	86.2
4	1458.0
5	1458.0
6	1670.5
7	1670.5
8	3208.5
9	3208.5
10	3415.0
11	3415.0
12	4125.6
13	4125.6
14	4270.3
15	4270.3
16	4556.1
17	4556.1
18	4682.1
19	4682.1
20	5378.9
21	5378.9
22	5751.7
23	5751.7
24	6253.7
25	6253.7
26	6451.9
27	6451.9
28	19217.4
29	19217.4
30	19442.1
31	19442.1
32	19878.2
33	19878.2
34	20225.1
35	20225.1
36	20364.3
37	20364.3
38	20600.7
39	20600.7
40	20656.0
41	20656.0

42	20712.6
43	20712.6
44	21128.4
45	21128.4
46	21248.1
47	21248.1
48	21289.3
49	21289.3
50	22148.0
51	22148.0
52	22632.5
53	22632.5
54	23043.0
55	23043.0
56	23184.7
57	23184.7
58	24373.2
59	24373.2
60	25622.6
61	25622.6
62	26072.6
63	26072.6
64	26284.9
65	26284.9
66	26857.5
67	26857.5
68	27252.8
69	27252.8
70	27466.3
71	27466.3
72	28360.0
73	28360.0
74	28378.2
75	28378.2
76	28492.5
77	28492.5
78	28945.0
79	28945.0
80	29285.2
81	29285.2
82	29530.3
83	29530.3
84	30180.3
85	30180.3
86	30296.3
87	30296.3
88	30664.4
89	30664.4
90	31511.6
91	31511.6
92	31929.5
93	31929.5
94	32664.6
95	32664.6
96	44488.1
97	44488.1
98	44936.4

99	44936.4
100	45040.7
101	45040.7
102	45897.8
103	45897.8
104	46054.9
105	46054.9
106	46264.6
107	46264.6
108	46420.7
109	46420.7
110	67962.6
111	67962.6
112	68697.6
113	68697.6
114	69917.7
115	69917.7
116	70682.3
117	70682.3
118	70999.1
119	70999.1

Table S86. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex C2 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	81.4
3	81.4
4	1758.0
5	1758.0
6	1934.1
7	1934.1
8	4792.5
9	4792.5
10	4961.5
11	4961.5
12	5595.5
13	5595.5
14	5743.3
15	5743.3
16	6244.5
17	6244.5
18	6470.5
19	6470.5
20	6987.6
21	6987.6
22	7384.7
23	7384.7
24	8198.2
25	8198.2
26	8355.0
27	8355.0
28	17730.2
29	17730.2
30	18119.9

31	18119.9
32	18517.3
33	18517.3
34	18666.0
35	18666.0
36	18711.1
37	18711.1
38	18957.3
39	18957.3
40	19085.8
41	19085.8
42	19443.8
43	19443.8
44	19507.7
45	19507.7
46	19644.7
47	19644.7
48	20313.1
49	20313.1
50	20992.5
51	20992.5
52	21141.8
53	21141.8
54	22126.1
55	22126.1
56	22166.7
57	22166.7
58	22627.6
59	22627.6
60	24058.9
61	24058.9
62	24477.6
63	24477.6
64	24888.8
65	24888.8
66	25383.6
67	25383.6
68	25589.1
69	25589.1
70	26202.0
71	26202.0
72	26550.9
73	26550.9
74	26696.7
75	26696.7
76	27187.0
77	27187.0
78	27730.6
79	27730.6
80	28525.1
81	28525.1
82	28602.3
83	28602.3
84	29041.7
85	29041.7
86	29319.0
87	29319.0

88	30366.5
89	30366.5
90	31149.8
91	31149.8
92	31413.8
93	31413.8
94	32670.0
95	32670.0
96	39675.7
97	39675.7
98	40086.9
99	40086.9
100	40479.9
101	40479.9
102	41292.7
103	41292.7
104	41642.0
105	41642.0
106	41862.4
107	41862.4
108	42333.1
109	42333.1
110	59207.1
111	59207.1
112	60537.4
113	60537.4
114	61273.8
115	61273.8
116	62327.9
117	62327.9
118	62538.7
119	62538.7

Table S87. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex A4 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	158.0
3	158.0
4	1024.8
5	1024.8
6	1291.4
7	1291.4
8	3921.4
9	3921.4
10	4328.8
11	4328.8
12	4651.9
13	4651.9
14	4707.1
15	4707.1
16	4903.9
17	4903.9
18	5168.1
19	5168.1

20	5345.9
21	5345.9
22	5728.4
23	5728.4
24	6739.2
25	6739.2
26	6927.3
27	6927.3
28	19307.8
29	19307.8
30	19904.8
31	19904.8
32	19921.0
33	19921.0
34	20433.7
35	20433.7
36	20725.0
37	20725.0
38	20907.4
39	20907.4
40	21062.4
41	21062.4
42	21079.6
43	21079.6
44	21235.6
45	21235.6
46	22635.7
47	22635.7
48	22716.8
49	22716.8
50	22831.2
51	22831.2
52	23037.1
53	23037.1
54	23234.1
55	23234.1
56	23357.9
57	23357.9
58	24790.5
59	24790.5
60	25729.8
61	25729.8
62	26044.5
63	26044.5
64	26415.6
65	26415.6
66	26619.6
67	26619.6
68	28665.1
69	28665.1
70	28696.3
71	28696.3
72	28989.5
73	28989.5
74	29194.3
75	29194.3
76	29268.6

77	29268.6
78	29372.1
79	29372.1
80	29598.5
81	29598.5
82	30871.5
83	30871.5
84	31301.1
85	31301.1
86	31744.6
87	31744.6
88	31963.8
89	31963.8
90	31998.2
91	31998.2
92	32966.3
93	32966.3
94	33050.8
95	33050.8
96	45288.0
97	45288.0
98	45491.3
99	45491.3
100	46145.7
101	46145.7
102	46397.1
103	46397.1
104	47102.0
105	47102.0
106	47355.5
107	47355.5
108	47362.0
109	47362.0
110	68606.4
111	68606.4
112	70007.5
113	70007.5
114	70324.3
115	70324.3
116	72390.5
117	72390.5
118	72999.0
119	72999.0

Table S88. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex A4 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	176.4
3	176.4
4	992.8
5	992.8
6	1260.3
7	1260.3
8	4904.5

9	4904.5
10	5291.8
11	5291.8
12	5644.8
13	5644.8
14	5711.5
15	5711.5
16	5811.3
17	5811.3
18	6063.4
19	6063.4
20	6286.1
21	6286.1
22	6691.2
23	6691.2
24	7691.4
25	7691.4
26	7880.4
27	7880.4
28	17436.2
29	17436.2
30	18018.1
31	18018.1
32	18460.9
33	18460.9
34	18916.5
35	18916.5
36	19050.2
37	19050.2
38	19066.5
39	19066.5
40	19285.7
41	19285.7
42	19453.6
43	19453.6
44	19770.4
45	19770.4
46	20170.8
47	20170.8
48	20254.7
49	20254.7
50	20578.1
51	20578.1
52	20774.3
53	20774.3
54	22275.9
55	22275.9
56	22548.3
57	22548.3
58	22783.3
59	22783.3
60	24026.0
61	24026.0
62	24097.1
63	24097.1
64	24629.8
65	24629.8

66 24780.2
67 24780.2
68 25786.0
69 25786.0
70 26581.4
71 26581.4
72 27058.9
73 27058.9
74 27551.2
75 27551.2
76 27666.0
77 27666.0
78 27898.2
79 27898.2
80 28011.8
81 28011.8
82 28324.5
83 28324.5
84 28924.0
85 28924.0
86 30544.5
87 30544.5
88 30967.0
89 30967.0
90 31322.9
91 31322.9
92 31526.0
93 31526.0
94 31961.8
95 31961.8
96 40117.6
97 40117.6
98 40296.3
99 40296.3
100 41260.3
101 41260.3
102 41517.2
103 41517.2
104 42189.0
105 42189.0
106 42451.8
107 42451.8
108 42893.7
109 42893.7
110 59677.4
111 59677.4
112 61498.6
113 61498.6
114 61819.0
115 61819.0
116 63617.1
117 63617.1
118 64247.0
119 64247.0

Table S89. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex B4 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	103.9
3	103.9
4	1353.4
5	1353.4
6	1573.0
7	1573.0
8	3661.7
9	3661.7
10	3917.1
11	3917.1
12	4391.5
13	4391.5
14	4575.5
15	4575.5
16	4965.6
17	4965.6
18	5229.4
19	5229.4
20	5344.4
21	5344.4
22	5708.4
23	5708.4
24	6665.9
25	6665.9
26	6868.8
27	6868.8
28	19410.5
29	19410.5
30	19819.7
31	19819.7
32	20087.0
33	20087.0
34	20548.6
35	20548.6
36	20656.7
37	20656.7
38	21010.6
39	21010.6
40	21104.4
41	21104.4
42	21167.8
43	21167.8
44	21500.0
45	21500.0
46	21589.9
47	21589.9
48	21703.9
49	21703.9
50	22667.1
51	22667.1
52	23176.6

53 23176.6
54 23733.4
55 23733.4
56 23891.1
57 23891.1
58 24619.6
59 24619.6
60 25779.3
61 25779.3
62 26280.2
63 26280.2
64 26350.0
65 26350.0
66 27250.2
67 27250.2
68 28044.6
69 28044.6
70 28391.3
71 28391.3
72 28748.6
73 28748.6
74 28981.3
75 28981.3
76 29219.6
77 29219.6
78 29317.1
79 29317.1
80 29743.1
81 29743.1
82 30610.8
83 30610.8
84 30906.3
85 30906.3
86 31320.8
87 31320.8
88 31438.2
89 31438.2
90 32084.2
91 32084.2
92 32740.4
93 32740.4
94 33160.3
95 33160.3
96 45209.7
97 45209.7
98 45580.7
99 45580.7
100 45789.0
101 45789.0
102 46649.8
103 46649.8
104 46937.8
105 46937.8
106 47219.0
107 47219.0
108 47270.6
109 47270.6

110	68595.8
111	68595.8
112	69333.4
113	69333.4
114	71302.8
115	71302.8
116	71874.6
117	71874.6
118	72724.7
119	72724.7

Table S90. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex B4 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	106.2
3	106.2
4	1445.5
5	1445.5
6	1647.3
7	1647.3
8	4602.8
9	4602.8
10	4804.5
11	4804.5
12	5480.3
13	5480.3
14	5714.1
15	5714.1
16	5996.4
17	5996.4
18	6282.8
19	6282.8
20	6355.5
21	6355.5
22	6770.4
23	6770.4
24	7805.8
25	7805.8
26	7996.6
27	7996.6
28	17502.0
29	17502.0
30	18325.5
31	18325.5
32	18479.7
33	18479.7
34	18900.0
35	18900.0
36	18932.2
37	18932.2
38	19021.6
39	19021.6
40	19222.4
41	19222.4

42	19298.3
43	19298.3
44	19381.2
45	19381.2
46	19680.8
47	19680.8
48	20267.4
49	20267.4
50	21519.3
51	21519.3
52	21702.8
53	21702.8
54	22141.9
55	22141.9
56	22191.5
57	22191.5
58	22666.5
59	22666.5
60	24048.4
61	24048.4
62	24453.4
63	24453.4
64	24727.8
65	24727.8
66	25454.4
67	25454.4
68	25982.4
69	25982.4
70	26020.3
71	26020.3
72	26748.2
73	26748.2
74	27382.8
75	27382.8
76	27613.7
77	27613.7
78	27671.5
79	27671.5
80	28179.3
81	28179.3
82	28497.8
83	28497.8
84	29213.3
85	29213.3
86	29573.7
87	29573.7
88	30755.9
89	30755.9
90	31164.1
91	31164.1
92	31186.6
93	31186.6
94	32267.9
95	32267.9
96	40154.3
97	40154.3
98	40499.2

99	40499.2
100	40860.4
101	40860.4
102	41981.8
103	41981.8
104	42138.9
105	42138.9
106	42428.0
107	42428.0
108	42831.2
109	42831.2
110	59731.8
111	59731.8
112	60721.5
113	60721.5
114	63057.2
115	63057.2
116	63162.9
117	63162.9
118	64099.6
119	64099.6

Table S91. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex C4 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	79.7
3	79.7
4	1590.1
5	1590.1
6	1791.0
7	1791.0
8	3747.3
9	3747.3
10	4071.6
11	4071.6
12	4173.4
13	4173.4
14	4237.8
15	4237.8
16	4942.9
17	4942.9
18	5216.8
19	5216.8
20	5418.5
21	5418.5
22	5842.2
23	5842.2
24	6547.4
25	6547.4
26	6728.9
27	6728.9
28	19708.5
29	19708.5
30	19980.7

31	19980.7
32	20202.8
33	20202.8
34	20653.6
35	20653.6
36	20700.6
37	20700.6
38	21084.9
39	21084.9
40	21289.7
41	21289.7
42	21293.4
43	21293.4
44	21545.9
45	21545.9
46	22268.7
47	22268.7
48	22398.2
49	22398.2
50	22507.0
51	22507.0
52	22623.6
53	22623.6
54	22765.1
55	22765.1
56	23117.9
57	23117.9
58	25289.8
59	25289.8
60	25989.5
61	25989.5
62	26364.3
63	26364.3
64	26659.2
65	26659.2
66	27079.0
67	27079.0
68	27881.6
69	27881.6
70	28439.4
71	28439.4
72	28835.2
73	28835.2
74	28902.6
75	28902.6
76	29066.8
77	29066.8
78	29327.7
79	29327.7
80	29615.3
81	29615.3
82	30335.1
83	30335.1
84	30796.7
85	30796.7
86	31078.6
87	31078.6

88	31300.3
89	31300.3
90	31847.2
91	31847.2
92	32878.4
93	32878.4
94	33033.5
95	33033.5
96	45248.7
97	45248.7
98	45561.6
99	45561.6
100	46043.0
101	46043.0
102	46268.5
103	46268.5
104	46790.2
105	46790.2
106	47018.2
107	47018.2
108	47065.1
109	47065.1
110	69016.8
111	69016.8
112	70392.8
113	70392.8
114	70453.9
115	70453.9
116	71363.8
117	71363.8
118	72078.6
119	72078.6

Table S92. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex C4 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	77.5
3	77.5
4	1798.5
5	1798.5
6	1974.5
7	1974.5
8	4817.4
9	4817.4
10	5117.3
11	5117.3
12	5222.1
13	5222.1
14	5284.5
15	5284.5
16	6177.1
17	6177.1
18	6439.6
19	6439.6

20	6648.3
21	6648.3
22	7060.0
23	7060.0
24	7858.2
25	7858.2
26	8028.2
27	8028.2
28	18131.8
29	18131.8
30	18580.3
31	18580.3
32	18611.6
33	18611.6
34	19151.5
35	19151.5
36	19190.9
37	19190.9
38	19325.0
39	19325.0
40	19391.1
41	19391.1
42	19897.6
43	19897.6
44	19974.8
45	19974.8
46	20136.1
47	20136.1
48	20242.0
49	20242.0
50	20406.3
51	20406.3
52	20505.6
53	20505.6
54	22196.4
55	22196.4
56	22675.9
57	22675.9
58	23039.8
59	23039.8
60	24255.0
61	24255.0
62	24498.2
63	24498.2
64	24954.4
65	24954.4
66	25202.0
67	25202.0
68	26067.5
69	26067.5
70	26552.1
71	26552.1
72	26668.1
73	26668.1
74	27277.5
75	27277.5
76	27573.0

77	27573.0
78	27840.1
79	27840.1
80	28180.3
81	28180.3
82	28824.0
83	28824.0
84	29154.8
85	29154.8
86	29511.3
87	29511.3
88	30449.4
89	30449.4
90	30922.7
91	30922.7
92	31636.6
93	31636.6
94	32342.2
95	32342.2
96	40239.3
97	40239.3
98	40523.2
99	40523.2
100	41272.4
101	41272.4
102	41490.4
103	41490.4
104	42089.6
105	42089.6
106	42333.1
107	42333.1
108	42723.4
109	42723.4
110	60198.9
111	60198.9
112	62077.7
113	62077.7
114	62140.0
115	62140.0
116	62659.5
117	62659.5
118	63543.4
119	63543.4

Table S93. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex A0 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	2.360957
6.06	2.389244
9.09	2.414911
12.12	2.440191
15.15	2.465357
18.18	2.490468
21.21	2.515516

24.24	2.540436
27.27	2.565117
30.30	2.589412
33.33	2.613157
36.36	2.636194
39.39	2.658379
42.42	2.679595
45.45	2.699753
48.48	2.718794
51.52	2.736684
54.55	2.753416
57.58	2.769001
60.61	2.783465
63.64	2.796849
66.67	2.809200
69.70	2.820573
72.73	2.831026
75.76	2.840617
78.79	2.849406
81.82	2.857453
84.85	2.864814
87.88	2.871543
90.91	2.877693
93.94	2.883313
96.97	2.888447
100.00	2.893139
103.03	2.897429
106.06	2.901351
109.09	2.904941
112.12	2.908229
115.15	2.911244
118.18	2.914010
121.21	2.916553
124.24	2.918893
127.27	2.921051
130.30	2.923043
133.33	2.924888
136.36	2.926598
139.39	2.928189
142.42	2.929672
145.45	2.931058
148.48	2.932358
151.52	2.933581
154.55	2.934734
157.58	2.935827
160.61	2.936864
163.64	2.937854
166.67	2.938800
169.70	2.939709
172.73	2.940585
175.76	2.941432
178.79	2.942254
181.82	2.943054
184.85	2.943836
187.88	2.944601
190.91	2.945353
193.94	2.946094

196.97	2.946826
200.00	2.947550
203.03	2.948268
206.06	2.948982
209.09	2.949692
212.12	2.950400
215.15	2.951108
218.18	2.951814
221.21	2.952522
224.24	2.953230
227.27	2.953940
230.30	2.954652
233.33	2.955366
236.36	2.956083
239.39	2.956804
242.42	2.957527
245.45	2.958254
248.48	2.958985
251.52	2.959719
254.55	2.960456
257.58	2.961198
260.61	2.961943
263.64	2.962691
266.67	2.963443
269.70	2.964198
272.73	2.964956
275.76	2.965718
278.79	2.966482
281.82	2.967249
284.85	2.968018
287.88	2.968790
290.91	2.969564
293.94	2.970340
296.97	2.971117
300.00	2.971896

Table S94. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex B0 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	3.023502
6.06	3.042194
9.09	3.056535
12.12	3.070232
15.15	3.083741
18.18	3.097177
21.21	3.110579
24.24	3.123962
27.27	3.137334
30.30	3.150698
33.33	3.164054
36.36	3.177401
39.39	3.190730
42.42	3.204033
45.45	3.217295

48.48	3.230497
51.52	3.243618
54.55	3.256635
57.58	3.269523
60.61	3.282256
63.64	3.294809
66.67	3.307157
69.70	3.319279
72.73	3.331153
75.76	3.342761
78.79	3.354086
81.82	3.365117
84.85	3.375841
87.88	3.386250
90.91	3.396338
93.94	3.406100
96.97	3.415534
100.00	3.424639
103.03	3.433415
106.06	3.441866
109.09	3.449993
112.12	3.457802
115.15	3.465297
118.18	3.472483
121.21	3.479367
124.24	3.485956
127.27	3.492256
130.30	3.498274
133.33	3.504019
136.36	3.509496
139.39	3.514714
142.42	3.519681
145.45	3.524403
148.48	3.528888
151.52	3.533144
154.55	3.537177
157.58	3.540995
160.61	3.544605
163.64	3.548012
166.67	3.551225
169.70	3.554248
172.73	3.557089
175.76	3.559754
178.79	3.562247
181.82	3.564576
184.85	3.566745
187.88	3.568760
190.91	3.570625
193.94	3.572347
196.97	3.573929
200.00	3.575377
203.03	3.576695
206.06	3.577887
209.09	3.578957
212.12	3.579910
215.15	3.580750
218.18	3.581480

221.21	3.582104
224.24	3.582626
227.27	3.583049
230.30	3.583377
233.33	3.583612
236.36	3.583758
239.39	3.583819
242.42	3.583796
245.45	3.583692
248.48	3.583512
251.52	3.583256
254.55	3.582929
257.58	3.582531
260.61	3.582067
263.64	3.581537
266.67	3.580946
269.70	3.580293
272.73	3.579583
275.76	3.578816
278.79	3.577996
281.82	3.577123
284.85	3.576201
287.88	3.575230
290.91	3.574212
293.94	3.573150
296.97	3.572045
300.00	3.570898

Table S95. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex C0 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	2.086966
6.06	2.134921
9.09	2.180873
12.12	2.226500
15.15	2.271836
18.18	2.316495
21.21	2.359865
24.24	2.401302
27.27	2.440272
30.30	2.476416
33.33	2.509553
36.36	2.539651
39.39	2.566794
42.42	2.591139
45.45	2.612893
48.48	2.632282
51.52	2.649536
54.55	2.664883
57.58	2.678533
60.61	2.690685
63.64	2.701515
66.67	2.711183
69.70	2.719832

72.73	2.727586
75.76	2.734556
78.79	2.740840
81.82	2.746521
84.85	2.751674
87.88	2.756364
90.91	2.760648
93.94	2.764574
96.97	2.768186
100.00	2.771522
103.03	2.774615
106.06	2.777494
109.09	2.780184
112.12	2.782708
115.15	2.785085
118.18	2.787332
121.21	2.789465
124.24	2.791496
127.27	2.793439
130.30	2.795302
133.33	2.797096
136.36	2.798829
139.39	2.800507
142.42	2.802138
145.45	2.803727
148.48	2.805279
151.52	2.806799
154.55	2.808291
157.58	2.809757
160.61	2.811203
163.64	2.812629
166.67	2.814040
169.70	2.815436
172.73	2.816821
175.76	2.818196
178.79	2.819563
181.82	2.820922
184.85	2.822276
187.88	2.823626
190.91	2.824972
193.94	2.826316
196.97	2.827658
200.00	2.828999
203.03	2.830339
206.06	2.831680
209.09	2.833022
212.12	2.834365
215.15	2.835709
218.18	2.837056
221.21	2.838405
224.24	2.839756
227.27	2.841110
230.30	2.842466
233.33	2.843826
236.36	2.845189
239.39	2.846556
242.42	2.847926

245.45	2.849299
248.48	2.850676
251.52	2.852056
254.55	2.853440
257.58	2.854827
260.61	2.856218
263.64	2.857613
266.67	2.859011
269.70	2.860413
272.73	2.861817
275.76	2.863226
278.79	2.864637
281.82	2.866052
284.85	2.867470
287.88	2.868890
290.91	2.870314
293.94	2.871741
296.97	2.873170
300.00	2.874602

Table S96. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex A2 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	3.011632
6.06	3.030715
9.09	3.045483
12.12	3.059611
15.15	3.073553
18.18	3.087423
21.21	3.101259
24.24	3.115076
27.27	3.128882
30.30	3.142680
33.33	3.156469
36.36	3.170246
39.39	3.184001
42.42	3.197722
45.45	3.211392
48.48	3.224990
51.52	3.238490
54.55	3.251867
57.58	3.265091
60.61	3.278137
63.64	3.290975
66.67	3.303580
69.70	3.315929
72.73	3.328001
75.76	3.339777
78.79	3.351241
81.82	3.362381
84.85	3.373187
87.88	3.383651
90.91	3.393768
93.94	3.403537

96.97	3.412955
100.00	3.422025
103.03	3.430749
106.06	3.439131
109.09	3.447175
112.12	3.454889
115.15	3.462278
118.18	3.469351
121.21	3.476114
124.24	3.482577
127.27	3.488748
130.30	3.494635
133.33	3.500248
136.36	3.505594
139.39	3.510683
142.42	3.515522
145.45	3.520122
148.48	3.524489
151.52	3.528631
154.55	3.532558
157.58	3.536276
160.61	3.539792
163.64	3.543115
166.67	3.546250
169.70	3.549205
172.73	3.551986
175.76	3.554599
178.79	3.557050
181.82	3.559345
184.85	3.561490
187.88	3.563490
190.91	3.565350
193.94	3.567075
196.97	3.568670
200.00	3.570138
203.03	3.571486
206.06	3.572717
209.09	3.573834
212.12	3.574842
215.15	3.575745
218.18	3.576546
221.21	3.577249
224.24	3.577857
227.27	3.578373
230.30	3.578801
233.33	3.579142
236.36	3.579402
239.39	3.579581
242.42	3.579683
245.45	3.579711
248.48	3.579666
251.52	3.579552
254.55	3.579371
257.58	3.579124
260.61	3.578815
263.64	3.578445
266.67	3.578016

269.70	3.577531
272.73	3.576992
275.76	3.576399
278.79	3.575756
281.82	3.575063
284.85	3.574323
287.88	3.573538
290.91	3.572708
293.94	3.571835
296.97	3.570922
300.00	3.569969

Table S97. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex B2 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	2.731009
6.06	2.755332
9.09	2.776127
12.12	2.796399
15.15	2.816520
18.18	2.836580
21.21	2.856611
24.24	2.876620
27.27	2.896596
30.30	2.916516
33.33	2.936335
36.36	2.955997
39.39	2.975432
42.42	2.994568
45.45	3.013329
48.48	3.031644
51.52	3.049449
54.55	3.066688
57.58	3.083315
60.61	3.099295
63.64	3.114603
66.67	3.129222
69.70	3.143147
72.73	3.156376
75.76	3.168918
78.79	3.180786
81.82	3.191995
84.85	3.202569
87.88	3.212528
90.91	3.221901
93.94	3.230712
96.97	3.238990
100.00	3.246764
103.03	3.254060
106.06	3.260907
109.09	3.267332
112.12	3.273361
115.15	3.279019
118.18	3.284331

121.21	3.289319
124.24	3.294007
127.27	3.298414
130.30	3.302561
133.33	3.306465
136.36	3.310145
139.39	3.313616
142.42	3.316893
145.45	3.319991
148.48	3.322923
151.52	3.325701
154.55	3.328337
157.58	3.330840
160.61	3.333220
163.64	3.335487
166.67	3.337649
169.70	3.339713
172.73	3.341686
175.76	3.343575
178.79	3.345386
181.82	3.347123
184.85	3.348793
187.88	3.350399
190.91	3.351947
193.94	3.353439
196.97	3.354879
200.00	3.356270
203.03	3.357616
206.06	3.358919
209.09	3.360181
212.12	3.361405
215.15	3.362593
218.18	3.363746
221.21	3.364867
224.24	3.365956
227.27	3.367015
230.30	3.368046
233.33	3.369050
236.36	3.370027
239.39	3.370978
242.42	3.371905
245.45	3.372808
248.48	3.373688
251.52	3.374546
254.55	3.375382
257.58	3.376196
260.61	3.376990
263.64	3.377763
266.67	3.378516
269.70	3.379250
272.73	3.379964
275.76	3.380660
278.79	3.381336
281.82	3.381995
284.85	3.382635
287.88	3.383257
290.91	3.383862

293.94	3.384449
296.97	3.385019
300.00	3.385571

Table S98. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex B2' measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	2.289815
6.06	2.323675
9.09	2.355111
12.12	2.386188
15.15	2.417157
18.18	2.448049
21.21	2.478799
24.24	2.509261
27.27	2.539226
30.30	2.568459
33.33	2.596733
36.36	2.623848
39.39	2.649647
42.42	2.674020
45.45	2.696902
48.48	2.718267
51.52	2.738125
54.55	2.756509
57.58	2.773474
60.61	2.789089
63.64	2.803431
66.67	2.816583
69.70	2.828628
72.73	2.839652
75.76	2.849735
78.79	2.858957
81.82	2.867391
84.85	2.875107
87.88	2.882172
90.91	2.888643
93.94	2.894578
96.97	2.900027
100.00	2.905036
103.03	2.909648
106.06	2.913902
109.09	2.917831
112.12	2.921469
115.15	2.924843
118.18	2.927980
121.21	2.930903
124.24	2.933635
127.27	2.936192
130.30	2.938595
133.33	2.940857
136.36	2.942993
139.39	2.945017
142.42	2.946939

145.45	2.948770
148.48	2.950520
151.52	2.952197
154.55	2.953808
157.58	2.955362
160.61	2.956863
163.64	2.958319
166.67	2.959733
169.70	2.961111
172.73	2.962457
175.76	2.963774
178.79	2.965066
181.82	2.966337
184.85	2.967588
187.88	2.968823
190.91	2.970043
193.94	2.971252
196.97	2.972449
200.00	2.973638
203.03	2.974819
206.06	2.975994
209.09	2.977164
212.12	2.978330
215.15	2.979493
218.18	2.980654
221.21	2.981813
224.24	2.982971
227.27	2.984129
230.30	2.985287
233.33	2.986446
236.36	2.987605
239.39	2.988765
242.42	2.989927
245.45	2.991090
248.48	2.992254
251.52	2.993420
254.55	2.994588
257.58	2.995758
260.61	2.996930
263.64	2.998103
266.67	2.999278
269.70	3.000455
272.73	3.001633
275.76	3.002813
278.79	3.003994
281.82	3.005176
284.85	3.006360
287.88	3.007544
290.91	3.008729
293.94	3.009915
296.97	3.011101
300.00	3.012288

Table S99. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex C2 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	2.030013
6.06	2.082193
9.09	2.132529
12.12	2.182535
15.15	2.232124
18.18	2.280724
21.21	2.327555
24.24	2.371871
27.27	2.413116
30.30	2.450966
33.33	2.485309
36.36	2.516201
39.39	2.543810
42.42	2.568373
45.45	2.590160
48.48	2.609455
51.52	2.626530
54.55	2.641644
57.58	2.655034
60.61	2.666915
63.64	2.677476
66.67	2.686886
69.70	2.695292
72.73	2.702823
75.76	2.709591
78.79	2.715693
81.82	2.721214
84.85	2.726228
87.88	2.730798
90.91	2.734980
93.94	2.738821
96.97	2.742363
100.00	2.745643
103.03	2.748692
106.06	2.751539
109.09	2.754207
112.12	2.756718
115.15	2.759089
118.18	2.761338
121.21	2.763479
124.24	2.765524
127.27	2.767485
130.30	2.769371
133.33	2.771191
136.36	2.772952
139.39	2.774663
142.42	2.776327
145.45	2.777952
148.48	2.779541
151.52	2.781098
154.55	2.782629

157.58	2.784135
160.61	2.785620
163.64	2.787087
166.67	2.788538
169.70	2.789976
172.73	2.791401
175.76	2.792816
178.79	2.794222
181.82	2.795621
184.85	2.797014
187.88	2.798402
190.91	2.799785
193.94	2.801166
196.97	2.802544
200.00	2.803921
203.03	2.805296
206.06	2.806671
209.09	2.808046
212.12	2.809421
215.15	2.810797
218.18	2.812174
221.21	2.813553
224.24	2.814933
227.27	2.816315
230.30	2.817700
233.33	2.819087
236.36	2.820476
239.39	2.821867
242.42	2.823262
245.45	2.824659
248.48	2.826059
251.52	2.827462
254.55	2.828868
257.58	2.830277
260.61	2.831689
263.64	2.833104
266.67	2.834522
269.70	2.835943
272.73	2.837367
275.76	2.838793
278.79	2.840223
281.82	2.841655
284.85	2.843091
287.88	2.844528
290.91	2.845969
293.94	2.847412
296.97	2.848858
300.00	2.850306

Table S100. Ab initio calculated temperature-dependent magnetic susceptibility
for S=3/2 ground state of Complex A4 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	2.626084

6.06	2.652657
9.09	2.675975
12.12	2.698812
15.15	2.721508
18.18	2.744149
21.21	2.766757
24.24	2.789326
27.27	2.811824
30.30	2.834191
33.33	2.856348
36.36	2.878196
39.39	2.899634
42.42	2.920559
45.45	2.940880
48.48	2.960516
51.52	2.979400
54.55	2.997481
57.58	3.014726
60.61	3.031113
63.64	3.046635
66.67	3.061295
69.70	3.075106
72.73	3.088088
75.76	3.100267
78.79	3.111675
81.82	3.122346
84.85	3.132316
87.88	3.141623
90.91	3.150304
93.94	3.158398
96.97	3.165942
100.00	3.172972
103.03	3.179524
106.06	3.185631
109.09	3.191326
112.12	3.196638
115.15	3.201597
118.18	3.206230
121.21	3.210562
124.24	3.214617
127.27	3.218416
130.30	3.221980
133.33	3.225329
136.36	3.228480
139.39	3.231449
142.42	3.234252
145.45	3.236902
148.48	3.239412
151.52	3.241794
154.55	3.244058
157.58	3.246216
160.61	3.248276
163.64	3.250245
166.67	3.252133
169.70	3.253946
172.73	3.255690
175.76	3.257371

178.79	3.258995
181.82	3.260566
184.85	3.262089
187.88	3.263569
190.91	3.265007
193.94	3.266409
196.97	3.267777
200.00	3.269113
203.03	3.270421
206.06	3.271702
209.09	3.272958
212.12	3.274192
215.15	3.275404
218.18	3.276597
221.21	3.277771
224.24	3.278928
227.27	3.280069
230.30	3.281194
233.33	3.282305
236.36	3.283403
239.39	3.284487
242.42	3.285558
245.45	3.286618
248.48	3.287666
251.52	3.288702
254.55	3.289727
257.58	3.290742
260.61	3.291746
263.64	3.292740
266.67	3.293723
269.70	3.294696
272.73	3.295659
275.76	3.296612
278.79	3.297556
281.82	3.298489
284.85	3.299412
287.88	3.300325
290.91	3.301229
293.94	3.302122
296.97	3.303005
300.00	3.303878

Table S101. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex B4 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	2.201941
6.06	2.243430
9.09	2.282708
12.12	2.321655
15.15	2.360469
18.18	2.399071
21.21	2.437210
24.24	2.474520
27.27	2.510606

30.30	2.545107
33.33	2.577741
36.36	2.608318
39.39	2.636735
42.42	2.662966
45.45	2.687047
48.48	2.709057
51.52	2.729106
54.55	2.747323
57.58	2.763846
60.61	2.778816
63.64	2.792370
66.67	2.804642
69.70	2.815756
72.73	2.825829
75.76	2.834966
78.79	2.843266
81.82	2.850816
84.85	2.857697
87.88	2.863979
90.91	2.869728
93.94	2.875000
96.97	2.879848
100.00	2.884316
103.03	2.888446
106.06	2.892274
109.09	2.895833
112.12	2.899151
115.15	2.902255
118.18	2.905167
121.21	2.907908
124.24	2.910496
127.27	2.912949
130.30	2.915279
133.33	2.917500
136.36	2.919625
139.39	2.921663
142.42	2.923624
145.45	2.925516
148.48	2.927347
151.52	2.929124
154.55	2.930852
157.58	2.932538
160.61	2.934185
163.64	2.935798
166.67	2.937382
169.70	2.938940
172.73	2.940475
175.76	2.941989
178.79	2.943487
181.82	2.944969
184.85	2.946438
187.88	2.947895
190.91	2.949344
193.94	2.950784
196.97	2.952218
200.00	2.953646

203.03	2.955070
206.06	2.956490
209.09	2.957908
212.12	2.959324
215.15	2.960740
218.18	2.962154
221.21	2.963569
224.24	2.964985
227.27	2.966401
230.30	2.967819
233.33	2.969238
236.36	2.970659
239.39	2.972082
242.42	2.973507
245.45	2.974935
248.48	2.976365
251.52	2.977798
254.55	2.979233
257.58	2.980671
260.61	2.982112
263.64	2.983555
266.67	2.985001
269.70	2.986450
272.73	2.987901
275.76	2.989354
278.79	2.990810
281.82	2.992268
284.85	2.993729
287.88	2.995191
290.91	2.996656
293.94	2.998122
296.97	2.999590
300.00	3.001060

Table S102. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex C4 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	2.042374
6.06	2.096561
9.09	2.148841
12.12	2.200752
15.15	2.252105
18.18	2.302184
21.21	2.350092
24.24	2.395040
27.27	2.436491
30.30	2.474180
33.33	2.508074
36.36	2.538306
39.39	2.565115
42.42	2.588798
45.45	2.609671
48.48	2.628051
51.52	2.644236

54.55	2.658499
57.58	2.671089
60.61	2.682225
63.64	2.692099
66.67	2.700880
69.70	2.708713
72.73	2.715724
75.76	2.722022
78.79	2.727701
81.82	2.732843
84.85	2.737517
87.88	2.741783
90.91	2.745693
93.94	2.749294
96.97	2.752623
100.00	2.755714
103.03	2.758597
106.06	2.761298
109.09	2.763838
112.12	2.766237
115.15	2.768512
118.18	2.770679
121.21	2.772749
124.24	2.774734
127.27	2.776646
130.30	2.778491
133.33	2.780279
136.36	2.782015
139.39	2.783707
142.42	2.785359
145.45	2.786977
148.48	2.788564
151.52	2.790125
154.55	2.791662
157.58	2.793179
160.61	2.794678
163.64	2.796161
166.67	2.797632
169.70	2.799091
172.73	2.800541
175.76	2.801982
178.79	2.803416
181.82	2.804845
184.85	2.806269
187.88	2.807689
190.91	2.809107
193.94	2.810522
196.97	2.811936
200.00	2.813349
203.03	2.814762
206.06	2.816175
209.09	2.817588
212.12	2.819003
215.15	2.820419
218.18	2.821836
221.21	2.823256
224.24	2.824677

227.27	2.826101
230.30	2.827527
233.33	2.828955
236.36	2.830386
239.39	2.831820
242.42	2.833257
245.45	2.834697
248.48	2.836139
251.52	2.837585
254.55	2.839034
257.58	2.840485
260.61	2.841940
263.64	2.843398
266.67	2.844858
269.70	2.846322
272.73	2.847789
275.76	2.849258
278.79	2.850731
281.82	2.852206
284.85	2.853684
287.88	2.855165
290.91	2.856648
293.94	2.858134
296.97	2.859623
300.00	2.861114

Table S103. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex A0 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	0.000000
808.08	0.170030
1616.16	0.337313
2424.24	0.499311
3232.32	0.653866
4040.40	0.799313
4848.48	0.934522
5656.57	1.058885
6464.65	1.172243
7272.73	1.274808
8080.81	1.367059
8888.89	1.449657
9696.97	1.523365
10505.05	1.588992
11313.13	1.647345
12121.21	1.699202
12929.29	1.745292
13737.37	1.786285
14545.45	1.822787
15353.54	1.855338
16161.62	1.884422
16969.70	1.910462
17777.78	1.933831
18585.86	1.954856
19393.94	1.973820
20202.02	1.990972

21010.10	2.006527
21818.18	2.020675
22626.26	2.033579
23434.34	2.045382
24242.42	2.056208
25050.51	2.066166
25858.59	2.075351
26666.67	2.083847
27474.75	2.091726
28282.83	2.099053
29090.91	2.105883
29898.99	2.112267
30707.07	2.118249
31515.15	2.123868
32323.23	2.129158
33131.31	2.134149
33939.39	2.138870
34747.47	2.143344
35555.56	2.147594
36363.64	2.151638
37171.72	2.155494
37979.80	2.159178
38787.88	2.162704
39595.96	2.166085
40404.04	2.169332
41212.12	2.172456
42020.20	2.175466
42828.28	2.178370
43636.36	2.181177
44444.44	2.183893
45252.53	2.186525
46060.61	2.189079
46868.69	2.191561
47676.77	2.193974
48484.85	2.196324
49292.93	2.198615
50101.01	2.200850
50909.09	2.203034
51717.17	2.205169
52525.25	2.207258
53333.33	2.209304
54141.41	2.211310
54949.49	2.213278
55757.58	2.215210
56565.66	2.217108
57373.74	2.218974
58181.82	2.220810
58989.90	2.222617
59797.98	2.224397
60606.06	2.226151
61414.14	2.227881
62222.22	2.229587
63030.30	2.231272
63838.38	2.232936
64646.46	2.234579
65454.55	2.236203
66262.63	2.237810

67070.71	2.239399
67878.79	2.240971
68686.87	2.242527
69494.95	2.244069
70303.03	2.245595
71111.11	2.247108
71919.19	2.248608
72727.27	2.250094
73535.35	2.251569
74343.43	2.253031
75151.52	2.254483
75959.60	2.255923
76767.68	2.257353
77575.76	2.258773
78383.84	2.260183
79191.92	2.261583
80000.00	2.262975

Table S104. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex B0 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	0.000000
808.08	0.218147
1616.16	0.431755
2424.24	0.636720
3232.32	0.829725
4040.40	1.008420
4848.48	1.171463
5656.57	1.318410
6464.65	1.449538
7272.73	1.565647
8080.81	1.667862
8888.89	1.757482
9696.97	1.835854
10505.05	1.904298
11313.13	1.964050
12121.21	2.016241
12929.29	2.061883
13737.37	2.101866
14545.45	2.136968
15353.54	2.167861
16161.62	2.195126
16969.70	2.219259
17777.78	2.240686
18585.86	2.259771
19393.94	2.276824
20202.02	2.292112
21010.10	2.305861
21818.18	2.318267
22626.26	2.329497
23434.34	2.339694
24242.42	2.348981
25050.51	2.357467
25858.59	2.365242
26666.67	2.372387

27474.75	2.378972
28282.83	2.385057
29090.91	2.390696
29898.99	2.395934
30707.07	2.400812
31515.15	2.405367
32323.23	2.409630
33131.31	2.413628
33939.39	2.417388
34747.47	2.420930
35555.56	2.424274
36363.64	2.427439
37171.72	2.430438
37979.80	2.433287
38787.88	2.435999
39595.96	2.438583
40404.04	2.441051
41212.12	2.443412
42020.20	2.445674
42828.28	2.447844
43636.36	2.449930
44444.44	2.451937
45252.53	2.453872
46060.61	2.455738
46868.69	2.457542
47676.77	2.459287
48484.85	2.460978
49292.93	2.462617
50101.01	2.464208
50909.09	2.465755
51717.17	2.467259
52525.25	2.468724
53333.33	2.470152
54141.41	2.471545
54949.49	2.472905
55757.58	2.474234
56565.66	2.475534
57373.74	2.476806
58181.82	2.478052
58989.90	2.479273
59797.98	2.480471
60606.06	2.481646
61414.14	2.482800
62222.22	2.483935
63030.30	2.485050
63838.38	2.486147
64646.46	2.487227
65454.55	2.488290
66262.63	2.489337
67070.71	2.490370
67878.79	2.491388
68686.87	2.492393
69494.95	2.493384
70303.03	2.494363
71111.11	2.495330
71919.19	2.496285
72727.27	2.497230

73535.35	2.498164
74343.43	2.499087
75151.52	2.500001
75959.60	2.500906
76767.68	2.501802
77575.76	2.502689
78383.84	2.503568
79191.92	2.504439
80000.00	2.505302

Table S105. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex C0 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	-0.000000
808.08	0.149742
1616.16	0.297382
2424.24	0.440958
3232.32	0.578766
4040.40	0.709442
4848.48	0.832004
5656.57	0.945849
6464.65	1.050718
7272.73	1.146646
8080.81	1.233893
8888.89	1.312888
9696.97	1.384166
10505.05	1.448322
11313.13	1.505976
12121.21	1.557745
12929.29	1.604219
13737.37	1.645956
14545.45	1.683471
15353.54	1.717232
16161.62	1.747665
16969.70	1.775148
17777.78	1.800021
18585.86	1.822582
19393.94	1.843096
20202.02	1.861798
21010.10	1.878893
21818.18	1.894562
22626.26	1.908962
23434.34	1.922235
24242.42	1.934502
25050.51	1.945871
25858.59	1.956437
26666.67	1.966284
27474.75	1.975485
28282.83	1.984106
29090.91	1.992204
29898.99	1.999830
30707.07	2.007029
31515.15	2.013842
32323.23	2.020304
33131.31	2.026447

33939.39	2.032300
34747.47	2.037888
35555.56	2.043234
36363.64	2.048359
37171.72	2.053280
37979.80	2.058015
38787.88	2.062579
39595.96	2.066984
40404.04	2.071245
41212.12	2.075370
42020.20	2.079372
42828.28	2.083258
43636.36	2.087037
44444.44	2.090718
45252.53	2.094306
46060.61	2.097808
46868.69	2.101231
47676.77	2.104579
48484.85	2.107858
49292.93	2.111071
50101.01	2.114223
50909.09	2.117319
51717.17	2.120361
52525.25	2.123353
53333.33	2.126297
54141.41	2.129197
54949.49	2.132056
55757.58	2.134875
56565.66	2.137657
57373.74	2.140404
58181.82	2.143117
58989.90	2.145800
59797.98	2.148452
60606.06	2.151077
61414.14	2.153675
62222.22	2.156248
63030.30	2.158797
63838.38	2.161323
64646.46	2.163827
65454.55	2.166311
66262.63	2.168775
67070.71	2.171221
67878.79	2.173648
68686.87	2.176059
69494.95	2.178453
70303.03	2.180831
71111.11	2.183195
71919.19	2.185545
72727.27	2.187881
73535.35	2.190203
74343.43	2.192513
75151.52	2.194812
75959.60	2.197098
76767.68	2.199374
77575.76	2.201638
78383.84	2.203893
79191.92	2.206137

80000.00	2.208372

Table S106. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex A2 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	0.000000
808.08	0.217280
1616.16	0.430057
2424.24	0.634260
3232.32	0.826592
4040.40	1.004719
4848.48	1.167297
5656.57	1.313878
6464.65	1.444730
7272.73	1.560639
8080.81	1.662717
8888.89	1.752248
9696.97	1.830572
10505.05	1.898996
11313.13	1.958751
12121.21	2.010961
12929.29	2.056632
13737.37	2.096653
14545.45	2.131798
15353.54	2.162737
16161.62	2.190050
16969.70	2.214233
17777.78	2.235709
18585.86	2.254844
19393.94	2.271948
20202.02	2.287285
21010.10	2.301085
21818.18	2.313540
22626.26	2.324820
23434.34	2.335066
24242.42	2.344404
25050.51	2.352939
25858.59	2.360765
26666.67	2.367961
27474.75	2.374596
28282.83	2.380732
29090.91	2.386422
29898.99	2.391712
30707.07	2.396642
31515.15	2.401249
32323.23	2.405564
33131.31	2.409615
33939.39	2.413427
34747.47	2.417022
35555.56	2.420419
36363.64	2.423636
37171.72	2.426688
37979.80	2.429589
38787.88	2.432352
39595.96	2.434989

40404.04	2.437508
41212.12	2.439920
42020.20	2.442233
42828.28	2.444453
43636.36	2.446589
44444.44	2.448646
45252.53	2.450629
46060.61	2.452544
46868.69	2.454396
47676.77	2.456188
48484.85	2.457925
49292.93	2.459610
50101.01	2.461247
50909.09	2.462838
51717.17	2.464387
52525.25	2.465895
53333.33	2.467366
54141.41	2.468801
54949.49	2.470202
55757.58	2.471572
56565.66	2.472912
57373.74	2.474223
58181.82	2.475508
58989.90	2.476767
59797.98	2.478002
60606.06	2.479214
61414.14	2.480405
62222.22	2.481575
63030.30	2.482725
63838.38	2.483856
64646.46	2.484970
65454.55	2.486066
66262.63	2.487147
67070.71	2.488211
67878.79	2.489261
68686.87	2.490297
69494.95	2.491319
70303.03	2.492328
71111.11	2.493324
71919.19	2.494309
72727.27	2.495282
73535.35	2.496244
74343.43	2.497196
75151.52	2.498137
75959.60	2.499069
76767.68	2.499991
77575.76	2.500904
78383.84	2.501809
79191.92	2.502706
80000.00	2.503594

Table S107. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex B2 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	0.000000

808.08	0.196872
1616.16	0.390054
2424.24	0.576179
3232.32	0.752460
4040.40	0.916847
4848.48	1.068069
5656.57	1.205575
6464.65	1.329416
7272.73	1.440100
8080.81	1.538443
8888.89	1.625446
9696.97	1.702190
10505.05	1.769766
11313.13	1.829223
12121.21	1.881539
12929.29	1.927607
13737.37	1.968226
14545.45	2.004103
15353.54	2.035859
16161.62	2.064035
16969.70	2.089100
17777.78	2.111460
18585.86	2.131466
19393.94	2.149419
20202.02	2.165579
21010.10	2.180171
21818.18	2.193387
22626.26	2.205394
23434.34	2.216337
24242.42	2.226339
25050.51	2.235509
25858.59	2.243941
26666.67	2.251716
27474.75	2.258906
28282.83	2.265573
29090.91	2.271772
29898.99	2.277551
30707.07	2.282952
31515.15	2.288012
32323.23	2.292764
33131.31	2.297237
33939.39	2.301457
34747.47	2.305448
35555.56	2.309230
36363.64	2.312821
37171.72	2.316237
37979.80	2.319494
38787.88	2.322605
39595.96	2.325581
40404.04	2.328434
41212.12	2.331173
42020.20	2.333806
42828.28	2.336343
43636.36	2.338790
44444.44	2.341154
45252.53	2.343441
46060.61	2.345656

46868.69	2.347804
47676.77	2.349890
48484.85	2.351918
49292.93	2.353892
50101.01	2.355815
50909.09	2.357691
51717.17	2.359523
52525.25	2.361313
53333.33	2.363063
54141.41	2.364777
54949.49	2.366457
55757.58	2.368104
56565.66	2.369720
57373.74	2.371307
58181.82	2.372867
58989.90	2.374401
59797.98	2.375910
60606.06	2.377396
61414.14	2.378860
62222.22	2.380303
63030.30	2.381726
63838.38	2.383130
64646.46	2.384516
65454.55	2.385885
66262.63	2.387238
67070.71	2.388575
67878.79	2.389897
68686.87	2.391205
69494.95	2.392499
70303.03	2.393780
71111.11	2.395049
71919.19	2.396306
72727.27	2.397551
73535.35	2.398786
74343.43	2.400010
75151.52	2.401223
75959.60	2.402428
76767.68	2.403622
77575.76	2.404808
78383.84	2.405985
79191.92	2.407154
80000.00	2.408315

Table S108. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex B2' at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	-0.000000
808.08	0.164752
1616.16	0.326962
2424.24	0.484274
3232.32	0.634671
4040.40	0.776575
4848.48	0.908897
5656.57	1.031020
6464.65	1.142744

7272.73	1.244218
8080.81	1.335847
8888.89	1.418212
9696.97	1.492004
10505.05	1.557964
11313.13	1.616842
12121.21	1.669367
12929.29	1.716228
13737.37	1.758061
14545.45	1.795446
15353.54	1.828908
16161.62	1.858911
16969.70	1.885870
17777.78	1.910149
18585.86	1.932069
19393.94	1.951910
20202.02	1.969918
21010.10	1.986308
21818.18	2.001267
22626.26	2.014960
23434.34	2.027529
24242.42	2.039099
25050.51	2.049781
25858.59	2.059669
26666.67	2.068849
27474.75	2.077394
28282.83	2.085369
29090.91	2.092833
29898.99	2.099834
30707.07	2.106419
31515.15	2.112627
32323.23	2.118493
33131.31	2.124049
33939.39	2.129323
34747.47	2.134339
35555.56	2.139119
36363.64	2.143685
37171.72	2.148053
37979.80	2.152240
38787.88	2.156261
39595.96	2.160129
40404.04	2.163854
41212.12	2.167449
42020.20	2.170923
42828.28	2.174284
43636.36	2.177542
44444.44	2.180702
45252.53	2.183772
46060.61	2.186758
46868.69	2.189666
47676.77	2.192500
48484.85	2.195265
49292.93	2.197966
50101.01	2.200607
50909.09	2.203191
51717.17	2.205721
52525.25	2.208202

53333.33	2.210635
54141.41	2.213023
54949.49	2.215369
55757.58	2.217675
56565.66	2.219944
57373.74	2.222177
58181.82	2.224375
58989.90	2.226542
59797.98	2.228678
60606.06	2.230785
61414.14	2.232864
62222.22	2.234916
63030.30	2.236944
63838.38	2.238948
64646.46	2.240928
65454.55	2.242887
66262.63	2.244825
67070.71	2.246742
67878.79	2.248641
68686.87	2.250521
69494.95	2.252384
70303.03	2.254229
71111.11	2.256058
71919.19	2.257872
72727.27	2.259671
73535.35	2.261455
74343.43	2.263225
75151.52	2.264982
75959.60	2.266726
76767.68	2.268457
77575.76	2.270177
78383.84	2.271884
79191.92	2.273581
80000.00	2.275267

Table S109. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex C2 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	0.000000
808.08	0.145523
1616.16	0.289109
2424.24	0.428944
3232.32	0.563443
4040.40	0.691322
4848.48	0.811639
5656.57	0.923793
6464.65	1.027501
7272.73	1.122749
8080.81	1.209740
8888.89	1.288839
9696.97	1.360515
10505.05	1.425307
11313.13	1.483779
12121.21	1.536502
12929.29	1.584028

13737.37	1.626883
14545.45	1.665555
15353.54	1.700494
16161.62	1.732107
16969.70	1.760764
17777.78	1.786792
18585.86	1.810486
19393.94	1.832107
20202.02	1.851885
21010.10	1.870025
21818.18	1.886705
22626.26	1.902087
23434.34	1.916308
24242.42	1.929493
25050.51	1.941751
25858.59	1.953178
26666.67	1.963859
27474.75	1.973868
28282.83	1.983272
29090.91	1.992131
29898.99	2.000496
30707.07	2.008413
31515.15	2.015925
32323.23	2.023068
33131.31	2.029874
33939.39	2.036374
34747.47	2.042593
35555.56	2.048555
36363.64	2.054282
37171.72	2.059792
37979.80	2.065103
38787.88	2.070230
39595.96	2.075187
40404.04	2.079987
41212.12	2.084642
42020.20	2.089163
42828.28	2.093557
43636.36	2.097835
44444.44	2.102005
45252.53	2.106073
46060.61	2.110046
46868.69	2.113931
47676.77	2.117732
48484.85	2.121455
49292.93	2.125106
50101.01	2.128687
50909.09	2.132204
51717.17	2.135659
52525.25	2.139057
53333.33	2.142400
54141.41	2.145692
54949.49	2.148934
55757.58	2.152131
56565.66	2.155284
57373.74	2.158394
58181.82	2.161466
58989.90	2.164499

59797.98	2.167497
60606.06	2.170460
61414.14	2.173391
62222.22	2.176290
63030.30	2.179160
63838.38	2.182001
64646.46	2.184815
65454.55	2.187603
66262.63	2.190365
67070.71	2.193104
67878.79	2.195819
68686.87	2.198513
69494.95	2.201184
70303.03	2.203836
71111.11	2.206467
71919.19	2.209080
72727.27	2.211674
73535.35	2.214251
74343.43	2.216810
75151.52	2.219353
75959.60	2.221880
76767.68	2.224392
77575.76	2.226889
78383.84	2.229371
79191.92	2.231839
80000.00	2.234294

Table S110. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex A4 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	0.000000
808.08	0.189234
1616.16	0.375063
2424.24	0.554367
3232.32	0.724546
4040.40	0.883658
4848.48	1.030469
5656.57	1.164401
6464.65	1.285437
7272.73	1.393992
8080.81	1.490780
8888.89	1.576698
9696.97	1.652735
10505.05	1.719900
11313.13	1.779173
12121.21	1.831475
12929.29	1.877655
13737.37	1.918474
14545.45	1.954614
15353.54	1.986673
16161.62	2.015177
16969.70	2.040583
17777.78	2.063290
18585.86	2.083641
19393.94	2.101933

20202.02	2.118425
21010.10	2.133337
21818.18	2.146862
22626.26	2.159166
23434.34	2.170394
24242.42	2.180669
25050.51	2.190100
25858.59	2.198782
26666.67	2.206796
27474.75	2.214216
28282.83	2.221102
29090.91	2.227512
29898.99	2.233493
30707.07	2.239087
31515.15	2.244334
32323.23	2.249266
33131.31	2.253913
33939.39	2.258301
34747.47	2.262454
35555.56	2.266393
36363.64	2.270137
37171.72	2.273701
37979.80	2.277103
38787.88	2.280354
39595.96	2.283468
40404.04	2.286455
41212.12	2.289325
42020.20	2.292087
42828.28	2.294751
43636.36	2.297322
44444.44	2.299808
45252.53	2.302216
46060.61	2.304550
46868.69	2.306815
47676.77	2.309018
48484.85	2.311161
49292.93	2.313249
50101.01	2.315286
50909.09	2.317274
51717.17	2.319218
52525.25	2.321119
53333.33	2.322981
54141.41	2.324806
54949.49	2.326595
55757.58	2.328352
56565.66	2.330078
57373.74	2.331775
58181.82	2.333444
58989.90	2.335088
59797.98	2.336707
60606.06	2.338302
61414.14	2.339876
62222.22	2.341429
63030.30	2.342962
63838.38	2.344477
64646.46	2.345974
65454.55	2.347453

66262.63	2.348917
67070.71	2.350366
67878.79	2.351799
68686.87	2.353219
69494.95	2.354626
70303.03	2.356020
71111.11	2.357401
71919.19	2.358772
72727.27	2.360131
73535.35	2.361479
74343.43	2.362817
75151.52	2.364146
75959.60	2.365465
76767.68	2.366775
77575.76	2.368076
78383.84	2.369369
79191.92	2.370654
80000.00	2.371931

Table S111. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex B4 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	-0.000000
808.08	0.158213
1616.16	0.314104
2424.24	0.465513
3232.32	0.610575
4040.40	0.747818
4848.48	0.876199
5656.57	0.995101
6464.65	1.104290
7272.73	1.203852
8080.81	1.294115
8888.89	1.375582
9696.97	1.448864
10505.05	1.514629
11313.13	1.573564
12121.21	1.626340
12929.29	1.673601
13737.37	1.715945
14545.45	1.753922
15353.54	1.788032
16161.62	1.818720
16969.70	1.846386
17777.78	1.871383
18585.86	1.894024
19393.94	1.914582
20202.02	1.933300
21010.10	1.950389
21818.18	1.966034
22626.26	1.980398
23434.34	1.993623
24242.42	2.005835
25050.51	2.017142
25858.59	2.027642

26666.67	2.037418
27474.75	2.046546
28282.83	2.055090
29090.91	2.063110
29898.99	2.070656
30707.07	2.077773
31515.15	2.084503
32323.23	2.090881
33131.31	2.096939
33939.39	2.102705
34747.47	2.108206
35555.56	2.113463
36363.64	2.118497
37171.72	2.123328
37979.80	2.127970
38787.88	2.132440
39595.96	2.136750
40404.04	2.140913
41212.12	2.144940
42020.20	2.148841
42828.28	2.152625
43636.36	2.156300
44444.44	2.159874
45252.53	2.163354
46060.61	2.166745
46868.69	2.170055
47676.77	2.173288
48484.85	2.176449
49292.93	2.179542
50101.01	2.182572
50909.09	2.185542
51717.17	2.188457
52525.25	2.191318
53333.33	2.194129
54141.41	2.196894
54949.49	2.199614
55757.58	2.202291
56565.66	2.204929
57373.74	2.207529
58181.82	2.210093
58989.90	2.212623
59797.98	2.215121
60606.06	2.217587
61414.14	2.220024
62222.22	2.222433
63030.30	2.224815
63838.38	2.227172
64646.46	2.229504
65454.55	2.231813
66262.63	2.234099
67070.71	2.236364
67878.79	2.238608
68686.87	2.240833
69494.95	2.243038
70303.03	2.245225
71111.11	2.247395
71919.19	2.249548

72727.27	2.251685
73535.35	2.253806
74343.43	2.255912
75151.52	2.258003
75959.60	2.260081
76767.68	2.262145
77575.76	2.264196
78383.84	2.266234
79191.92	2.268260
80000.00	2.270274

Table S112. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex C4 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	-0.000000
808.08	0.146366
1616.16	0.290732
2424.24	0.431229
3232.32	0.566226
4040.40	0.694413
4848.48	0.814834
5656.57	0.926892
6464.65	1.030317
7272.73	1.125116
8080.81	1.211519
8888.89	1.289917
9696.97	1.360808
10505.05	1.424753
11313.13	1.482339
12121.21	1.534155
12929.29	1.580768
13737.37	1.622715
14545.45	1.660494
15353.54	1.694561
16161.62	1.725329
16969.70	1.753170
17777.78	1.778414
18585.86	1.801357
19393.94	1.822260
20202.02	1.841353
21010.10	1.858840
21818.18	1.874900
22626.26	1.889690
23434.34	1.903349
24242.42	1.916000
25050.51	1.927750
25858.59	1.938694
26666.67	1.948916
27474.75	1.958489
28282.83	1.967478
29090.91	1.975942
29898.99	1.983931
30707.07	1.991491
31515.15	1.998662
32323.23	2.005480

33131.31	2.011978
33939.39	2.018183
34747.47	2.024123
35555.56	2.029818
36363.64	2.035291
37171.72	2.040560
37979.80	2.045641
38787.88	2.050549
39595.96	2.055299
40404.04	2.059901
41212.12	2.064369
42020.20	2.068711
42828.28	2.072937
43636.36	2.077055
44444.44	2.081073
45252.53	2.084997
46060.61	2.088836
46868.69	2.092593
47676.77	2.096274
48484.85	2.099885
49292.93	2.103430
50101.01	2.106912
50909.09	2.110336
51717.17	2.113706
52525.25	2.117024
53333.33	2.120294
54141.41	2.123518
54949.49	2.126699
55757.58	2.129839
56565.66	2.132941
57373.74	2.136007
58181.82	2.139037
58989.90	2.142035
59797.98	2.145002
60606.06	2.147940
61414.14	2.150849
62222.22	2.153732
63030.30	2.156589
63838.38	2.159422
64646.46	2.162232
65454.55	2.165019
66262.63	2.167786
67070.71	2.170532
67878.79	2.173259
68686.87	2.175967
69494.95	2.178658
70303.03	2.181331
71111.11	2.183988
71919.19	2.186629
72727.27	2.189255
73535.35	2.191867
74343.43	2.194465
75151.52	2.197049
75959.60	2.199620
76767.68	2.202179
77575.76	2.204725
78383.84	2.207260

79191.92	2.209784
80000.00	2.212296

Part 2: Optimized structures, g-tensors, excitation energies, temperature-dependent magnetic susceptibility, and field-dependent molar magnetization for Co(II) 1,2-dicarba-closo-hexaborane complexes (Figure 3 in the main text).

Table S113. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex A0 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
B	-0.772002	0.370914	0.046726
B	0.704606	-0.507847	0.344451
B	-0.635587	-1.280616	-0.396706
B	-0.295003	-0.016082	1.648947
C	-0.216229	-1.593493	1.169650
C	-1.537901	-0.806458	0.901779
S	-0.200310	-3.085645	2.097038
S	-3.088271	-1.371377	1.504157
H	-1.175329	1.356332	-0.495974
H	1.878047	-0.460679	0.119983
H	-0.232576	0.456277	2.739717
H	-0.902832	-2.029776	-1.282497
B	-5.011498	-7.013662	4.261993
B	-4.811754	-6.085991	5.725027
B	-5.497472	-5.369999	4.325227
B	-3.445795	-6.575728	4.810188
C	-3.962986	-5.008824	4.816552
C	-4.143111	-5.839661	3.506680
S	-3.075428	-3.492509	4.834982
S	-3.469569	-5.307244	1.974309
H	-5.509934	-8.023028	3.860918
H	-5.096943	-6.104220	6.885800
H	-2.349721	-7.020204	4.943478
H	-6.383608	-4.649750	3.989061
Co	-2.456118	-3.315507	2.602925

Table S114. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex B0 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
C	-0.810419	0.165131	0.118034
C	0.521587	-0.627026	0.386216
B	-0.725542	-1.393120	-0.296367
B	-0.298256	-0.022207	1.640205
B	-0.266688	-1.760746	1.365059
B	-1.716898	-0.897003	1.073569
S	-0.040479	-3.237260	2.352986
S	-3.360252	-1.259619	1.686931
H	-0.887118	1.057337	-0.497745
H	1.493909	-0.359313	-0.017985
H	0.011294	0.778449	2.470973
H	-0.835445	-1.935930	-1.353777
B	-4.962787	-6.964393	4.156679
B	-4.796225	-6.074369	5.656218
B	-5.463515	-5.332597	4.266573

B	-3.417139	-6.546310	4.760620
C	-3.932482	-4.971752	4.794528
C	-4.082645	-5.765204	3.457101
S	-3.066854	-3.455486	4.936988
S	-3.401930	-5.242937	1.930586
H	-5.449551	-7.963467	3.715919
H	-5.105391	-6.126767	6.810201
H	-2.322728	-6.992896	4.903505
H	-6.345535	-4.605347	3.933505
Co	-2.426236	-3.241944	2.683889

Table S115. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex C0 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
C	-0.850652	0.152440	0.115808
C	0.504890	-0.593606	0.395430
B	-0.709752	-1.404605	-0.292538
B	-0.345142	-0.015232	1.642024
B	-0.254680	-1.754137	1.373944
B	-1.730318	-0.939260	1.067615
S	0.012223	-3.220032	2.365107
S	-3.365854	-1.351777	1.665393
H	-0.951876	1.039216	-0.504570
H	1.470683	-0.290567	0.000083
H	-0.068386	0.798920	2.472062
H	-0.793031	-1.951810	-1.350653
C	-4.929295	-6.805848	4.170493
C	-4.757446	-6.015180	5.518333
B	-5.403662	-5.264102	4.242920
B	-3.442401	-6.565128	4.756796
B	-3.782450	-4.837310	4.785873
B	-3.969686	-5.699322	3.316231
S	-2.864357	-3.327482	5.071231
S	-3.295210	-5.303526	1.706562
H	-5.507543	-7.719239	4.058221
H	-5.197813	-6.307557	6.467747
H	-2.599588	-7.338237	5.103308
H	-6.475235	-4.761795	4.084685
Co	-2.380741	-3.299606	2.702308

Table S116. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex A2 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
B	-0.961966	0.172562	0.244218
B	0.538162	-0.757086	0.487564
B	-0.825130	-1.448507	-0.267252
B	-0.407428	-0.230221	1.805002
C	-0.395299	-1.833538	1.311692
C	-1.709523	-1.020786	1.092632
O	-0.415528	-2.966836	1.985147
O	-2.854570	-1.456570	1.579072
H	-1.316454	1.185385	-0.283576
H	1.699271	-0.681433	0.209980
H	-0.314550	0.211074	2.910385
H	-1.134335	-2.179455	-1.159353

B	-4.848343	-6.865853	4.142536
B	-4.708393	-5.900217	5.595396
B	-5.375607	-5.238424	4.165052
B	-3.313842	-6.390059	4.733576
C	-3.856648	-4.827650	4.686554
C	-3.984452	-5.688485	3.389354
S	-3.024679	-3.285475	4.756678
S	-3.293361	-5.232964	1.843858
H	-5.313964	-7.894570	3.751348
H	-5.027244	-5.900817	6.747454
H	-2.212851	-6.808845	4.906060
H	-6.266151	-4.543156	3.789387
Co	-2.364438	-3.192855	2.511650

Table S117. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex B2 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
C	-0.897607	0.044987	0.227423
C	0.432410	-0.743900	0.511382
B	-0.791801	-1.503561	-0.219307
B	-0.423680	-0.174235	1.757418
B	-0.373026	-1.906730	1.443868
B	-1.821709	-1.046057	1.135113
S	-0.154415	-3.403986	2.403330
S	-3.480017	-1.428539	1.696076
H	-0.964023	0.950148	-0.370288
H	1.412321	-0.459203	0.138366
H	-0.141195	0.609173	2.614019
H	-0.870157	-2.021174	-1.292418
B	-4.825738	-6.780672	4.029932
B	-4.629981	-5.866564	5.547122
B	-5.348229	-5.164034	4.169669
B	-3.283231	-6.378853	4.635677
C	-3.783688	-4.774872	4.650647
C	-3.957742	-5.576502	3.320298
O	-3.117658	-3.639909	4.666466
O	-3.441487	-5.128354	2.195685
H	-5.336600	-7.793464	3.649275
H	-4.941909	-5.956809	6.699023
H	-2.179569	-6.817946	4.756166
H	-6.232862	-4.431886	3.842153
Co	-2.535733	-3.381837	2.727317

Table S118. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex B2' with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
C	-0.935262	-0.000781	0.231138
C	0.401282	-0.790364	0.502746
B	-0.846777	-1.560587	-0.169420
B	-0.409157	-0.163910	1.751035
B	-0.409561	-1.943531	1.531614
B	-1.859832	-1.083084	1.236202
O	-0.295003	-3.039854	2.292279
O	-3.065733	-1.398665	1.727953
H	-0.957627	0.881109	-0.404671

H	1.346409	-0.480347	0.063995
H	-0.078420	0.669242	2.548829
H	-0.947818	-2.097713	-1.236043
B	-4.874951	-6.846436	4.061262
B	-4.708391	-5.963426	5.565723
B	-5.375390	-5.215604	4.179739
B	-3.330050	-6.432405	4.668306
C	-3.844224	-4.857129	4.709141
C	-3.994101	-5.644136	3.368164
S	-2.977544	-3.342115	4.861396
S	-3.314956	-5.115507	1.842919
H	-5.362289	-7.843468	3.615884
H	-5.018368	-6.021862	6.719431
H	-2.235392	-6.879418	4.809288
H	-6.256662	-4.485994	3.849087
Co	-2.337507	-3.118794	2.608415

Table S119. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex C2 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
C	-0.982093	-0.005432	0.245357
C	0.386673	-0.734193	0.523116
B	-0.806375	-1.552526	-0.186752
B	-0.472458	-0.182243	1.770914
B	-0.400113	-1.957797	1.515685
B	-1.874612	-1.148524	1.201395
O	-0.249772	-3.062584	2.254146
O	-3.076671	-1.521196	1.660397
H	-1.035773	0.888275	-0.371756
H	1.320841	-0.362906	0.107862
H	-0.200264	0.647487	2.594725
H	-0.864016	-2.066098	-1.268948
C	-4.833951	-6.692745	4.101380
C	-4.661507	-5.886166	5.439557
B	-5.315511	-5.152429	4.157365
B	-3.346476	-6.437374	4.679715
B	-3.694802	-4.710822	4.689963
B	-3.882131	-5.591004	3.230722
S	-2.784529	-3.192823	4.959210
S	-3.216026	-5.212657	1.613262
H	-5.407385	-7.610882	4.003306
H	-5.098654	-6.170557	6.392935
H	-2.500164	-7.203915	5.033004
H	-6.391222	-4.658640	3.997992
Co	-2.300331	-3.197026	2.589859

Table S120. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex A4 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
B	-1.048398	0.039846	0.320645
B	0.454531	-0.879461	0.597213
B	-0.891654	-1.584141	-0.177235
B	-0.517161	-0.348713	1.894634
C	-0.486301	-1.956215	1.411156
C	-1.802471	-1.150920	1.165847

O	-0.510385	-3.085656	2.090309
O	-2.952509	-1.591132	1.635468
H	-1.400362	1.048575	-0.216871
H	1.620278	-0.800087	0.339813
H	-0.448874	0.101320	2.998454
H	-1.180629	-2.327071	-1.066476
B	-4.730335	-6.681706	3.998326
B	-4.551028	-5.710873	5.483667
B	-5.266230	-5.063910	4.077912
B	-3.194564	-6.245400	4.597143
C	-3.707668	-4.648254	4.553183
C	-3.870431	-5.496320	3.251873
O	-3.049201	-3.506505	4.528671
O	-3.348949	-5.081813	2.114471
H	-5.230983	-7.710350	3.649880
H	-4.867069	-5.760260	6.636355
H	-2.087299	-6.669203	4.737722
H	-6.153808	-4.349741	3.719762
Co	-2.465817	-3.316785	2.592490

Table S121. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex B4 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
C	-1.020409	-0.118328	0.338182
C	0.312429	-0.907146	0.620971
B	-0.917544	-1.669374	-0.093818
B	-0.527503	-0.312662	1.864890
B	-0.514248	-2.089739	1.606726
B	-1.964519	-1.228069	1.299214
O	-0.397380	-3.201531	2.344472
O	-3.183476	-1.548398	1.753659
H	-1.032487	0.776350	-0.279777
H	1.264687	-0.582961	0.208672
H	-0.218627	0.503530	2.688859
H	-0.992106	-2.181608	-1.175337
B	-4.737809	-6.666960	3.932372
B	-4.549932	-5.759867	5.456344
B	-5.262592	-5.051830	4.079065
B	-3.199109	-6.267668	4.548734
C	-3.700000	-4.663301	4.569118
C	-3.867264	-5.458261	3.233466
O	-3.034990	-3.528555	4.593434
O	-3.346314	-5.003830	2.114686
H	-5.246514	-7.678565	3.544543
H	-4.868001	-5.857079	6.606353
H	-2.095591	-6.707097	4.672505
H	-6.146693	-4.318667	3.751080
Co	-2.441331	-3.253162	2.655999

Table S122. DFT/B3LYP Optimized geometry for S=3/2 ground state of Complex C4 with the def2-TZVP basis set. Cartesian coordinates in Angstroms.

	X	Y	Z
C	-1.062652	-0.123266	0.333620
C	0.301460	-0.861199	0.604449
B	-0.899265	-1.671488	-0.101307

B	-0.549417	-0.307945	1.857355
B	-0.492708	-2.085387	1.600406
B	-1.963457	-1.262754	1.290893
O	-0.341527	-3.192226	2.334190
O	-3.169541	-1.621032	1.748054
H	-1.111032	0.772544	-0.281105
H	1.235680	-0.493099	0.186064
H	-0.268503	0.519282	2.681579
H	-0.963292	-2.182067	-1.185188
C	-4.713883	-6.527810	3.979939
C	-4.539222	-5.730557	5.325478
B	-5.199459	-4.990174	4.053154
B	-3.226861	-6.280729	4.563539
B	-3.539015	-4.511990	4.550833
B	-3.733992	-5.385443	3.089544
O	-2.846995	-3.377982	4.707535
O	-3.219979	-5.052799	1.899939
H	-5.300044	-7.442740	3.933008
H	-4.997783	-6.070929	6.251015
H	-2.397797	-7.071496	4.923435
H	-6.291477	-4.514228	3.911389
Co	-2.396563	-3.309263	2.676596

Table S123. g-values and tensor from CASSCF calculation on Complex A0 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	1.448128	1.460068	3.534909
		g-tensor	
X	0.6870140	0.5134667	0.5141631
Y	0.0228506	-0.7225020	0.6909911
Z	0.7262848	-0.4629716	-0.5081020

Table S124. g-values and tensor from CASSCF/NEVPT2 calculation on Complex A0 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	1.635731	1.646132	3.495778
		g-tensor	
X	0.6864860	0.5141359	0.5141997
Y	0.0235532	-0.7225020	0.6909675
Z	0.7267615	-0.4622285	-0.5080970

Table S125. g-values and tensor from CASSCF calculation on Complex B0 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.262129	2.362085	2.855103
		g-tensor	
X	0.2174269	0.8296687	0.5141745
Y	0.3939478	-0.5565575	0.7314704
Z	0.8930457	0.0435166	-0.4478567

Table S126. g-values and tensor from CASSCF/NEVPT2 calculation on Complex B0 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.181130	2.252475	2.666131
		g-tensor	
X	0.2106687	0.8311428	0.5146069
Y	0.4007467	-0.5535816	0.7300339
Z	0.8916394	0.0524317	-0.4497001

Table S127. g-values and tensor from CASSCF calculation on Complex C0 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.434856	2.444952	2.632757
		g-tensor	
X	0.5836716	0.6772695	-0.4479214
Y	-0.6269772	0.0253759	-0.7786242
Z	-0.5159720	0.7352973	0.4394437

Table S128. g-values and tensor from CASSCF/NEVPT2 calculation on Complex C0 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.292833	2.299458	2.461485
		g-tensor	
X	0.5800009	0.6762825	-0.4541376
Y	-0.6351423	0.0263403	-0.7719459
Z	-0.5100914	0.7361713	0.4448130

Table S129. g-values and tensor from CASSCF calculation on Complex A2 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.120261	2.251105	3.062596
		g-tensor	
X	0.3760444	0.7735490	0.5101104
Y	0.3550759	-0.6287924	0.6917668
Z	0.8558690	-0.0790071	-0.5111224

Table S130. g-values and tensor from CASSCF/NEVPT2 calculation on Complex A2 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.082735	2.165888	3.007797
		g-tensor	
X	0.3606944	0.7807224	0.5102667
Y	0.3673011	-0.6217870	0.6917159
Z	0.8573152	-0.0620766	-0.5110353

Table S131. g-values and tensor from CASSCF calculation
on Complex B2 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.293848	2.365413	2.777183
		g-tensor	
X	0.8524787	0.0445435	-0.5208608
Y	-0.4646931	0.5209679	-0.7159977
Z	0.2394587	0.8524132	0.4648131

Table S132. g-values and tensor from CASSCF/NEVPT2 calculation
on Complex B2 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.228445	2.259371	2.643760
		g-tensor	
X	0.8522551	0.0499342	-0.5207378
Y	-0.4670708	0.5209412	-0.7144684
Z	0.2355974	0.8521308	0.4672976

Table S133. g-values and tensor from CASSCF calculation
on Complex B2' with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.190769	2.408814	2.707650
		g-tensor	
X	0.1358102	0.8518892	0.505806
Y	0.4617994	-0.5061155	0.728415
Z	0.8765254	0.1346550	-0.462137

Table S134. g-values and tensor from CASSCF/NEVPT2 calculation
on Complex B2' with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.150181	2.292614	2.598208
		g-tensor	
X	-0.1295694	0.8516522	-0.507838
Y	-0.4661362	-0.5043515	-0.726874
Z	-0.8751736	0.1425414	0.462334

Table S135. g-values and tensor from CASSCF calculation
on Complex C2 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.290640	2.507303	2.589745
		g-tensor	
X	0.0874860	0.9693891	0.2294146
Y	0.5163361	-0.2410741	0.8217544

Z	0.8519056	0.0465630	-0.5216212

Table S136. g-values and tensor from CASSCF/NEVPT2 calculation on Complex C2 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.226104	2.353087	2.469162
		g-tensor	
X	0.0899865	0.9417481	0.3240570
Y	0.5156089	-0.3224303	0.7938427
Z	0.8520856	0.0956515	-0.5145880

Table S137. g-values and tensor from CASSCF calculation on Complex A4 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.189341	2.231030	2.951514
		g-tensor	
X	0.6974534	0.4983693	0.5149628
Y	0.0124732	-0.7269228	0.6866059
Z	0.7165216	-0.4724524	-0.5132111

Table S138. g-values and tensor from CASSCF/NEVPT2 calculation on Complex A4 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.149896	2.182199	2.898893
		g-tensor	
X	0.6974704	0.4983172	0.5149902
Y	0.0123801	-0.7269159	0.6866149
Z	0.7165066	-0.4725180	-0.5131715

Table S139. g-values and tensor from CASSCF calculation on Complex B4 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.241548	2.352820	2.686618
		g-tensor	
X	0.1408060	0.8439833	0.5175576
Y	0.4776412	-0.5158135	0.7111929
Z	0.8671981	0.1470666	-0.4757508

Table S140. g-values and tensor from CASSCF/NEVPT2 calculation on Complex B4 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.195155	2.287480	2.599979
		g-tensor	
X	0.1420106	0.8436845	0.5177157
Y	0.4773182	-0.5165584	0.7108690

Z	0.8671795	0.1461642	-0.4760627

Table S141. g-values and tensor from CASSCF calculation on Complex C4 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.346546	2.352984	2.567507
		g-tensor	
X	0.7120172	0.5338763	-0.4560784
Y	-0.6340656	0.2098266	-0.7442671
Z	-0.3016492	0.8191147	0.4879128

Table S142. g-values and tensor from CASSCF/NEVPT2 calculation on Complex C4 with DFT(BP86) optimized geometry.

	g1	g2	g3
		g-values	
	2.276773	2.281772	2.480651
		g-tensor	
X	0.7120227	0.5317727	-0.4585210
Y	-0.6355402	0.2104586	-0.7428296
Z	-0.2985168	0.8203200	0.4878143

Table S143. D-values and tensor from CASSCF calculation on Complex A0 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
	D-values	
46.656138	46.739281	-93.395419
	D-tensor	
0.511686	0.688523	-0.513919
-0.722313	0.020842	-0.691252
-0.465232	0.724915	0.507994

D = -140.093128 cm-1
E/D = 0.000297

Table S144. D-values and tensor from CASSCF/NEVPT2 calculation on Complex A0 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
	D-values	
48.103078	48.279147	-96.382225
	D-tensor	
0.504073	0.693944	-0.514151
-0.722698	0.012957	-0.691043
-0.472883	0.719912	0.508043

D = -144.573337 cm-1
E/D = 0.000609

Table S145. D-values and tensor from CASSCF calculation on Complex B0 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
	D-values	
11.753342	18.148953	-29.902295
	D-tensor	
0.828814	0.221332	-0.513886
-0.558275	0.388437	-0.733106
0.037353	0.894499	0.445506

D = -44.853442 cm-1
E/D = 0.071295

Table S146. D-values and tensor from CASSCF/NEVPT2 calculation on Complex B0 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
	D-values	
9.538065	15.440607	-24.978672
	D-tensor	
0.835280	0.194825	-0.514151
-0.545700	0.408091	-0.731897
0.067228	0.891911	0.447186

D = -37.468008 cm-1
E/D = 0.078768

Table S147. D-values and tensor from CASSCF calculation on Complex C0 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
	D-values	
4.402546	5.211374	-9.613920
	D-tensor	
0.678410	0.587771	-0.440778
0.023673	-0.617133	-0.786503
0.734302	-0.523137	0.432583

D = -14.420879 cm-1
E/D = 0.028044

Table S148. D-values and tensor from CASSCF/NEVPT2 calculation on Complex C0 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
	D-values	
4.122338	4.674333	-8.796671
	D-tensor	
0.675387	0.585665	-0.448161
0.027153	-0.627043	-0.778511
0.736963	-0.513628	0.439400

D = -13.195006 cm-1
E/D = 0.020917

Table S149. D-values and tensor from CASSCF calculation on Complex A2 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz

```
                D-values
   21.620825    29.942526   -51.563351
                D-tensor
    0.781259     0.359914    -0.509996
   -0.621200     0.368206    -0.691762
   -0.061192     0.857255     0.511243

D   =  -77.345026  cm-1
E/D =    0.053796
```

Table S150. D-values and tensor from CASSCF/NEVPT2 calculation on Complex A2 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
   23.096821    29.036928   -52.133749
                D-tensor
    0.791869     0.335718    -0.510134
   -0.609702     0.387090    -0.691683
   -0.034743     0.858752     0.511212

D   =  -78.200624  cm-1
E/D =    0.037980
```

Table S151. D-values and tensor from CASSCF calculation on Complex B2 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
    9.192442    15.371465   -24.563906
                D-tensor
    0.051630     0.851993    -0.521001
    0.514576    -0.469807    -0.717282
    0.855889     0.231061     0.462671

D   =  -36.845860  cm-1
E/D =    0.083850
```

Table S152. D-values and tensor from CASSCF/NEVPT2 calculation on Complex B2 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
    9.742268    12.467632   -22.209900
                D-tensor
    0.052915     0.852026    -0.520819
    0.516949    -0.469598    -0.715710
    0.854379     0.231365     0.465303

D   =  -33.314850  cm-1
E/D =    0.040903
```

Table S153. D-values and tensor from CASSCF calculation on Complex B2' with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
```

```
    2.479318    20.013212   -22.492530
                 D-tensor
    0.853244     0.132147    -0.504491
   -0.503161     0.462954    -0.729728
    0.137125     0.876476     0.461504

D   =  -33.738795  cm-1
E/D =    0.259848
```

Table S154. D-values and tensor from CASSCF/NEVPT2 calculation on Complex B2' with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                 D-values
    3.942780    17.044826   -20.987606
                 D-tensor
    0.853704     0.121653    -0.506350
   -0.498939     0.469585    -0.728389
    0.149163     0.874466     0.461584

D   =  -31.481409  cm-1
E/D =    0.208092
```

Table S155. D-values and tensor from CASSCF calculation on Complex C2 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                 D-values
   -4.044105    -9.898968    13.943073
                 D-tensor
    0.985631    -0.144306     0.087790
   -0.168911    -0.840037     0.515564
    0.000652     0.522985     0.852342

D   =   20.914609  cm-1
E/D =    0.139971
```

Table S156. D-values and tensor from CASSCF/NEVPT2 calculation on Complex C2 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                 D-values
   -0.993105    -9.632222    10.625328
                 D-tensor
    0.953804    -0.286416     0.090688
   -0.291104    -0.806451     0.514681
    0.074278     0.517304     0.852572

D   =   15.937992  cm-1
E/D =    0.271023
```

Table S157. D-values and tensor from CASSCF calculation on Complex A4 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                 D-values
   20.175078    23.079793   -43.254871
```

```
                D-tensor
    0.498038     0.697718    -0.514924
   -0.726936     0.012178    -0.686597
   -0.472781     0.716269     0.513262

D   =  -64.882306  cm-1
E/D =    0.022384
```

Table S158. D-values and tensor from CASSCF/NEVPT2 calculation on Complex A4 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
   20.150148    22.485494   -42.635642
                D-tensor
    0.497783     0.697887    -0.514942
   -0.726931     0.011881    -0.686607
   -0.473057     0.716109     0.513230

D   =  -63.953463  cm-1
E/D =    0.018258
```

Table S159. D-values and tensor from CASSCF calculation on Complex B4 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
    6.237292    15.318948   -21.556241
                D-tensor
    0.844469     0.138913    -0.517277
   -0.514602     0.478228    -0.711676
    0.148516     0.867180     0.475333

D   =  -32.334361  cm-1
E/D =    0.140434
```

Table S160. D-values and tensor from CASSCF/NEVPT2 calculation on Complex B4 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
    5.807368    14.077756   -19.885123
                D-tensor
    0.844619     0.137580    -0.517388
   -0.513889     0.479335    -0.711446
    0.150122     0.866781     0.475556

D   =  -29.827685  cm-1
E/D =    0.138636
```

Table S161. D-values and tensor from CASSCF calculation on Complex C4 with DFT(BP86) optimized geometry. D in cm-1.

```
       Dxx         Dyy          Dzz
                D-values
    5.454085     5.989316   -11.443401
                D-tensor
```

0.526835	0.720436	-0.451017
0.218058	-0.627431	-0.747517
0.821520	-0.295471	0.487649

D = -17.165101 cm-1
E/D = 0.015591

Table S162. D-values and tensor from CASSCF/NEVPT2 calculation on Complex C4 with DFT(BP86) optimized geometry. D in cm-1.

Dxx	Dyy	Dzz
	D-values	
5.176142	5.603261	-10.779403
	D-tensor	
0.516749	0.726089	-0.453614
0.225815	-0.626669	-0.745851
0.825820	-0.282985	0.487792

D = -16.169105 cm-1
E/D = 0.013208

Table S163. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex A0 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	-0.000
1	4	33.1	-170.995	-0.000
2	4	4205.6	10.488	-10.467
3	4	4283.6	5.440	5.402
4	4	4697.2	2.885	-2.819
5	4	4705.3	7.312	7.287
6	4	6344.9	0.000	-0.000
7	4	20657.6	0.000	-0.000
8	4	21416.1	0.001	-0.001
9	4	21547.3	0.002	0.002
0'	2	18599.3	-0.629	0.626
1'	2	18729.4	-0.579	-0.577
2'	2	18826.4	-0.001	-0.001
3'	2	18939.9	0.025	0.000
4'	2	19151.0	-0.000	0.000
5'	2	19730.0	0.001	-0.000
6'	2	19767.4	7.061	0.000
7'	2	22176.5	-1.962	1.961
8'	2	22180.2	-1.920	-1.919
9'	2	23565.1	0.004	0.000
10'	2	24918.1	0.002	0.000
11'	2	25095.0	1.202	0.000
12'	2	25191.3	-0.007	0.009
13'	2	25218.4	-0.008	-0.008
14'	2	27162.4	-0.005	-0.005
15'	2	27163.4	-0.009	0.009
16'	2	27902.2	-0.007	-0.007
17'	2	27906.1	-0.000	0.000
18'	2	28090.3	-0.120	-0.120

19'	2	28099.2	-0.002	-0.002
20'	2	28127.8	-0.126	0.125
21'	2	29744.2	-1.199	-1.194
22'	2	29772.0	-1.129	1.124
23'	2	30323.7	-0.000	-0.000
24'	2	30395.1	0.000	0.000
25'	2	30983.7	-0.000	-0.000
26'	2	31991.2	0.001	-0.000
27'	2	32108.0	0.318	0.000
28'	2	43348.3	0.000	0.000
29'	2	43640.2	0.326	0.000
30'	2	44441.5	-0.077	0.077
31'	2	44514.6	-0.073	-0.072
32'	2	45183.8	-0.045	0.045
33'	2	45184.5	-0.045	-0.044
34'	2	45699.3	0.000	-0.000
35'	2	66398.2	-0.000	-0.000
36'	2	68194.6	-0.024	-0.024
37'	2	68325.0	-0.024	0.024
38'	2	69090.8	0.000	-0.000
39'	2	69489.1	0.046	0.000

Table S164. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex A0 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	146.2	-166.374	-0.000
1	4	0.0	0.000	0.000
2	4	6498.5	4.101	4.088
3	4	6603.5	7.102	-7.100
4	4	7522.0	4.060	4.029
5	4	7572.1	1.382	-1.328
6	4	9362.9	0.000	0.000
7	4	19810.0	0.000	0.000
8	4	20152.4	0.003	0.003
9	4	20308.3	0.002	-0.002
0'	2	16345.6	-0.857	-0.856
1'	2	16605.1	-0.826	0.825
2'	2	17589.1	0.027	0.001
3'	2	17669.8	-0.000	-0.000
4'	2	18064.9	0.003	0.000
5'	2	18636.7	7.441	0.000
6'	2	18559.4	0.001	0.000
7'	2	23196.5	-1.653	-1.651
8'	2	23198.0	-1.691	1.688
9'	2	20999.6	-0.000	-0.000
10'	2	23082.4	1.345	0.000
11'	2	23326.5	0.002	-0.000
12'	2	24756.7	-0.009	-0.009
13'	2	24745.9	-0.012	0.013
14'	2	26870.5	-0.012	0.012
15'	2	26873.2	-0.004	-0.004
16'	2	28395.1	-0.026	0.026
17'	2	28476.8	-0.010	-0.009

18'	2	26714.3	-0.131	0.131
19'	2	26691.0	-0.002	0.001
20'	2	26682.2	-0.131	-0.131
21'	2	29068.2	-1.224	1.220
22'	2	29135.6	-1.274	-1.271
23'	2	32335.3	0.000	0.000
24'	2	32629.6	-0.000	-0.000
25'	2	31022.1	0.000	0.000
26'	2	33796.3	0.285	-0.000
27'	2	34001.1	0.001	-0.000
28'	2	38746.4	0.381	0.000
29'	2	39039.9	0.001	-0.000
30'	2	40456.9	-0.086	-0.086
31'	2	40557.5	-0.084	0.084
32'	2	41484.2	-0.057	-0.057
33'	2	41485.6	-0.058	0.057
34'	2	42914.3	0.000	-0.000
35'	2	57477.1	0.000	0.000
36'	2	60497.1	-0.032	0.032
37'	2	60675.1	-0.032	-0.032
38'	2	61356.0	0.054	0.000
39'	2	61733.1	0.000	-0.000

Table S165. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex B0 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	-0.000
1	4	1119.5	-87.364	0.007
2	4	2691.5	15.559	-15.445
3	4	3160.4	14.884	14.901
4	4	4014.9	6.531	-5.634
5	4	4824.2	0.025	0.007
6	4	5022.0	0.000	-0.001
7	4	20149.6	0.000	0.000
8	4	20789.7	0.000	-0.000
9	4	21243.0	0.005	-0.004
0'	2	19262.4	0.068	-0.000
1'	2	19334.9	0.001	0.004
2'	2	19403.1	-0.256	0.256
3'	2	19590.0	-0.002	0.001
4'	2	19639.5	-0.004	-0.008
5'	2	19661.2	-0.036	-0.035
6'	2	20490.0	6.502	-0.004
7'	2	21183.0	-3.136	-2.692
8'	2	21314.1	-1.982	1.554
9'	2	24578.6	0.007	0.000
10'	2	25328.5	-0.026	-0.020
11'	2	25461.1	-0.069	-0.041
12'	2	25756.6	0.861	-0.000
13'	2	25910.5	-0.198	0.188
14'	2	25975.8	-0.013	0.020
15'	2	25991.5	-0.006	0.006
16'	2	26954.0	-0.005	0.003
17'	2	27204.9	-0.026	-0.029

18'	2	27713.4	0.112	-0.001
19'	2	27727.8	0.031	-0.000
20'	2	27908.6	-0.119	-0.107
21'	2	28064.2	-0.195	0.180
22'	2	28334.4	-0.005	0.004
23'	2	28929.7	-1.002	-0.977
24'	2	29936.0	-0.824	0.787
25'	2	30018.6	0.231	0.002
26'	2	30784.6	0.533	-0.000
27'	2	31247.7	0.000	0.000
28'	2	43541.8	0.000	0.000
29'	2	43972.7	0.247	-0.005
30'	2	44158.1	-0.089	-0.092
31'	2	44545.1	-0.149	0.133
32'	2	44618.3	-0.002	0.002
33'	2	44794.5	-0.002	-0.001
34'	2	45044.0	0.000	0.000
35'	2	67281.8	0.005	-0.000
36'	2	67841.5	-0.000	0.001
37'	2	68132.7	-0.014	0.012
38'	2	68565.0	0.049	-0.000
39'	2	69239.9	-0.035	-0.033

Table S166. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex B0 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	0.000
1	4	1648.5	-64.830	0.004
2	4	4234.7	10.058	-9.878
3	4	4982.4	9.577	9.598
4	4	6371.8	4.135	-3.698
5	4	7468.8	0.016	0.003
6	4	7772.8	0.000	-0.000
7	4	18380.0	0.000	0.000
8	4	19374.4	0.000	-0.000
9	4	19839.5	0.005	-0.005
0'	2	18009.1	0.072	-0.000
1'	2	18281.4	0.001	0.005
2'	2	18220.3	-0.273	0.272
3'	2	18688.9	-0.002	0.001
4'	2	18834.4	-0.004	-0.009
5'	2	18662.1	-0.038	-0.036
6'	2	19945.5	6.681	-0.004
7'	2	21327.9	-3.116	-2.774
8'	2	21699.7	-1.946	1.603
9'	2	22093.6	0.008	0.000
10'	2	23685.9	-0.027	-0.020
11'	2	24112.9	-0.073	-0.047
12'	2	24353.5	0.910	-0.000
13'	2	24886.9	-0.206	0.199
14'	2	24675.5	-0.013	0.022
15'	2	25110.9	-0.006	0.005
16'	2	26347.3	-0.006	0.003

17'	2	26878.0	-0.026	-0.029
18'	2	27516.9	0.112	-0.001
19'	2	27147.2	0.031	-0.000
20'	2	26863.6	-0.124	-0.115
21'	2	27498.3	-0.199	0.188
22'	2	28958.1	-0.005	0.004
23'	2	27831.3	-1.042	-1.029
24'	2	29436.6	-0.838	0.815
25'	2	30039.6	0.231	0.002
26'	2	31183.7	0.526	-0.000
27'	2	32236.1	0.000	0.000
28'	2	38960.4	0.000	0.000
29'	2	39445.8	0.276	-0.006
30'	2	39814.0	-0.100	-0.105
31'	2	40291.4	-0.165	0.151
32'	2	40653.4	-0.002	0.002
33'	2	40813.2	-0.002	-0.001
34'	2	41390.7	0.000	0.000
35'	2	58483.1	0.006	-0.000
36'	2	59345.9	-0.001	0.001
37'	2	60113.3	-0.016	0.015
38'	2	60306.2	0.056	-0.000
39'	2	61609.8	-0.040	-0.038

Table S167. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex C0 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	-0.000
1	4	1670.0	-64.734	0.111
2	4	2374.8	23.043	-23.038
3	4	2416.3	22.184	22.436
4	4	3874.0	0.536	0.533
5	4	3897.7	0.493	-0.478
6	4	3978.9	0.003	-0.003
7	4	20144.8	0.002	-0.002
8	4	20170.6	0.002	0.002
9	4	20983.5	0.000	0.000
0'	2	19418.8	-0.000	0.000
1'	2	19455.3	0.001	-0.000
2'	2	19492.3	-0.001	0.001
3'	2	19676.8	-0.003	0.003
4'	2	19679.1	-0.001	-0.001
5'	2	19815.5	-0.000	0.000
6'	2	20693.2	6.091	-0.025
7'	2	20929.0	-2.851	2.847
8'	2	20942.1	-2.793	-2.821
9'	2	24950.8	-0.074	0.071
10'	2	24955.7	-0.071	-0.069
11'	2	25013.2	-0.002	-0.003
12'	2	25692.7	-0.099	0.099
13'	2	25735.6	-0.046	-0.082
14'	2	25808.5	0.758	-0.012
15'	2	26487.0	-0.001	0.001
16'	2	26584.9	-0.001	0.001

17'	2	26996.1	-0.032	-0.032
18'	2	27006.1	-0.040	0.037
19'	2	27153.2	-0.010	-0.010
20'	2	27445.6	-0.101	-0.100
21'	2	27468.3	-0.101	0.100
22'	2	27642.3	-0.000	-0.000
23'	2	29072.8	-0.872	-0.112
24'	2	29075.6	-0.871	0.104
25'	2	29590.8	-0.001	0.001
26'	2	29741.7	1.306	-0.004
27'	2	30456.4	-0.000	0.000
28'	2	43528.3	-0.000	0.000
29'	2	44053.6	0.048	-0.069
30'	2	44087.3	-0.137	0.136
31'	2	44130.7	0.073	-0.064
32'	2	44541.7	-0.011	0.011
33'	2	44545.6	-0.012	-0.012
34'	2	44792.0	-0.000	-0.000
35'	2	67170.1	-0.000	0.000
36'	2	67853.5	0.060	-0.000
37'	2	68028.5	-0.000	0.000
38'	2	68818.7	-0.026	-0.026
39'	2	68858.1	-0.026	0.026

Table S168. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex C0 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	0.000
1	4	2550.9	-44.693	0.047
2	4	3866.1	14.572	-14.565
3	4	3933.3	14.091	14.195
4	4	6146.6	0.341	0.336
5	4	6173.5	0.311	-0.301
6	4	6455.7	0.002	-0.002
7	4	18426.7	0.002	-0.002
8	4	18446.3	0.002	0.002
9	4	19503.3	0.000	0.000
0'	2	18456.6	-0.000	0.000
1'	2	18634.1	0.001	-0.000
2'	2	18417.4	-0.001	0.001
3'	2	18889.3	-0.003	0.003
4'	2	18898.0	-0.001	-0.001
5'	2	19539.8	-0.000	0.000
6'	2	20548.1	6.154	-0.019
7'	2	21154.7	-2.821	2.815
8'	2	21177.7	-2.777	-2.793
9'	2	23428.7	-0.078	0.076
10'	2	23426.2	-0.076	-0.074
11'	2	22614.7	-0.002	-0.003
12'	2	24231.1	-0.104	0.104
13'	2	24266.9	-0.052	-0.088
14'	2	24377.0	0.808	-0.011
15'	2	25400.8	-0.001	0.001

16'	2	26005.3	-0.001	0.001
17'	2	25969.7	-0.034	-0.033
18'	2	25856.7	-0.041	0.039
19'	2	27461.5	-0.010	-0.010
20'	2	27085.1	-0.102	-0.102
21'	2	27149.6	-0.102	0.102
22'	2	26731.3	-0.000	-0.000
23'	2	28051.0	-0.907	-0.126
24'	2	28057.6	-0.905	0.116
25'	2	29361.9	-0.001	0.001
26'	2	29362.0	1.327	-0.003
27'	2	30941.0	-0.000	0.000
28'	2	38913.4	-0.000	0.000
29'	2	39624.1	0.059	-0.075
30'	2	39675.0	-0.152	0.151
31'	2	39745.3	0.076	-0.073
32'	2	40513.2	-0.012	0.012
33'	2	40506.8	-0.014	-0.014
34'	2	40917.3	-0.000	-0.000
35'	2	58331.2	-0.000	0.000
36'	2	59439.8	0.069	-0.000
37'	2	59376.8	-0.000	0.000
38'	2	60961.6	-0.029	-0.029
39'	2	61008.8	-0.029	0.029

Table S169. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex A2 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	0.000
1	4	776.3	-110.930	0.000
2	4	3528.5	17.328	-16.611
3	4	4261.7	1.190	0.697
4	4	4759.5	10.301	9.577
5	4	5167.9	0.351	0.304
6	4	6220.3	-0.001	0.000
7	4	20872.1	0.007	0.007
8	4	20986.4	0.000	0.000
9	4	23014.4	0.001	-0.001
0'	2	19096.0	-0.680	-0.218
1'	2	19370.4	0.638	0.000
2'	2	19518.6	0.108	0.000
3'	2	19721.8	0.044	0.000
4'	2	19775.6	-0.324	0.107
5'	2	20196.2	0.000	0.000
6'	2	20735.2	6.054	0.000
7'	2	22329.4	-2.177	1.881
8'	2	22418.6	-2.186	-1.987
9'	2	23918.1	0.034	0.000
10'	2	25402.3	-0.015	0.011
11'	2	25727.2	-0.009	0.002
12'	2	25948.5	1.029	-0.000
13'	2	26486.5	0.047	-0.000
14'	2	27243.9	-0.063	0.050
15'	2	27371.7	-0.022	0.001

16'	2	28372.6	-0.125	0.124
17'	2	28486.2	0.004	-0.001
18'	2	28509.1	-0.075	-0.071
19'	2	28695.8	-0.003	-0.003
20'	2	28842.2	-0.113	0.053
21'	2	30018.3	0.057	-0.000
22'	2	30054.4	-1.270	-1.256
23'	2	30430.4	-0.078	0.077
24'	2	30438.9	-0.694	0.675
25'	2	31503.3	0.002	-0.000
26'	2	31910.0	0.460	0.000
27'	2	32306.5	0.001	0.000
28'	2	44319.8	0.000	0.000
29'	2	44685.2	0.321	0.000
30'	2	44941.2	-0.101	-0.057
31'	2	45751.8	-0.061	0.034
32'	2	46013.8	-0.065	0.050
33'	2	46071.9	-0.021	-0.005
34'	2	46352.6	0.004	-0.000
35'	2	67712.6	0.002	0.000
36'	2	68481.1	-0.018	0.010
37'	2	70202.4	0.001	-0.000
38'	2	70331.7	-0.033	-0.024
39'	2	70844.6	0.047	-0.000

Table S170. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex A2 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	0.000
1	4	881.2	-103.114	0.000
2	4	5057.8	12.238	-11.496
3	4	6050.5	0.839	0.448
4	4	6488.9	7.593	6.875
5	4	6772.4	0.268	0.223
6	4	8208.4	-0.001	0.000
7	4	19018.9	0.008	0.007
8	4	19425.0	0.000	0.000
9	4	21001.0	0.001	-0.001
0'	2	17124.8	-0.758	-0.287
1'	2	18109.5	0.683	-0.000
2'	2	18220.6	0.116	0.000
3'	2	18525.1	0.047	0.000
4'	2	18240.1	-0.351	0.137
5'	2	18887.1	0.000	0.000
6'	2	19590.0	6.407	0.000
7'	2	22427.9	-2.168	1.802
8'	2	22520.3	-2.176	-1.918
9'	2	21614.1	0.038	0.000
10'	2	24401.3	-0.016	0.010
11'	2	24463.0	-0.009	0.003
12'	2	24083.5	1.108	-0.000
13'	2	24648.1	0.050	-0.000
14'	2	26067.8	-0.066	0.054

15'	2	26406.2	-0.023	-0.001
16'	2	26472.2	-0.134	0.134
17'	2	26442.5	0.004	-0.001
18'	2	27705.7	-0.077	-0.075
19'	2	27104.0	-0.003	-0.003
20'	2	28198.7	-0.116	0.060
22'	2	28214.4	0.057	-0.000
21'	2	29969.9	-1.353	-1.347
23'	2	30815.6	-0.077	0.077
24'	2	29307.7	-0.720	0.710
25'	2	30789.2	0.002	-0.000
26'	2	32077.4	0.458	0.000
27'	2	32606.7	0.001	0.000
28'	2	39511.3	0.000	0.000
29'	2	39857.3	0.360	0.000
30'	2	40497.0	-0.112	-0.069
31'	2	41265.4	-0.068	0.041
32'	2	41649.0	-0.072	0.058
33'	2	41722.8	-0.023	-0.007
34'	2	42495.4	0.004	-0.000
35'	2	58979.3	0.002	0.000
36'	2	60456.2	-0.021	0.012
37'	2	61771.8	0.001	-0.000
38'	2	62210.3	-0.037	-0.028
39'	2	62409.7	0.054	-0.000

Table S171. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex B2 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	-0.000
1	4	1330.8	-78.309	-0.008
2	4	2747.3	19.282	-19.154
3	4	2894.8	8.543	8.051
4	4	4083.0	9.417	9.398
5	4	5155.9	0.001	0.001
6	4	5310.3	0.201	-0.195
7	4	20753.4	0.004	0.004
8	4	20874.4	0.007	0.007
9	4	21695.1	0.003	-0.003
0'	2	19257.9	0.579	0.001
1'	2	19556.3	-0.364	-0.358
2'	2	19660.0	-0.001	-0.001
3'	2	19990.0	0.001	-0.000
4'	2	20013.3	-0.051	0.052
5'	2	20050.8	0.057	0.000
6'	2	20943.8	5.970	0.001
7'	2	21398.7	-2.961	2.955
8'	2	21670.1	-2.082	-2.079
9'	2	24615.5	0.001	0.000
10'	2	25493.1	-0.012	-0.002
11'	2	25606.0	-0.079	0.076
12'	2	26311.7	0.833	0.001
13'	2	26692.8	-0.203	-0.201
14'	2	26709.1	-0.014	0.012

15'	2	26726.6	-0.002	-0.002
16'	2	27520.3	-0.025	-0.025
17'	2	27847.6	-0.130	0.129
18'	2	28179.4	0.000	-0.000
19'	2	28377.6	0.024	0.001
20'	2	28520.9	-0.011	0.011
21'	2	28626.1	-0.001	-0.001
22'	2	29039.9	-0.001	-0.001
23'	2	29572.6	-0.901	0.893
24'	2	30009.2	-1.150	-1.143
25'	2	30602.9	0.742	0.000
26'	2	30953.6	0.180	0.000
27'	2	31305.2	-0.000	-0.000
28'	2	44282.8	-0.000	-0.000
29'	2	44597.3	0.312	0.001
30'	2	44869.5	-0.127	-0.124
31'	2	45170.4	-0.113	0.112
32'	2	45465.4	-0.020	-0.020
33'	2	45573.1	-0.007	0.007
34'	2	45649.0	0.000	-0.000
35'	2	68197.3	0.001	0.000
36'	2	69091.9	-0.029	0.029
37'	2	69267.9	-0.000	-0.000
38'	2	69594.7	-0.023	-0.022
39'	2	69930.8	0.054	0.000

Table S172. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex B2 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	-0.000
1	4	1759.4	-62.539	-0.004
2	4	4074.8	13.250	-13.160
3	4	4107.9	6.065	5.717
4	4	5645.8	6.847	6.833
5	4	6967.3	0.001	0.001
6	4	6973.8	0.153	-0.149
7	4	18891.4	0.004	0.004
8	4	19049.0	0.007	0.007
9	4	19413.6	0.004	-0.004
0'	2	17929.3	0.622	0.001
1'	2	18171.6	-0.392	-0.385
2'	2	18527.2	-0.001	-0.001
3'	2	18701.2	0.001	-0.000
4'	2	18885.8	-0.054	0.055
5'	2	19282.8	0.059	0.000
6'	2	20168.4	6.200	0.000
7'	2	21122.1	-3.000	2.993
8'	2	21513.8	-2.097	-2.094
9'	2	22298.6	0.001	0.000
10'	2	23864.5	-0.013	-0.002
11'	2	23852.1	-0.085	0.082
12'	2	24714.0	0.888	0.000
13'	2	25352.4	-0.214	-0.212

14'	2	25249.8	-0.015	0.013
15'	2	25263.9	-0.002	-0.002
16'	2	26425.6	-0.026	-0.026
17'	2	26616.7	-0.136	0.135
18'	2	26199.4	0.000	-0.000
19'	2	27607.1	0.024	0.001
20'	2	27461.9	-0.011	0.012
21'	2	27205.6	-0.001	-0.001
22'	2	28936.5	-0.001	-0.001
23'	2	27746.7	-0.960	0.952
24'	2	28449.7	-1.213	-1.206
25'	2	29795.3	0.762	0.000
26'	2	30189.1	0.185	0.000
27'	2	31141.9	-0.000	-0.000
28'	2	39456.5	-0.000	-0.000
29'	2	39776.8	0.350	0.001
30'	2	40366.4	-0.141	-0.138
31'	2	40438.4	-0.126	0.125
32'	2	40982.9	-0.022	-0.022
33'	2	41148.2	-0.008	0.008
34'	2	41455.7	0.000	-0.000
35'	2	59508.9	0.001	0.000
37'	2	60534.5	-0.033	0.033
36'	2	61134.1	-0.000	-0.000
38'	2	61210.7	-0.026	-0.025
39'	2	61356.9	0.061	0.000

Table S173. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex B2' with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	0.000
1	4	1486.9	-70.685	-0.002
2	4	3154.3	21.127	-21.053
3	4	4088.2	11.088	10.971
4	4	4751.4	0.840	-0.776
5	4	5086.2	0.066	0.045
6	4	5887.4	0.000	0.000
7	4	19906.3	0.010	0.011
8	4	21650.3	0.000	0.000
9	4	23144.7	0.000	-0.000
0'	2	19641.3	0.006	0.000
1'	2	19714.2	0.422	-0.001
2'	2	19900.3	-0.154	-0.136
3'	2	20092.1	-0.195	0.192
4'	2	20192.1	0.000	0.000
5'	2	20291.2	0.009	0.000
6'	2	21205.9	6.028	-0.001
7'	2	22001.5	-3.278	-3.004
8'	2	22069.3	-2.019	1.622
9'	2	24476.1	0.001	0.000
10'	2	25889.6	-0.031	-0.034
11'	2	25955.4	-0.106	0.106
12'	2	26192.4	0.773	0.016

13'	2	26209.4	0.065	0.082
14'	2	26412.1	-0.008	-0.004
15'	2	27196.2	0.000	0.000
16'	2	27872.3	-0.041	0.041
17'	2	28044.7	-0.067	-0.068
18'	2	28372.9	0.001	-0.000
19'	2	28526.8	0.349	-0.001
20'	2	28863.7	-0.098	-0.098
21'	2	29081.3	-0.364	0.361
22'	2	29430.3	-0.013	-0.009
23'	2	29603.4	-0.979	-0.979
24'	2	30989.7	0.164	0.000
25'	2	31127.9	-0.464	0.463
26'	2	31875.7	0.413	0.000
27'	2	32670.9	0.000	0.000
28'	2	44380.3	0.000	0.000
29'	2	44804.1	-0.111	-0.111
30'	2	45073.0	0.244	-0.000
31'	2	45693.2	-0.067	0.067
32'	2	45892.6	-0.001	-0.001
33'	2	45992.8	-0.083	0.083
34'	2	46276.7	0.000	0.000
35'	2	67852.6	0.016	-0.000
36'	2	68449.3	-0.010	0.010
37'	2	69152.1	0.000	0.000
38'	2	70618.8	0.038	0.000
39'	2	71442.6	-0.041	-0.040

Table S174. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex B2' with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	-0.000
1	4	1887.5	-57.940	-0.001
2	4	4606.4	14.722	-14.631
3	4	5507.8	8.280	8.159
4	4	6492.3	0.615	-0.574
5	4	7336.1	0.046	0.032
6	4	8141.9	0.000	0.000
7	4	18011.3	0.012	0.012
8	4	20052.6	0.000	0.000
9	4	21410.7	0.000	-0.000
0'	2	18429.1	0.007	0.000
1'	2	18537.8	0.449	-0.001
2'	2	18497.5	-0.166	-0.148
3'	2	18976.7	-0.206	0.204
4'	2	18922.9	0.000	0.000
5'	2	19604.0	0.010	0.000
6'	2	20349.8	6.282	-0.001
7'	2	21762.4	-3.314	-3.069
8'	2	22136.9	-2.013	1.646
9'	2	22222.9	0.001	0.000
10'	2	25174.2	-0.031	-0.036
11'	2	23883.7	-0.115	0.115

12'	2	24617.3	0.823	0.016
13'	2	25044.0	0.067	0.087
14'	2	25306.4	-0.008	-0.004
15'	2	25456.9	0.000	0.000
16'	2	26375.9	-0.044	0.043
17'	2	27103.0	-0.069	-0.071
18'	2	27266.2	0.001	-0.000
19'	2	27919.1	0.357	-0.001
20'	2	26988.3	-0.105	-0.105
21'	2	28198.0	-0.376	0.374
22'	2	29462.4	-0.013	-0.009
23'	2	28347.6	-1.023	-1.023
24'	2	30697.8	0.166	0.000
25'	2	30393.0	-0.475	0.475
26'	2	31724.1	0.415	0.000
27'	2	32994.0	0.000	0.000
28'	2	39780.9	0.000	0.000
29'	2	40314.9	-0.124	-0.124
30'	2	40490.3	0.271	-0.000
31'	2	41399.6	-0.074	0.074
32'	2	41658.7	-0.001	-0.001
33'	2	41639.6	-0.092	0.092
34'	2	42259.1	0.000	0.000
35'	2	59339.9	0.018	-0.000
36'	2	60414.0	-0.012	0.012
37'	2	60619.4	0.000	0.000
38'	2	62047.3	0.043	0.000
39'	2	63641.4	-0.045	-0.045

Table S175. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex C2 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	0.000
1	4	1883.1	29.727	25.215
2	4	2410.5	25.919	-21.228
3	4	3058.5	-26.453	-0.004
4	4	4188.5	-5.832	0.000
5	4	4696.0	-0.018	0.000
6	4	4838.7	0.000	-0.000
7	4	19782.4	-0.031	-0.000
8	4	21597.6	-0.000	-0.000
9	4	21901.2	0.000	-0.000
0'	2	19545.1	-0.269	-0.173
1'	2	19649.9	0.003	-0.000
2'	2	19988.1	0.094	0.000
3'	2	20044.0	0.003	0.000
4'	2	20089.3	-0.004	0.004
5'	2	20302.0	-0.002	-0.000
6'	2	21262.4	-2.834	-2.592
7'	2	21396.9	-2.719	2.521
8'	2	21586.3	5.943	0.000
9'	2	24894.2	0.000	-0.000
10'	2	25411.2	-0.055	0.042
11'	2	25516.3	0.255	-0.000

12'	2	26022.7	0.039	0.013
13'	2	26068.9	0.039	0.007
14'	2	26419.6	-0.392	-0.287
15'	2	27240.4	0.002	-0.000
16'	2	27423.2	-0.081	-0.041
17'	2	27636.8	0.178	0.001
18'	2	27681.6	-0.165	0.111
19'	2	28149.5	0.013	0.000
20'	2	28215.6	-0.000	0.000
21'	2	28526.7	0.015	0.000
22'	2	28745.6	-0.194	0.166
23'	2	29544.1	2.037	0.000
24'	2	30099.8	-0.548	0.408
25'	2	30421.6	-0.177	-0.142
26'	2	30634.2	-0.393	-0.292
27'	2	31499.7	0.000	0.000
28'	2	44264.0	0.000	-0.000
29'	2	44662.6	0.280	-0.000
30'	2	44886.1	-0.124	-0.059
31'	2	45161.9	-0.114	0.052
32'	2	45401.6	0.001	0.000
33'	2	45615.9	-0.039	0.025
34'	2	45766.9	0.000	0.000
35'	2	68103.2	-0.015	-0.012
36'	2	68327.2	-0.000	-0.000
37'	2	68952.5	-0.019	0.014
38'	2	70031.6	-0.016	-0.008
39'	2	70765.3	0.063	0.000

Table S176. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex C2 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	0.000
1	4	2540.6	22.769	21.970
2	4	3688.9	17.439	-16.565
3	4	4230.1	-19.317	-0.005
4	4	6047.8	-4.047	0.000
6	4	6535.4	-0.013	0.000
5	4	6663.1	0.000	-0.000
7	4	17843.9	-0.035	0.000
8	4	19853.6	-0.000	-0.000
9	4	19915.7	0.000	-0.000
0'	2	18330.3	-0.287	-0.240
1'	2	18534.7	0.003	-0.000
2'	2	18860.5	0.099	0.000
3'	2	18881.9	0.003	0.000
4'	2	19131.9	-0.005	0.003
5'	2	19801.5	-0.002	-0.001
6'	2	20754.4	-2.904	-2.882
7'	2	21265.1	-2.735	2.726
8'	2	21384.4	5.999	0.001
9'	2	22500.9	0.000	-0.000
10'	2	23606.2	-0.060	0.054

11'	2	24040.9	0.271	-0.000
12'	2	24601.5	0.042	0.017
13'	2	24650.4	0.041	0.012
14'	2	24945.2	-0.415	-0.372
15'	2	26331.7	0.002	-0.000
16'	2	26368.1	-0.084	-0.062
17'	2	26701.6	0.185	0.001
18'	2	25817.6	-0.178	0.153
19'	2	26395.8	0.013	0.000
20'	2	26924.1	-0.000	0.000
21'	2	27619.3	0.016	0.000
22'	2	28121.8	-0.198	0.192
23'	2	28223.5	2.133	0.000
24'	2	28826.4	-0.572	0.519
25'	2	29902.7	-0.180	-0.169
26'	2	29644.7	-0.407	-0.367
27'	2	31373.8	0.000	0.000
28'	2	39566.3	0.000	-0.000
29'	2	40053.8	0.312	-0.000
30'	2	40267.1	-0.138	-0.098
31'	2	40639.6	-0.126	0.087
32'	2	41109.2	0.001	0.000
33'	2	41233.6	-0.043	0.036
34'	2	41550.8	0.000	-0.000
36'	2	59495.5	-0.017	-0.016
35'	2	59653.0	-0.000	-0.000
37'	2	60943.5	-0.022	0.019
38'	2	61360.5	-0.018	-0.013
39'	2	62724.0	0.072	0.000

Table S177. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex A4 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	-0.000
1	4	996.5	-96.641	0.000
2	4	3942.2	15.027	-15.027
3	4	4506.4	13.136	13.136
4	4	4748.0	0.181	0.181
5	4	5141.0	0.056	-0.056
6	4	6322.3	-0.003	0.000
7	4	21048.1	-0.000	0.000
8	4	22245.5	0.000	-0.000
9	4	22836.0	0.000	0.000
0'	2	19572.6	-0.608	0.607
1'	2	19903.9	-0.433	-0.433
2'	2	19957.2	0.000	-0.000
3'	2	20112.7	0.195	-0.000
4'	2	20215.3	0.000	0.000
5'	2	20496.2	-0.000	0.000
6'	2	21111.7	6.638	-0.000
7'	2	22756.2	-2.236	2.236
8'	2	22819.4	-2.211	-2.211
9'	2	24710.4	0.058	0.000
10'	2	25763.8	-0.027	0.027

11'	2	26011.9	-0.019	-0.019
12'	2	26100.9	0.994	-0.000
13'	2	26342.0	0.000	0.000
14'	2	28299.9	-0.058	-0.058
15'	2	28410.4	-0.055	0.055
16'	2	28795.1	0.003	0.000
17'	2	28871.9	-0.001	-0.000
18'	2	28882.3	-0.001	0.001
19'	2	29043.7	-0.002	-0.002
20'	2	29170.1	-0.017	0.017
21'	2	30733.3	-1.185	-1.185
22'	2	30734.3	-0.003	-0.003
23'	2	30812.5	-1.015	1.015
24'	2	31262.2	0.006	-0.000
25'	2	31950.0	0.539	0.000
26'	2	32419.5	0.000	0.000
27'	2	32454.3	0.000	0.000
28'	2	45087.3	0.000	-0.000
29'	2	45322.3	0.367	-0.000
30'	2	45892.6	-0.080	0.080
31'	2	46156.7	-0.072	-0.072
32'	2	46845.3	-0.040	-0.039
33'	2	46845.8	-0.050	0.049
34'	2	47014.1	0.003	0.000
35'	2	68624.5	-0.000	0.000
36'	2	69808.5	-0.027	-0.027
37'	2	70366.3	-0.027	0.027
38'	2	71789.3	-0.000	0.000
39'	2	72235.3	0.049	-0.000

Table S178. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex A4 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	0.000
1	4	1110.1	-89.852	0.000
2	4	4993.7	11.947	-11.946
3	4	5693.0	10.454	10.454
4	4	5940.5	0.145	0.145
5	4	6379.8	0.045	-0.045
6	4	7589.4	-0.003	0.000
7	4	19218.5	-0.000	0.000
8	4	20003.9	0.000	-0.000
9	4	20594.3	0.000	0.000
0'	2	17681.8	-0.672	0.672
1'	2	18200.3	-0.474	-0.473
2'	2	18591.2	0.000	-0.000
3'	2	18720.8	0.210	-0.000
4'	2	18930.5	0.000	0.000
5'	2	19141.6	-0.000	0.000
6'	2	19889.0	7.046	-0.000
7'	2	22393.2	-2.272	2.272
8'	2	22474.1	-2.245	-2.245
9'	2	22462.6	0.064	0.000

10'	2	24316.1	-0.029	0.029
11'	2	24507.2	-0.020	-0.020
12'	2	24190.8	1.072	-0.000
13'	2	24443.2	0.000	0.000
14'	2	26623.7	-0.062	-0.062
15'	2	26877.9	-0.058	0.058
16'	2	25993.0	0.003	0.000
17'	2	27843.3	-0.001	-0.000
18'	2	27405.9	-0.001	0.001
19'	2	27234.4	-0.003	-0.003
20'	2	27809.0	-0.018	0.018
21'	2	28461.0	-1.279	-1.279
22'	2	29898.4	-0.003	-0.003
23'	2	28541.0	-1.096	1.095
24'	2	31152.8	0.006	-0.000
25'	2	31152.8	0.553	0.000
26'	2	31374.7	0.000	0.000
27'	2	31714.0	0.000	-0.000
28'	2	40126.3	0.000	-0.000
29'	2	40343.0	0.413	-0.000
30'	2	41211.3	-0.089	0.089
31'	2	41507.3	-0.081	-0.081
32'	2	42206.7	-0.044	-0.044
33'	2	42215.3	-0.055	0.054
34'	2	42817.4	0.003	0.000
35'	2	59909.2	0.000	0.000
36'	2	61583.1	-0.031	-0.031
37'	2	62174.2	-0.030	0.030
38'	2	63226.3	-0.000	0.000
39'	2	63806.9	0.056	-0.000

Table S179. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex B4 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	0.000	0.000
1	4	1598.0	-68.056	0.000
2	4	3443.3	17.355	-17.153
3	4	3788.8	13.313	13.100
4	4	4621.8	1.898	-1.870
5	4	5448.7	0.043	0.043
6	4	5903.6	-0.000	-0.000
7	4	21166.5	0.000	0.000
8	4	21507.1	-0.000	0.000
9	4	22650.5	0.001	-0.001
0'	2	20081.0	0.002	-0.000
1'	2	20134.7	0.002	0.001
2'	2	20246.4	-0.272	0.248
3'	2	20302.3	-0.128	-0.088
4'	2	20415.6	0.002	0.000
5'	2	20648.8	0.002	-0.000
6'	2	21429.2	6.560	-0.000
7'	2	22200.1	-3.182	-3.140
8'	2	22357.1	-2.043	1.997
9'	2	25407.8	0.002	0.000

10'	2	26236.5	-0.053	-0.052
11'	2	26308.1	-0.027	-0.027
12'	2	26490.9	0.874	-0.000
13'	2	27102.8	-0.030	0.030
14'	2	27116.1	-0.212	0.211
15'	2	27328.8	-0.004	-0.003
16'	2	28326.3	-0.001	0.000
17'	2	28453.1	-0.009	-0.009
18'	2	28715.0	-0.000	0.000
19'	2	29101.1	-0.020	-0.020
20'	2	29135.7	0.190	-0.000
21'	2	29392.3	-0.130	0.129
22'	2	29936.4	-0.000	-0.000
23'	2	30130.3	-1.036	-1.033
24'	2	31006.7	-0.803	0.800
25'	2	31573.4	0.587	-0.000
26'	2	31952.5	0.123	-0.000
27'	2	32530.9	0.000	0.000
28'	2	45049.8	0.000	0.000
29'	2	45493.0	0.295	-0.001
30'	2	45608.0	-0.102	-0.104
31'	2	46162.3	-0.123	0.122
32'	2	46310.3	-0.026	0.026
33'	2	46464.4	-0.007	-0.007
34'	2	46638.2	0.000	0.000
35'	2	69154.9	0.005	-0.000
36'	2	69677.3	-0.016	0.016
37'	2	70459.9	0.000	0.000
38'	2	71144.8	-0.021	-0.030
39'	2	71193.2	0.033	-0.007

Table S180. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex B4 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	-0.000
1	4	1923.6	-58.209	0.000
2	4	4377.9	13.778	-13.610
3	4	4856.8	10.456	10.282
4	4	5951.6	1.475	-1.454
5	4	6865.1	0.034	0.034
6	4	7378.4	-0.000	-0.000
7	4	18819.4	0.000	0.000
8	4	19583.9	-0.000	0.000
9	4	20619.1	0.001	-0.001
0'	2	18710.3	0.002	-0.000
1'	2	18778.9	0.003	0.001
2'	2	18867.6	-0.292	0.265
3'	2	18880.3	-0.138	-0.094
4'	2	19090.0	0.002	0.000
5'	2	19731.5	0.002	-0.000
6'	2	20439.8	6.877	-0.000
7'	2	21620.4	-3.267	-3.226
8'	2	21961.9	-2.080	2.035

9'	2	23016.1	0.002	0.000
10'	2	24562.0	-0.057	-0.056
11'	2	24431.3	-0.029	-0.029
12'	2	24705.1	0.938	-0.000
13'	2	25313.0	-0.032	0.032
14'	2	25342.8	-0.227	0.226
15'	2	25761.2	-0.004	-0.003
16'	2	26874.8	-0.001	0.000
17'	2	27407.3	-0.009	-0.009
18'	2	26576.1	-0.000	0.000
19'	2	27106.2	-0.022	-0.022
20'	2	27984.1	0.198	-0.000
21'	2	28055.8	-0.137	0.135
22'	2	29554.2	-0.000	-0.000
23'	2	28022.9	-1.113	-1.111
24'	2	29310.4	-0.849	0.846
26'	2	30669.9	0.602	-0.000
25'	2	30752.4	0.128	-0.000
27'	2	31968.0	0.000	0.000
28'	2	40176.4	0.000	0.000
29'	2	40644.8	0.330	-0.001
30'	2	40818.4	-0.114	-0.116
31'	2	41529.2	-0.137	0.136
32'	2	41742.4	-0.028	0.028
33'	2	41902.0	-0.008	-0.007
34'	2	42306.8	0.000	0.000
35'	2	60458.4	0.006	-0.000
36'	2	61352.0	-0.019	0.018
37'	2	61777.6	0.000	0.000
39'	2	62833.2	-0.024	-0.034
38'	2	63070.5	0.037	-0.008

Table S181. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF method on Complex C4 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	0.000
1	4	2017.4	-56.614	0.012
2	4	3177.5	17.925	-17.129
3	4	3220.1	17.595	16.799
4	4	4948.1	0.429	0.347
5	4	4974.1	0.394	-0.319
6	4	5278.4	0.007	0.007
7	4	21268.0	0.002	-0.001
8	4	21321.7	0.002	0.001
9	4	22115.7	0.000	0.000
0'	2	20123.6	-0.000	0.000
1'	2	20197.9	-0.002	0.002
2'	2	20221.9	0.001	-0.000
3'	2	20480.5	-0.024	0.013
4'	2	20485.7	-0.019	-0.007
5'	2	20823.1	-0.000	0.000
6'	2	21589.4	6.346	-0.002
7'	2	22019.1	-2.845	2.480
8'	2	22032.3	-2.842	-2.484

9'	2	25890.9	0.002	-0.000
10'	2	26051.0	-0.087	0.084
11'	2	26056.3	-0.085	-0.083
12'	2	26702.0	-0.075	0.074
13'	2	26745.9	0.796	0.001
14'	2	26757.7	0.014	-0.071
15'	2	27589.9	-0.001	0.001
16'	2	28111.9	-0.000	-0.000
17'	2	28296.6	-0.068	0.027
18'	2	28306.0	-0.069	-0.029
19'	2	28769.8	-0.027	-0.016
20'	2	28854.3	-0.066	-0.063
21'	2	28885.4	-0.077	0.077
22'	2	29032.3	-0.001	0.001
23'	2	30409.5	-0.794	0.054
24'	2	30427.9	-0.796	-0.062
25'	2	31291.6	1.041	-0.002
26'	2	31355.1	0.003	0.000
27'	2	32275.7	-0.000	0.000
28'	2	44999.9	-0.000	0.000
29'	2	45545.7	0.186	-0.020
30'	2	45621.7	-0.126	0.130
31'	2	45643.9	-0.083	-0.107
32'	2	46118.9	-0.004	0.003
33'	2	46124.8	-0.006	-0.004
34'	2	46412.7	0.000	0.000
35'	2	69292.5	-0.000	0.000
36'	2	69841.0	0.060	-0.000
37'	2	70070.7	0.000	-0.000
38'	2	70672.0	-0.026	-0.014
39'	2	70742.6	-0.025	0.014

Table S182. Calculated delta excitation energies (in cm-1) and individual contributions to D and E parameters arising from the CASSCF/NEVPT2 method on Complex C4 with DFT(BP86) optimized geometry before including the spin-orbit effects. The Roots correspond to ten S=3/2 and forty S=1/2 (') configurations.

Root	Mult	delta	D	E
0	4	0.0	-0.000	0.000
1	4	2498.2	-46.771	0.008
2	4	4137.3	13.924	-13.188
3	4	4191.4	13.671	12.934
4	4	6394.5	0.333	0.263
5	4	6419.7	0.306	-0.242
6	4	6854.4	0.005	0.005
7	4	19133.1	0.003	-0.001
8	4	19184.5	0.003	0.002
9	4	20186.7	0.000	0.000
0'	2	18809.6	-0.000	0.000
1'	2	18827.5	-0.002	0.002
2'	2	19018.1	0.001	-0.000
3'	2	19260.4	-0.025	0.013
4'	2	19272.1	-0.020	-0.007
5'	2	20074.8	-0.000	0.000
6'	2	20797.8	6.590	-0.002
7'	2	21573.6	-2.904	2.492

8'	2	21591.0	-2.900	-2.496
9'	2	23257.3	0.002	-0.000
10'	2	24276.3	-0.093	0.091
11'	2	24290.1	-0.091	-0.090
12'	2	24959.7	-0.081	0.078
13'	2	24969.5	0.852	0.001
14'	2	24995.5	0.016	-0.075
15'	2	25930.0	-0.001	0.001
16'	2	26947.0	-0.000	-0.000
18'	2	26152.2	-0.074	0.031
17'	2	26154.6	-0.074	-0.033
19'	2	27904.4	-0.028	-0.016
20'	2	27996.1	-0.068	-0.066
21'	2	27976.6	-0.080	0.080
22'	2	27838.0	-0.001	0.001
23'	2	28672.4	-0.843	0.034
24'	2	28686.6	-0.845	-0.044
25'	2	30131.2	1.081	-0.002
26'	2	30278.0	0.003	0.000
27'	2	31729.0	-0.000	0.000
28'	2	40156.8	-0.000	0.000
29'	2	40779.8	0.209	-0.023
30'	2	40860.9	-0.141	0.144
31'	2	40898.8	-0.094	-0.118
33'	2	41634.6	-0.005	0.003
32'	2	41636.7	-0.007	-0.004
34'	2	42044.3	0.000	0.000
35'	2	60493.6	-0.000	0.000
36'	2	61323.0	0.068	-0.000
37'	2	61457.5	0.000	-0.000
38'	2	62558.5	-0.029	-0.015
39'	2	62638.8	-0.029	0.015

Table S183. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex A0 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	280.2
3	280.2
4	615.0
5	615.0
6	997.0
7	997.0
8	4394.0
9	4394.0
10	4601.5
11	4601.5
12	4619.9
13	4619.9
14	4695.5
15	4695.5
16	4996.4
17	4996.4
18	5012.5
19	5012.5

20	5510.1
21	5510.1
22	5985.9
23	5985.9
24	6973.1
25	6973.1
26	7124.3
27	7124.3
28	18705.2
29	18705.2
30	19000.6
31	19000.6
32	19322.9
33	19322.9
34	19780.2
35	19780.2
36	20005.2
37	20005.2
38	20222.3
39	20222.3
40	20281.0
41	20281.0
42	21081.3
43	21081.3
44	21103.4
45	21103.4
46	21735.8
47	21735.8
48	21858.6
49	21858.6
50	21990.5
51	21990.5
52	22249.5
53	22249.5
54	22475.2
55	22475.2
56	22916.8
57	22916.8
58	24155.9
59	24155.9
60	25336.3
61	25336.3
62	25455.9
63	25455.9
64	25997.5
65	25997.5
66	26147.9
67	26147.9
68	27459.4
69	27459.4
70	27930.3
71	27930.3
72	28256.6
73	28256.6
74	28295.3
75	28295.3
76	28465.5

77	28465.5
78	28721.3
79	28721.3
80	29090.1
81	29090.1
82	30282.7
83	30282.7
84	30422.6
85	30422.6
86	30974.2
87	30974.2
88	31034.4
89	31034.4
90	31825.5
91	31825.5
92	32255.6
93	32255.6
94	33149.0
95	33149.0
96	43878.3
97	43878.3
98	44169.8
99	44169.8
100	44879.6
101	44879.6
102	45152.6
103	45152.6
104	45631.7
105	45631.7
106	45864.7
107	45864.7
108	46270.6
109	46270.6
110	66956.2
111	66956.2
112	68773.5
113	68773.5
114	68907.7
115	68907.7
116	69578.4
117	69578.4
118	70156.6
119	70156.6

Table S184. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex A0 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	289.1
3	289.1
4	655.0
5	655.0
6	1015.0
7	1015.0
8	6740.5

9	6740.5
10	6845.4
11	6845.4
12	6968.9
13	6968.9
14	7211.9
15	7211.9
16	7293.5
17	7293.5
18	7771.7
19	7771.7
20	8275.9
21	8275.9
22	8750.4
23	8750.4
24	9888.6
25	9888.6
26	10012.1
27	10012.1
28	16594.1
29	16594.1
30	17146.2
31	17146.2
32	17700.5
33	17700.5
34	18408.4
35	18408.4
36	18764.5
37	18764.5
38	19001.7
39	19001.7
40	19081.4
41	19081.4
42	20124.1
43	20124.1
44	20158.6
45	20158.6
46	20404.7
47	20404.7
48	20512.3
49	20512.3
50	20620.6
51	20620.6
52	20948.4
53	20948.4
54	21766.9
55	21766.9
56	23428.9
57	23428.9
58	23434.4
59	23434.4
60	23907.5
61	23907.5
62	23964.5
63	23964.5
64	25113.7
65	25113.7

66 25562.8
67 25562.8
68 26861.9
69 26861.9
70 27068.5
71 27068.5
72 27109.3
73 27109.3
74 27574.3
75 27574.3
76 27641.8
77 27641.8
78 28773.7
79 28773.7
80 29156.0
81 29156.0
82 29592.8
83 29592.8
84 29760.8
85 29760.8
86 31693.2
87 31693.2
88 32883.4
89 32883.4
90 33173.3
91 33173.3
92 34028.9
93 34028.9
94 34866.0
95 34866.0
96 39219.4
97 39219.4
98 39517.6
99 39517.6
100 40849.9
101 40849.9
102 41125.8
103 41125.8
104 41856.6
105 41856.6
106 42105.9
107 42105.9
108 43411.1
109 43411.1
110 57989.7
111 57989.7
112 61014.3
113 61014.3
114 61196.0
115 61196.0
116 61782.6
117 61782.6
118 62347.9
119 62347.9

Table S185. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex B0 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	90.4
3	90.4
4	1217.5
5	1217.5
6	1468.1
7	1468.1
8	2847.9
9	2847.9
10	2961.3
11	2961.3
12	3175.0
13	3175.0
14	3367.9
15	3367.9
16	4172.8
17	4172.8
18	4273.9
19	4273.9
20	4920.1
21	4920.1
22	5297.6
23	5297.6
24	5491.6
25	5491.6
26	5744.8
27	5744.8
28	19120.9
29	19120.9
30	19195.6
31	19195.6
32	19608.4
33	19608.4
34	19972.3
35	19972.3
36	20094.1
37	20094.1
38	20230.5
39	20230.5
40	20295.9
41	20295.9
42	20307.7
43	20307.7
44	20674.6
45	20674.6
46	20911.7
47	20911.7
48	21004.6
49	21004.6
50	21278.4
51	21278.4
52	21413.7

53 21413.7
54 21601.4
55 21601.4
56 21747.6
57 21747.6
58 24755.6
59 24755.6
60 25434.2
61 25434.2
62 25832.7
63 25832.7
64 25929.2
65 25929.2
66 26119.9
67 26119.9
68 26432.5
69 26432.5
70 26557.4
71 26557.4
72 27047.8
73 27047.8
74 27669.4
75 27669.4
76 27797.8
77 27797.8
78 27942.7
79 27942.7
80 28213.9
81 28213.9
82 28568.1
83 28568.1
84 28732.5
85 28732.5
86 29302.4
87 29302.4
88 30117.6
89 30117.6
90 30624.8
91 30624.8
92 30954.0
93 30954.0
94 31961.7
95 31961.7
96 43779.8
97 43779.8
98 44211.2
99 44211.2
100 44394.8
101 44394.8
102 44762.7
103 44762.7
104 44911.3
105 44911.3
106 45124.2
107 45124.2
108 45366.0
109 45366.0

110	67541.1
111	67541.1
112	68090.2
113	68090.2
114	68459.7
115	68459.7
116	68889.6
117	68889.6
118	69559.1
119	69559.1

Table S186. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex B0 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	75.6
3	75.6
4	1733.3
5	1733.3
6	1916.5
7	1916.5
8	4341.8
9	4341.8
10	4427.6
11	4427.6
12	4989.5
13	4989.5
14	5125.3
15	5125.3
16	6443.6
17	6443.6
18	6555.3
19	6555.3
20	7455.5
21	7455.5
22	7822.9
23	7822.9
24	8094.8
25	8094.8
26	8347.4
27	8347.4
28	17880.4
29	17880.4
30	18086.0
31	18086.0
32	18430.2
33	18430.2
34	18468.1
35	18468.1
36	18603.5
37	18603.5
38	18786.7
39	18786.7
40	19081.8
41	19081.8

42	19269.8
43	19269.8
44	19435.7
45	19435.7
46	19518.8
47	19518.8
48	19918.3
49	19918.3
50	20087.2
51	20087.2
52	20122.4
53	20122.4
54	21407.2
55	21407.2
56	21965.8
57	21965.8
58	22337.7
59	22337.7
60	23845.7
61	23845.7
62	24371.5
63	24371.5
64	24527.0
65	24527.0
66	24918.3
67	24918.3
68	25204.6
69	25204.6
70	25473.9
71	25473.9
72	26416.2
73	26416.2
74	26936.3
75	26936.3
76	27153.7
77	27153.7
78	27283.6
79	27283.6
80	27738.7
81	27738.7
82	27891.4
83	27891.4
84	28313.9
85	28313.9
86	29197.2
87	29197.2
88	29656.1
89	29656.1
90	30484.1
91	30484.1
92	31367.7
93	31367.7
94	32681.3
95	32681.3
96	39136.9
97	39136.9
98	39637.2

99	39637.2
100	39995.9
101	39995.9
102	40470.7
103	40470.7
104	40852.1
105	40852.1
106	41063.1
107	41063.1
108	41622.8
109	41622.8
110	58698.6
111	58698.6
112	59548.4
113	59548.4
114	60355.4
115	60355.4
116	60572.7
117	60572.7
118	61856.7
119	61856.7

Table S187. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex C0 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	28.9
3	28.9
4	1636.3
5	1636.3
6	1856.9
7	1856.9
8	2371.8
9	2371.8
10	2596.7
11	2596.7
12	2608.1
13	2608.1
14	2643.3
15	2643.3
16	3519.3
17	3519.3
18	3916.0
19	3916.0
20	4152.3
21	4152.3
22	4527.8
23	4527.8
24	4656.0
25	4656.0
26	4771.0
27	4771.0
28	19217.9
29	19217.9
30	19427.9

31 19427.9
32 19450.0
33 19450.0
34 20036.1
35 20036.1
36 20090.6
37 20090.6
38 20146.4
39 20146.4
40 20229.6
41 20229.6
42 20292.2
43 20292.2
44 20414.2
45 20414.2
46 20483.7
47 20483.7
48 20750.0
49 20750.0
50 20948.2
51 20948.2
52 21127.5
53 21127.5
54 21285.6
55 21285.6
56 21453.2
57 21453.2
58 24889.2
59 24889.2
60 25081.2
61 25081.2
62 25541.3
63 25541.3
64 25687.9
65 25687.9
66 26099.5
67 26099.5
68 26168.6
69 26168.6
70 26790.4
71 26790.4
72 26874.9
73 26874.9
74 27140.4
75 27140.4
76 27172.7
77 27172.7
78 27567.8
79 27567.8
80 27689.4
81 27689.4
82 27797.4
83 27797.4
84 28075.4
85 28075.4
86 29221.2
87 29221.2

88	29255.1
89	29255.1
90	29953.7
91	29953.7
92	30264.9
93	30264.9
94	31107.4
95	31107.4
96	43727.4
97	43727.4
98	44196.5
99	44196.5
100	44277.4
101	44277.4
102	44402.3
103	44402.3
104	44775.7
105	44775.7
106	44832.7
107	44832.7
108	45088.7
109	45088.7
110	67390.5
111	67390.5
112	68140.7
113	68140.7
114	68234.2
115	68234.2
116	69105.7
117	69105.7
118	69156.6
119	69156.6

Table S188. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex C0 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	26.4
3	26.4
4	2543.6
5	2543.6
6	2708.8
7	2708.8
8	3866.2
9	3866.2
10	4005.4
11	4005.4
12	4018.3
13	4018.3
14	4080.9
15	4080.9
16	5709.7
17	5709.7
18	6086.9
19	6086.9

20	6393.1
21	6393.1
22	6817.9
23	6817.9
24	6931.8
25	6931.8
26	6946.0
27	6946.0
28	18261.9
29	18261.9
30	18298.4
31	18298.4
32	18376.0
33	18376.0
34	18430.9
35	18430.9
36	18524.0
37	18524.0
38	18689.3
39	18689.3
40	18696.4
41	18696.4
42	19149.4
43	19149.4
44	19228.5
45	19228.5
46	19608.5
47	19608.5
48	19705.8
49	19705.8
50	19907.6
51	19907.6
52	20573.1
53	20573.1
54	21096.7
55	21096.7
56	21556.9
57	21556.9
58	22771.0
59	22771.0
60	23306.2
61	23306.2
62	23964.6
63	23964.6
64	24173.2
65	24173.2
66	24581.5
67	24581.5
68	24688.2
69	24688.2
70	25629.0
71	25629.0
72	25953.1
73	25953.1
74	26120.1
75	26120.1
76	26337.6

77	26337.6
78	26760.4
79	26760.4
80	27259.5
81	27259.5
82	27501.9
83	27501.9
84	27747.0
85	27747.0
86	28221.5
87	28221.5
88	28318.9
89	28318.9
90	29596.3
91	29596.3
92	29810.7
93	29810.7
94	31327.7
95	31327.7
96	39053.7
97	39053.7
98	39730.1
99	39730.1
100	39828.9
101	39828.9
102	39934.9
103	39934.9
104	40662.9
105	40662.9
106	40712.7
107	40712.7
108	41129.8
109	41129.8
110	58506.6
111	58506.6
112	59545.5
113	59545.5
114	59659.0
115	59659.0
116	61166.9
117	61166.9
118	61235.6
119	61235.6

Table S189. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex A2 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	155.4
3	155.4
4	994.3
5	994.3
6	1263.6
7	1263.6
8	3570.9

9	3570.9
10	3792.0
11	3792.0
12	4447.0
13	4447.0
14	4640.7
15	4640.7
16	4752.7
17	4752.7
18	4965.2
19	4965.2
20	5508.5
21	5508.5
22	5906.4
23	5906.4
24	6640.8
25	6640.8
26	6823.8
27	6823.8
28	19076.4
29	19076.4
30	19342.8
31	19342.8
32	19857.2
33	19857.2
34	20195.1
35	20195.1
36	20273.4
37	20273.4
38	20577.7
39	20577.7
40	20948.9
41	20948.9
42	21013.8
43	21013.8
44	21056.8
45	21056.8
46	21256.7
47	21256.7
48	21400.2
49	21400.2
50	22428.8
51	22428.8
52	22897.5
53	22897.5
54	23158.4
55	23158.4
56	23312.0
57	23312.0
58	24302.7
59	24302.7
60	25653.8
61	25653.8
62	26160.9
63	26160.9
64	26271.5
65	26271.5

66 27002.3
67 27002.3
68 27367.6
69 27367.6
70 27890.1
71 27890.1
72 28497.5
73 28497.5
74 28591.0
75 28591.0
76 28784.5
77 28784.5
78 29118.8
79 29118.8
80 29434.0
81 29434.0
82 30288.8
83 30288.8
84 30541.9
85 30541.9
86 30823.2
87 30823.2
88 30881.8
89 30881.8
90 32032.9
91 32032.9
92 32131.3
93 32131.3
94 33033.9
95 33033.9
96 44617.3
97 44617.3
98 44978.7
99 44978.7
100 45238.5
101 45238.5
102 46062.8
103 46062.8
104 46250.7
105 46250.7
106 46499.6
107 46499.6
108 46706.9
109 46706.9
110 68032.2
111 68032.2
112 68840.6
113 68840.6
114 70469.2
115 70469.2
116 70696.7
117 70696.7
118 71254.4
119 71254.4

Table S190. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex A2 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	156.7
3	156.7
4	1096.4
5	1096.4
6	1338.6
7	1338.6
8	5100.8
9	5100.8
10	5282.2
11	5282.2
12	6178.1
13	6178.1
14	6304.5
15	6304.5
16	6449.7
17	6449.7
18	6632.6
19	6632.6
20	7113.6
21	7113.6
22	7527.8
23	7527.8
24	8572.1
25	8572.1
26	8732.2
27	8732.2
28	17231.7
29	17231.7
30	18032.5
31	18032.5
32	18332.1
33	18332.1
34	18792.3
35	18792.3
36	18959.5
37	18959.5
38	19134.9
39	19134.9
40	19175.0
41	19175.0
42	19283.5
43	19283.5
44	19621.4
45	19621.4
46	19734.6
47	19734.6
48	19860.7
49	19860.7
50	21106.9
51	21106.9
52	21281.1

53 21281.1
54 22047.6
55 22047.6
56 22493.0
57 22493.0
58 22949.5
59 22949.5
60 24263.9
61 24263.9
62 24550.0
63 24550.0
64 24883.1
65 24883.1
66 25295.7
67 25295.7
68 26216.4
69 26216.4
70 26583.9
71 26583.9
72 26700.7
73 26700.7
74 26868.0
75 26868.0
76 27470.1
77 27470.1
78 28009.0
79 28009.0
80 28543.1
81 28543.1
82 28694.9
83 28694.9
84 29643.5
85 29643.5
86 30377.9
87 30377.9
88 31091.7
89 31091.7
90 31341.7
91 31341.7
92 32231.7
93 32231.7
94 33207.2
95 33207.2
96 39784.2
97 39784.2
98 40131.1
99 40131.1
100 40765.0
101 40765.0
102 41559.8
103 41559.8
104 41853.7
105 41853.7
106 42118.1
107 42118.1
108 42805.1
109 42805.1

110	59286.7
111	59286.7
112	60783.0
113	60783.0
114	62027.8
115	62027.8
116	62524.3
117	62524.3
118	62808.7
119	62808.7

Table S191. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex B2 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	74.5
3	74.5
4	1397.6
5	1397.6
6	1638.7
7	1638.7
8	2663.5
9	2663.5
10	2932.7
11	2932.7
12	3078.7
13	3078.7
14	3325.0
15	3325.0
16	4259.9
17	4259.9
18	4333.8
19	4333.8
20	5129.5
21	5129.5
22	5467.6
23	5467.6
24	5812.4
25	5812.4
26	6037.8
27	6037.8
28	19180.0
29	19180.0
30	19493.5
31	19493.5
32	19904.2
33	19904.2
34	20176.6
35	20176.6
36	20382.1
37	20382.1
38	20635.9
39	20635.9
40	20773.2
41	20773.2

42	20862.7
43	20862.7
44	21000.8
45	21000.8
46	21132.1
47	21132.1
48	21181.1
49	21181.1
50	21505.8
51	21505.8
52	21834.2
53	21834.2
54	21998.6
55	21998.6
56	22062.3
57	22062.3
58	24812.6
59	24812.6
60	25648.9
61	25648.9
62	26111.1
63	26111.1
64	26463.8
65	26463.8
66	26652.5
67	26652.5
68	27157.9
69	27157.9
70	27256.8
71	27256.8
72	27603.7
73	27603.7
74	28157.8
75	28157.8
76	28313.6
77	28313.6
78	28697.8
79	28697.8
80	28808.6
81	28808.6
82	29004.9
83	29004.9
84	29414.5
85	29414.5
86	29843.4
87	29843.4
88	30299.6
89	30299.6
90	30854.9
91	30854.9
92	31452.8
93	31452.8
94	31989.1
95	31989.1
96	44503.3
97	44503.3
98	44820.4

99	44820.4
100	45069.7
101	45069.7
102	45424.1
103	45424.1
104	45695.6
105	45695.6
106	45879.0
107	45879.0
108	45964.5
109	45964.5
110	68437.9
111	68437.9
112	69367.0
113	69367.0
114	69503.2
115	69503.2
116	69902.4
117	69902.4
118	70261.4
119	70261.4

Table S192. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex B2 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	66.8
3	66.8
4	1822.8
5	1822.8
6	2012.4
7	2012.4
8	3907.2
9	3907.2
10	4163.5
11	4163.5
12	4275.5
13	4275.5
14	4502.9
15	4502.9
16	5755.5
17	5755.5
18	5833.6
19	5833.6
20	6789.2
21	6789.2
22	7158.9
23	7158.9
24	7438.2
25	7438.2
26	7700.7
27	7700.7
28	17815.0
29	17815.0
30	18262.0

31	18262.0
32	18632.6
33	18632.6
34	18829.6
35	18829.6
36	18871.0
37	18871.0
38	18955.6
39	18955.6
40	19085.2
41	19085.2
42	19130.8
43	19130.8
44	19339.6
45	19339.6
46	19537.4
47	19537.4
48	19671.2
49	19671.2
50	19795.9
51	19795.9
52	20296.8
53	20296.8
54	21188.6
55	21188.6
56	21797.9
57	21797.9
58	22524.7
59	22524.7
60	23906.8
61	23906.8
62	24345.8
63	24345.8
64	24856.8
65	24856.8
66	25196.5
67	25196.5
68	25636.8
69	25636.8
70	25811.9
71	25811.9
72	26289.0
73	26289.0
74	26425.6
75	26425.6
76	26992.5
77	26992.5
78	27406.5
79	27406.5
80	27695.1
81	27695.1
82	27882.6
83	27882.6
84	28117.5
85	28117.5
86	28779.8
87	28779.8

88	29219.4
89	29219.4
90	30064.9
91	30064.9
92	30555.0
93	30555.0
94	31597.3
95	31597.3
96	39631.3
97	39631.3
98	39963.6
99	39963.6
100	40482.8
101	40482.8
102	40695.2
103	40695.2
104	41161.9
105	41161.9
106	41406.5
107	41406.5
108	41690.8
109	41690.8
110	59717.7
111	59717.7
112	60719.2
113	60719.2
114	61368.3
115	61368.3
116	61460.9
117	61460.9
118	61649.3
119	61649.3

Table S193. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex B2' with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	74.0
3	74.0
4	1566.4
5	1566.4
6	1773.7
7	1773.7
8	3299.1
9	3299.1
10	3399.6
11	3399.6
12	3972.1
13	3972.1
14	4174.8
15	4174.8
16	4733.8
17	4733.8
18	4946.2
19	4946.2

20	5351.9
21	5351.9
22	5780.4
23	5780.4
24	6226.1
25	6226.1
26	6431.4
27	6431.4
28	19503.2
29	19503.2
30	19686.5
31	19686.5
32	19950.4
33	19950.4
34	20010.3
35	20010.3
36	20049.0
37	20049.0
38	20465.6
39	20465.6
40	20555.9
41	20555.9
42	20833.4
43	20833.4
44	21355.3
45	21355.3
46	21770.5
47	21770.5
48	21826.2
49	21826.2
50	22045.2
51	22045.2
52	22475.3
53	22475.3
54	23219.2
55	23219.2
56	23360.8
57	23360.8
58	24718.7
59	24718.7
60	26003.6
61	26003.6
62	26112.5
63	26112.5
64	26415.1
65	26415.1
66	26542.3
67	26542.3
68	26817.4
69	26817.4
70	27581.2
71	27581.2
72	27936.3
73	27936.3
74	28313.9
75	28313.9
76	28447.1

77	28447.1
78	28917.2
79	28917.2
80	29010.3
81	29010.3
82	29619.0
83	29619.0
84	29752.9
85	29752.9
86	30003.8
87	30003.8
88	31228.1
89	31228.1
90	31529.6
91	31529.6
92	32073.3
93	32073.3
94	33247.4
95	33247.4
96	44582.4
97	44582.4
98	45028.8
99	45028.8
100	45278.2
101	45278.2
102	45870.2
103	45870.2
104	46130.3
105	46130.3
106	46255.2
107	46255.2
108	46577.6
109	46577.6
110	68081.0
111	68081.0
112	68714.9
113	68714.9
114	69411.3
115	69411.3
116	70862.4
117	70862.4
118	71731.9
119	71731.9

Table S194. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex B2' with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	66.9
3	66.9
4	1966.7
5	1966.7
6	2131.1
7	2131.1
8	4715.1

9	4715.1
10	4782.5
11	4782.5
12	5420.9
13	5420.9
14	5587.1
15	5587.1
16	6544.6
17	6544.6
18	6673.5
19	6673.5
20	7459.6
21	7459.6
22	7788.6
23	7788.6
24	8407.0
25	8407.0
26	8587.6
27	8587.6
28	18071.9
29	18071.9
30	18107.6
31	18107.6
32	18283.8
33	18283.8
34	18452.1
35	18452.1
36	18673.3
37	18673.3
38	19230.3
39	19230.3
40	19300.5
41	19300.5
42	19965.5
43	19965.5
44	20136.6
45	20136.6
46	20184.4
47	20184.4
48	20476.1
49	20476.1
50	21424.2
51	21424.2
52	21588.2
53	21588.2
54	21834.6
55	21834.6
56	22346.5
57	22346.5
58	22562.0
59	22562.0
60	24046.9
61	24046.9
62	24731.5
63	24731.5
64	25127.2
65	25127.2

66 25480.3
67 25480.3
68 25608.9
69 25608.9
70 25877.2
71 25877.2
72 26466.8
73 26466.8
74 27119.2
75 27119.2
76 27240.4
77 27240.4
78 27531.4
79 27531.4
80 28223.1
81 28223.1
82 28532.8
83 28532.8
84 28755.2
85 28755.2
86 29708.3
87 29708.3
88 30545.3
89 30545.3
90 31091.7
91 31091.7
92 31917.0
93 31917.0
94 33404.5
95 33404.5
96 39945.3
97 39945.3
98 40495.7
99 40495.7
100 40668.9
101 40668.9
102 41540.5
103 41540.5
104 41789.2
105 41789.2
106 41934.2
107 41934.2
108 42493.1
109 42493.1
110 59542.0
111 59542.0
112 60613.1
113 60613.1
114 60864.6
115 60864.6
116 62270.1
117 62270.1
118 63879.1
119 63879.1

Table S195. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex C2 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	43.0
3	43.0
4	1863.4
5	1863.4
6	2074.5
7	2074.5
8	2495.9
9	2495.9
10	2666.3
11	2666.3
12	3109.6
13	3109.6
14	3294.3
15	3294.3
16	4098.0
17	4098.0
18	4380.6
19	4380.6
20	4806.4
21	4806.4
22	5113.1
23	5113.1
24	5383.6
25	5383.6
26	5532.4
27	5532.4
28	19407.0
29	19407.0
30	19735.4
31	19735.4
32	19829.0
33	19829.0
34	19893.5
35	19893.5
36	19914.5
37	19914.5
38	20378.7
39	20378.7
40	20539.7
41	20539.7
42	20826.2
43	20826.2
44	21319.2
45	21319.2
46	21468.7
47	21468.7
48	21641.2
49	21641.2
50	21718.1
51	21718.1
52	21999.7

53 21999.7
54 22029.7
55 22029.7
56 22215.2
57 22215.2
58 25066.8
59 25066.8
60 25397.1
61 25397.1
62 25953.9
63 25953.9
64 26076.5
65 26076.5
66 26495.7
67 26495.7
68 26759.8
69 26759.8
70 27535.5
71 27535.5
72 27625.9
73 27625.9
74 27665.1
75 27665.1
76 28011.3
77 28011.3
78 28294.3
79 28294.3
80 28599.1
81 28599.1
82 28779.7
83 28779.7
84 29208.2
85 29208.2
86 29792.1
87 29792.1
88 30226.1
89 30226.1
90 30802.1
91 30802.1
92 31084.4
93 31084.4
94 32089.5
95 32089.5
96 44453.2
97 44453.2
98 44865.3
99 44865.3
100 45079.4
101 45079.4
102 45340.0
103 45340.0
104 45679.4
105 45679.4
106 45821.2
107 45821.2
108 46070.8
109 46070.8

110	68278.3
111	68278.3
112	68620.0
113	68620.0
114	69218.7
115	69218.7
116	70252.9
117	70252.9
118	71056.6
119	71056.6

Table S196. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex C2 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	35.2
3	35.2
4	2539.1
5	2539.1
6	2705.4
7	2705.4
8	3732.8
9	3732.8
10	3841.5
11	3841.5
12	4257.7
13	4257.7
14	4409.5
15	4409.5
16	5824.8
17	5824.8
18	6141.8
19	6141.8
20	6571.8
21	6571.8
22	6942.4
23	6942.4
24	7099.1
25	7099.1
26	7257.3
27	7257.3
28	17887.5
29	17887.5
30	17920.9
31	17920.9
32	18187.1
33	18187.1
34	18658.3
35	18658.3
36	18724.7
37	18724.7
38	19201.9
39	19201.9
40	19419.7
41	19419.7

42	19769.9
43	19769.9
44	19894.9
45	19894.9
46	20032.0
47	20032.0
48	20122.1
49	20122.1
50	20283.2
51	20283.2
52	20797.2
53	20797.2
54	21245.2
55	21245.2
56	21726.7
57	21726.7
58	22712.8
59	22712.8
60	23646.0
61	23646.0
62	24367.1
63	24367.1
64	24593.1
65	24593.1
66	24983.8
67	24983.8
68	25278.1
69	25278.1
70	25815.1
71	25815.1
72	26431.2
73	26431.2
74	26571.9
75	26571.9
76	26704.5
77	26704.5
78	27026.5
79	27026.5
80	27180.0
81	27180.0
82	27749.2
83	27749.2
84	28438.0
85	28438.0
86	28520.4
87	28520.4
88	28974.0
89	28974.0
90	29941.1
91	29941.1
92	30295.3
93	30295.3
94	31759.2
95	31759.2
96	39708.3
97	39708.3
98	40210.2

99	40210.2
100	40423.8
101	40423.8
102	40784.4
103	40784.4
104	41304.8
105	41304.8
106	41403.6
107	41403.6
108	41779.8
109	41779.8
110	59618.5
111	59618.5
112	59917.9
113	59917.9
114	61145.5
115	61145.5
116	61561.6
117	61561.6
118	62951.2
119	62951.2

Table S197. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex A4 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	129.9
3	129.9
4	1173.5
5	1173.5
6	1415.9
7	1415.9
8	3846.1
9	3846.1
10	4142.8
11	4142.8
12	4592.8
13	4592.8
14	4681.1
15	4681.1
16	4886.8
17	4886.8
18	5087.3
19	5087.3
20	5451.1
21	5451.1
22	5833.6
23	5833.6
24	6714.5
25	6714.5
26	6899.2
27	6899.2
28	19472.9
29	19472.9
30	19923.4

31	19923.4
32	20097.8
33	20097.8
34	20553.7
35	20553.7
36	20710.3
37	20710.3
38	20955.7
39	20955.7
40	21215.8
41	21215.8
42	21233.4
43	21233.4
44	21367.6
45	21367.6
46	22374.0
47	22374.0
48	22453.3
49	22453.3
50	22788.4
51	22788.4
52	22989.3
53	22989.3
54	23158.9
55	23158.9
56	23295.9
57	23295.9
58	24974.6
59	24974.6
60	25918.7
61	25918.7
62	26276.2
63	26276.2
64	26577.6
65	26577.6
66	26914.5
67	26914.5
68	28347.3
69	28347.3
70	28809.2
71	28809.2
72	28924.1
73	28924.1
74	29021.2
75	29021.2
76	29193.4
77	29193.4
78	29421.7
79	29421.7
80	29663.9
81	29663.9
82	30846.9
83	30846.9
84	31026.1
85	31026.1
86	31498.8
87	31498.8

88	31639.1
89	31639.1
90	32090.2
91	32090.2
92	32959.2
93	32959.2
94	33125.7
95	33125.7
96	45349.7
97	45349.7
98	45582.4
99	45582.4
100	46125.8
101	46125.8
102	46466.7
103	46466.7
104	47021.2
105	47021.2
106	47267.7
107	47267.7
108	47323.7
109	47323.7
110	68912.8
111	68912.8
112	70127.6
113	70127.6
114	70685.1
115	70685.1
116	72009.3
117	72009.3
118	72636.2
119	72636.2

Table S198. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex A4 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	128.0
3	128.0
4	1282.5
5	1282.5
6	1502.4
7	1502.4
8	4908.6
9	4908.6
10	5167.7
11	5167.7
12	5737.0
13	5737.0
14	5831.1
15	5831.1
16	6053.0
17	6053.0
18	6239.3
19	6239.3

20	6643.7
21	6643.7
22	7015.5
23	7015.5
24	7946.3
25	7946.3
26	8126.7
27	8126.7
28	17689.2
29	17689.2
30	18373.2
31	18373.2
32	18545.9
33	18545.9
34	19078.3
35	19078.3
36	19286.8
37	19286.8
38	19362.1
39	19362.1
40	19421.4
41	19421.4
42	19585.5
43	19585.5
44	20052.3
45	20052.3
46	20147.0
47	20147.0
48	20223.5
49	20223.5
50	20732.8
51	20732.8
52	20907.3
53	20907.3
54	22405.4
55	22405.4
56	22755.3
57	22755.3
58	22899.4
59	22899.4
60	24317.3
61	24317.3
62	24415.9
63	24415.9
64	24926.7
65	24926.7
66	25143.9
67	25143.9
68	26180.3
69	26180.3
70	26697.0
71	26697.0
72	27314.0
73	27314.0
74	27424.9
75	27424.9
76	27629.4

77	27629.4
78	28080.1
79	28080.1
80	28218.5
81	28218.5
82	28637.9
83	28637.9
84	29149.5
85	29149.5
86	30298.7
87	30298.7
88	31252.0
89	31252.0
90	31477.1
91	31477.1
92	31844.9
93	31844.9
94	32289.6
95	32289.6
96	40369.1
97	40369.1
98	40586.5
99	40586.5
100	41429.1
101	41429.1
102	41792.9
103	41792.9
104	42356.4
105	42356.4
106	42613.5
107	42613.5
108	43095.9
109	43095.9
110	60187.4
111	60187.4
112	61880.1
113	61880.1
114	62471.2
115	62471.2
116	63445.6
117	63445.6
118	64173.7
119	64173.7

Table S199. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex B4 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	66.6
3	66.6
4	1666.8
5	1666.8
6	1871.6
7	1871.6
8	3537.8

9	3537.8
10	3660.5
11	3660.5
12	3700.1
13	3700.1
14	3920.6
15	3920.6
16	4772.6
17	4772.6
18	4888.2
19	4888.2
20	5538.0
21	5538.0
22	5920.2
23	5920.2
24	6263.3
25	6263.3
26	6507.8
27	6507.8
28	19917.4
29	19917.4
30	19988.9
31	19988.9
32	20271.3
33	20271.3
34	20742.2
35	20742.2
36	20826.0
37	20826.0
38	21150.2
39	21150.2
40	21227.7
41	21227.7
42	21270.7
43	21270.7
44	21547.2
45	21547.2
46	21655.2
47	21655.2
48	21743.2
49	21743.2
50	22245.0
51	22245.0
52	22731.5
53	22731.5
54	22758.3
55	22758.3
56	22894.8
57	22894.8
58	25542.8
59	25542.8
60	26259.9
61	26259.9
62	26695.3
63	26695.3
64	26856.0
65	26856.0

66 27167.2
67 27167.2
68 27516.7
69 27516.7
70 27710.8
71 27710.8
72 28387.4
73 28387.4
74 28676.2
75 28676.2
76 28932.4
77 28932.4
78 29179.3
79 29179.3
80 29540.9
81 29540.9
82 29803.8
83 29803.8
84 30254.5
85 30254.5
86 30502.3
87 30502.3
88 31205.2
89 31205.2
90 31852.2
91 31852.2
92 32324.4
93 32324.4
94 33132.5
95 33132.5
96 45242.8
97 45242.8
98 45682.4
99 45682.4
100 45815.6
101 45815.6
102 46344.2
103 46344.2
104 46518.1
105 46518.1
106 46757.2
107 46757.2
108 46915.7
109 46915.7
110 69362.5
111 69362.5
112 69951.1
113 69951.1
114 70666.9
115 70666.9
116 71352.9
117 71352.9
118 71543.6
119 71543.6

Table S200. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex B4 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	61.4
3	61.4
4	1990.4
5	1990.4
6	2162.7
7	2162.7
8	4469.7
9	4469.7
10	4557.1
11	4557.1
12	4755.4
13	4755.4
14	4960.6
15	4960.6
16	6057.2
17	6057.2
18	6158.6
19	6158.6
20	6904.4
21	6904.4
22	7268.8
23	7268.8
24	7680.4
25	7680.4
26	7912.8
27	7912.8
28	18512.0
29	18512.0
30	18663.6
31	18663.6
32	18845.5
33	18845.5
34	18876.8
35	18876.8
36	18915.5
37	18915.5
38	19332.1
39	19332.1
40	19457.8
41	19457.8
42	19689.0
43	19689.0
44	19765.2
45	19765.2
46	20120.2
47	20120.2
48	20545.9
49	20545.9
50	20697.3
51	20697.3
52	20836.6

53 20836.6
54 21675.0
55 21675.0
56 22237.3
57 22237.3
58 23198.4
59 23198.4
60 24442.5
61 24442.5
62 24881.3
63 24881.3
64 25028.5
65 25028.5
66 25409.0
67 25409.0
68 25714.9
69 25714.9
70 26081.7
71 26081.7
72 26611.8
73 26611.8
74 26987.8
75 26987.8
76 27282.4
77 27282.4
78 27724.4
79 27724.4
80 28114.9
81 28114.9
82 28293.3
83 28293.3
84 28655.3
85 28655.3
86 29496.4
87 29496.4
88 29830.5
89 29830.5
90 30912.5
91 30912.5
92 31108.6
93 31108.6
94 32400.2
95 32400.2
96 40341.7
97 40341.7
98 40815.0
99 40815.0
100 41001.5
101 41001.5
102 41692.7
103 41692.7
104 41907.3
105 41907.3
106 42166.3
107 42166.3
108 42535.9
109 42535.9

110	60656.0
111	60656.0
112	61581.0
113	61581.0
114	61984.3
115	61984.3
116	63049.9
117	63049.9
118	63341.9
119	63341.9

Table S201. Calculated Delta excitation energies (in cm-1) arising from the CASSCF method on Complex C4 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	34.3
3	34.3
4	2018.0
5	2018.0
6	2214.4
7	2214.4
8	3166.6
9	3166.6
10	3346.3
11	3346.3
12	3355.2
13	3355.2
14	3401.7
15	3401.7
16	4566.2
17	4566.2
18	4943.9
19	4943.9
20	5262.2
21	5262.2
22	5682.3
23	5682.3
24	5809.6
25	5809.6
26	5840.0
27	5840.0
28	19936.7
29	19936.7
30	20161.0
31	20161.0
32	20201.5
33	20201.5
34	20791.2
35	20791.2
36	20907.9
37	20907.9
38	21204.9
39	21204.9
40	21267.9
41	21267.9

42	21308.1
43	21308.1
44	21459.6
45	21459.6
46	21585.5
47	21585.5
48	21649.9
49	21649.9
50	22000.2
51	22000.2
52	22228.2
53	22228.2
54	22388.2
55	22388.2
56	22476.7
57	22476.7
58	25956.8
59	25956.8
60	25978.0
61	25978.0
62	26589.2
63	26589.2
64	26640.7
65	26640.7
66	27058.4
67	27058.4
68	27194.6
69	27194.6
70	27864.0
71	27864.0
72	28284.8
73	28284.8
74	28321.5
75	28321.5
76	28603.8
77	28603.8
78	28979.7
79	28979.7
80	29177.4
81	29177.4
82	29253.8
83	29253.8
84	29371.0
85	29371.0
86	30578.4
87	30578.4
88	30652.3
89	30652.3
90	31507.8
91	31507.8
92	31880.2
93	31880.2
94	32810.5
95	32810.5
96	45169.1
97	45169.1
98	45676.2

99	45676.2
100	45759.6
101	45759.6
102	45887.9
103	45887.9
104	46345.7
105	46345.7
106	46358.4
107	46358.4
108	46670.2
109	46670.2
110	69469.2
111	69469.2
112	70107.8
113	70107.8
114	70230.4
115	70230.4
116	70938.5
117	70938.5
118	71013.8
119	71013.8

Table S202. Calculated Delta excitation energies (in cm-1) arising from the CASSCF/NEVPT2 method on Complex C4 with DFT(BP86) optimized geometry after including the spin-orbit effects.

State	Delta
1	0.0
2	32.3
3	32.3
4	2509.7
5	2509.7
6	2672.3
7	2672.3
8	4132.7
9	4132.7
10	4267.5
11	4267.5
12	4277.9
13	4277.9
14	4337.4
15	4337.4
16	5967.4
17	5967.4
18	6339.7
19	6339.7
20	6682.4
21	6682.4
22	7155.5
23	7155.5
24	7220.5
25	7220.5
26	7315.0
27	7315.0
28	18638.3
29	18638.3
30	18791.9

31	18791.9
32	19024.6
33	19024.6
34	19041.6
35	19041.6
36	19130.4
37	19130.4
38	19228.8
39	19228.8
40	19402.1
41	19402.1
42	19590.0
43	19590.0
44	19633.7
45	19633.7
46	20282.3
47	20282.3
48	20366.9
49	20366.9
50	20462.5
51	20462.5
52	20848.5
53	20848.5
54	21514.0
55	21514.0
56	21960.6
57	21960.6
58	23423.5
59	23423.5
60	24155.6
61	24155.6
62	24801.2
63	24801.2
64	24848.4
65	24848.4
66	25284.0
67	25284.0
68	25361.2
69	25361.2
70	25955.8
71	25955.8
72	26441.4
73	26441.4
74	26471.4
75	26471.4
76	27207.1
77	27207.1
78	27805.7
79	27805.7
80	28120.1
81	28120.1
82	28203.6
83	28203.6
84	28342.4
85	28342.4
86	28873.0
87	28873.0

88	29029.9
89	29029.9
90	30355.4
91	30355.4
92	30700.8
93	30700.8
94	32111.9
95	32111.9
96	40297.2
97	40297.2
98	40895.5
99	40895.5
100	40993.4
101	40993.4
102	41101.9
103	41101.9
104	41819.2
105	41819.2
106	41826.1
107	41826.1
108	42258.4
109	42258.4
110	60660.7
111	60660.7
112	61549.7
113	61549.7
114	61620.8
115	61620.8
116	62780.3
117	62780.3
118	62868.6
119	62868.6

Table S203. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex A0 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	3.016110
6.06	3.034871
9.09	3.049303
12.12	3.063093
15.15	3.076697
18.18	3.090228
21.21	3.103725
24.24	3.117203
27.27	3.130670
30.30	3.144129
33.33	3.157580
36.36	3.171020
39.39	3.184440
42.42	3.197830
45.45	3.211173
48.48	3.224450
51.52	3.237637
54.55	3.250710

57.58	3.263642
60.61	3.276405
63.64	3.288974
66.67	3.301323
69.70	3.313430
72.73	3.325273
75.76	3.336834
78.79	3.348097
81.82	3.359049
84.85	3.369679
87.88	3.379981
90.91	3.389948
93.94	3.399576
96.97	3.408865
100.00	3.417815
103.03	3.426428
106.06	3.434706
109.09	3.442655
112.12	3.450279
115.15	3.457585
118.18	3.464579
121.21	3.471269
124.24	3.477661
127.27	3.483765
130.30	3.489587
133.33	3.495137
136.36	3.500422
139.39	3.505451
142.42	3.510231
145.45	3.514771
148.48	3.519079
151.52	3.523163
154.55	3.527029
157.58	3.530686
160.61	3.534141
163.64	3.537400
166.67	3.540471
169.70	3.543360
172.73	3.546073
175.76	3.548617
178.79	3.550997
181.82	3.553219
184.85	3.555288
187.88	3.557211
190.91	3.558991
193.94	3.560635
196.97	3.562146
200.00	3.563529
203.03	3.564789
206.06	3.565930
209.09	3.566956
212.12	3.567871
215.15	3.568678
218.18	3.569382
221.21	3.569986
224.24	3.570493
227.27	3.570907

230.30	3.571230
233.33	3.571466
236.36	3.571618
239.39	3.571688
242.42	3.571680
245.45	3.571596
248.48	3.571439
251.52	3.571211
254.55	3.570914
257.58	3.570552
260.61	3.570125
263.64	3.569637
266.67	3.569090
269.70	3.568485
272.73	3.567824
275.76	3.567111
278.79	3.566345
281.82	3.565530
284.85	3.564667
287.88	3.563758
290.91	3.562804
293.94	3.561807
296.97	3.560768
300.00	3.559690

Table S204. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex B0 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	2.030350
6.06	2.086444
9.09	2.140679
12.12	2.194530
15.15	2.247737
18.18	2.299493
21.21	2.348829
24.24	2.394927
27.27	2.437256
30.30	2.475581
33.33	2.509910
36.36	2.540417
39.39	2.567380
42.42	2.591128
45.45	2.612005
48.48	2.630346
51.52	2.646467
54.55	2.660652
57.58	2.673158
60.61	2.684208
63.64	2.694000
66.67	2.702704
69.70	2.710468
72.73	2.717418
75.76	2.723663
78.79	2.729299

81.82	2.734404
84.85	2.739049
87.88	2.743294
90.91	2.747190
93.94	2.750782
96.97	2.754108
100.00	2.757202
103.03	2.760092
106.06	2.762804
109.09	2.765360
112.12	2.767778
115.15	2.770075
118.18	2.772266
121.21	2.774364
124.24	2.776379
127.27	2.778322
130.30	2.780201
133.33	2.782024
136.36	2.783797
139.39	2.785527
142.42	2.787218
145.45	2.788876
148.48	2.790504
151.52	2.792106
154.55	2.793685
157.58	2.795245
160.61	2.796788
163.64	2.798315
166.67	2.799830
169.70	2.801334
172.73	2.802828
175.76	2.804315
178.79	2.805795
181.82	2.807269
184.85	2.808739
187.88	2.810205
190.91	2.811668
193.94	2.813129
196.97	2.814589
200.00	2.816048
203.03	2.817507
206.06	2.818966
209.09	2.820425
212.12	2.821886
215.15	2.823347
218.18	2.824810
221.21	2.826275
224.24	2.827741
227.27	2.829210
230.30	2.830681
233.33	2.832155
236.36	2.833630
239.39	2.835109
242.42	2.836590
245.45	2.838074
248.48	2.839561
251.52	2.841050

254.55	2.842542
257.58	2.844037
260.61	2.845535
263.64	2.847036
266.67	2.848539
269.70	2.850045
272.73	2.851554
275.76	2.853066
278.79	2.854580
281.82	2.856097
284.85	2.857616
287.88	2.859138
290.91	2.860662
293.94	2.862189
296.97	2.863718
300.00	2.865249

Table S205. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex C0 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	1.860519
6.06	2.020654
9.09	2.165321
12.12	2.281847
15.15	2.369048
18.18	2.432515
21.21	2.478644
24.24	2.512562
27.27	2.537940
30.30	2.557305
33.33	2.572384
36.36	2.584360
39.39	2.594055
42.42	2.602050
45.45	2.608757
48.48	2.614477
51.52	2.619432
54.55	2.623786
57.58	2.627664
60.61	2.631161
63.64	2.634351
66.67	2.637291
69.70	2.640026
72.73	2.642592
75.76	2.645019
78.79	2.647329
81.82	2.649540
84.85	2.651670
87.88	2.653729
90.91	2.655730
93.94	2.657680
96.97	2.659587
100.00	2.661456
103.03	2.663294

106.06	2.665105
109.09	2.666892
112.12	2.668658
115.15	2.670406
118.18	2.672139
121.21	2.673859
124.24	2.675566
127.27	2.677264
130.30	2.678952
133.33	2.680633
136.36	2.682307
139.39	2.683975
142.42	2.685638
145.45	2.687297
148.48	2.688951
151.52	2.690602
154.55	2.692250
157.58	2.693895
160.61	2.695539
163.64	2.697180
166.67	2.698820
169.70	2.700458
172.73	2.702095
175.76	2.703732
178.79	2.705367
181.82	2.707002
184.85	2.708636
187.88	2.710270
190.91	2.711903
193.94	2.713537
196.97	2.715170
200.00	2.716803
203.03	2.718436
206.06	2.720070
209.09	2.721703
212.12	2.723337
215.15	2.724970
218.18	2.726605
221.21	2.728239
224.24	2.729873
227.27	2.731508
230.30	2.733144
233.33	2.734779
236.36	2.736415
239.39	2.738052
242.42	2.739689
245.45	2.741326
248.48	2.742964
251.52	2.744602
254.55	2.746240
257.58	2.747879
260.61	2.749519
263.64	2.751159
266.67	2.752799
269.70	2.754440
272.73	2.756081
275.76	2.757722

278.79	2.759364
281.82	2.761007
284.85	2.762650
287.88	2.764293
290.91	2.765937
293.94	2.767581
296.97	2.769225
300.00	2.770870

Table S206. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex A2 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	2.495292
6.06	2.524045
9.09	2.549874
12.12	2.575270
15.15	2.600540
18.18	2.625757
21.21	2.650927
24.24	2.676017
27.27	2.700952
30.30	2.725620
33.33	2.749890
36.36	2.773623
39.39	2.796683
42.42	2.818952
45.45	2.840329
48.48	2.860740
51.52	2.880132
54.55	2.898473
57.58	2.915752
60.61	2.931975
63.64	2.947161
66.67	2.961338
69.70	2.974545
72.73	2.986825
75.76	2.998226
78.79	3.008799
81.82	3.018593
84.85	3.027660
87.88	3.036049
90.91	3.043810
93.94	3.050989
96.97	3.057631
100.00	3.063777
103.03	3.069468
106.06	3.074741
109.09	3.079630
112.12	3.084167
115.15	3.088383
118.18	3.092306
121.21	3.095960
124.24	3.099370
127.27	3.102557

130.30	3.105540
133.33	3.108340
136.36	3.110971
139.39	3.113449
142.42	3.115789
145.45	3.118003
148.48	3.120103
151.52	3.122100
154.55	3.124003
157.58	3.125822
160.61	3.127564
163.64	3.129237
166.67	3.130847
169.70	3.132401
172.73	3.133904
175.76	3.135362
178.79	3.136778
181.82	3.138158
184.85	3.139504
187.88	3.140821
190.91	3.142111
193.94	3.143376
196.97	3.144621
200.00	3.145846
203.03	3.147054
206.06	3.148247
209.09	3.149425
212.12	3.150592
215.15	3.151747
218.18	3.152893
221.21	3.154030
224.24	3.155158
227.27	3.156280
230.30	3.157395
233.33	3.158504
236.36	3.159607
239.39	3.160705
242.42	3.161799
245.45	3.162888
248.48	3.163973
251.52	3.165054
254.55	3.166131
257.58	3.167204
260.61	3.168274
263.64	3.169340
266.67	3.170402
269.70	3.171461
272.73	3.172516
275.76	3.173567
278.79	3.174614
281.82	3.175658
284.85	3.176697
287.88	3.177732
290.91	3.178762
293.94	3.179788
296.97	3.180809
300.00	3.181826

Table S207. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex B2 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	2.013026
6.06	2.076995
9.09	2.139121
12.12	2.200678
15.15	2.260941
18.18	2.318596
21.21	2.372389
24.24	2.421474
27.27	2.465478
30.30	2.504413
33.33	2.538551
36.36	2.568308
39.39	2.594159
42.42	2.616587
45.45	2.636049
48.48	2.652960
51.52	2.667689
54.55	2.680554
57.58	2.691832
60.61	2.701756
63.64	2.710527
66.67	2.718313
69.70	2.725257
72.73	2.731481
75.76	2.737087
78.79	2.742162
81.82	2.746779
84.85	2.751002
87.88	2.754884
90.91	2.758470
93.94	2.761799
96.97	2.764906
100.00	2.767819
103.03	2.770562
106.06	2.773157
109.09	2.775623
112.12	2.777976
115.15	2.780230
118.18	2.782397
121.21	2.784487
124.24	2.786510
127.27	2.788474
130.30	2.790386
133.33	2.792253
136.36	2.794080
139.39	2.795871
142.42	2.797632
145.45	2.799365
148.48	2.801075
151.52	2.802764

154.55	2.804435
157.58	2.806089
160.61	2.807731
163.64	2.809360
166.67	2.810979
169.70	2.812589
172.73	2.814191
175.76	2.815788
178.79	2.817379
181.82	2.818965
184.85	2.820548
187.88	2.822128
190.91	2.823706
193.94	2.825282
196.97	2.826858
200.00	2.828432
203.03	2.830006
206.06	2.831581
209.09	2.833156
212.12	2.834732
215.15	2.836308
218.18	2.837886
221.21	2.839465
224.24	2.841046
227.27	2.842629
230.30	2.844213
233.33	2.845800
236.36	2.847388
239.39	2.848978
242.42	2.850571
245.45	2.852166
248.48	2.853763
251.52	2.855363
254.55	2.856964
257.58	2.858568
260.61	2.860175
263.64	2.861783
266.67	2.863394
269.70	2.865008
272.73	2.866623
275.76	2.868241
278.79	2.869861
281.82	2.871483
284.85	2.873107
287.88	2.874734
290.91	2.876362
293.94	2.877992
296.97	2.879625
300.00	2.881259

Table S208. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex B2' measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	1.912840

6.06	1.977923
9.09	2.041467
12.12	2.104490
15.15	2.166241
18.18	2.225390
21.21	2.280657
24.24	2.331171
27.27	2.376534
30.30	2.416740
33.33	2.452051
36.36	2.482877
39.39	2.509694
42.42	2.532990
45.45	2.553228
48.48	2.570829
51.52	2.586168
54.55	2.599573
57.58	2.611326
60.61	2.621668
63.64	2.630804
66.67	2.638908
69.70	2.646130
72.73	2.652593
75.76	2.658405
78.79	2.663655
81.82	2.668420
84.85	2.672767
87.88	2.676750
90.91	2.680417
93.94	2.683810
96.97	2.686963
100.00	2.689908
103.03	2.692669
106.06	2.695270
109.09	2.697730
112.12	2.700066
115.15	2.702294
118.18	2.704426
121.21	2.706473
124.24	2.708445
127.27	2.710352
130.30	2.712200
133.33	2.713997
136.36	2.715748
139.39	2.717459
142.42	2.719135
145.45	2.720778
148.48	2.722394
151.52	2.723985
154.55	2.725554
157.58	2.727104
160.61	2.728637
163.64	2.730155
166.67	2.731660
169.70	2.733154
172.73	2.734637
175.76	2.736112

178.79	2.737579
181.82	2.739040
184.85	2.740496
187.88	2.741946
190.91	2.743393
193.94	2.744836
196.97	2.746277
200.00	2.747715
203.03	2.749152
206.06	2.750588
209.09	2.752023
212.12	2.753457
215.15	2.754891
218.18	2.756326
221.21	2.757760
224.24	2.759196
227.27	2.760632
230.30	2.762069
233.33	2.763507
236.36	2.764946
239.39	2.766387
242.42	2.767829
245.45	2.769273
248.48	2.770719
251.52	2.772166
254.55	2.773615
257.58	2.775065
260.61	2.776518
263.64	2.777972
266.67	2.779428
269.70	2.780886
272.73	2.782346
275.76	2.783808
278.79	2.785272
281.82	2.786737
284.85	2.788205
287.88	2.789674
290.91	2.791145
293.94	2.792618
296.97	2.794093
300.00	2.795569

Table S209. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex C2 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	1.791632
6.06	1.920195
9.09	2.044314
12.12	2.156851
15.15	2.252067
18.18	2.329059
21.21	2.389898
24.24	2.437593
27.27	2.475030

30.30	2.504611
33.33	2.528207
36.36	2.547241
39.39	2.562775
42.42	2.575608
45.45	2.586337
48.48	2.595413
51.52	2.603180
54.55	2.609901
57.58	2.615779
60.61	2.620975
63.64	2.625611
66.67	2.629789
69.70	2.633586
72.73	2.637066
75.76	2.640282
78.79	2.643274
81.82	2.646078
84.85	2.648721
87.88	2.651228
90.91	2.653618
93.94	2.655907
96.97	2.658110
100.00	2.660238
103.03	2.662302
106.06	2.664308
109.09	2.666266
112.12	2.668181
115.15	2.670058
118.18	2.671902
121.21	2.673717
124.24	2.675507
127.27	2.677274
130.30	2.679021
133.33	2.680751
136.36	2.682465
139.39	2.684166
142.42	2.685855
145.45	2.687532
148.48	2.689201
151.52	2.690860
154.55	2.692513
157.58	2.694158
160.61	2.695798
163.64	2.697433
166.67	2.699063
169.70	2.700689
172.73	2.702311
175.76	2.703930
178.79	2.705547
181.82	2.707161
184.85	2.708773
187.88	2.710383
190.91	2.711991
193.94	2.713599
196.97	2.715204
200.00	2.716809

203.03	2.718414
206.06	2.720017
209.09	2.721620
212.12	2.723222
215.15	2.724825
218.18	2.726427
221.21	2.728028
224.24	2.729630
227.27	2.731232
230.30	2.732834
233.33	2.734436
236.36	2.736038
239.39	2.737640
242.42	2.739243
245.45	2.740846
248.48	2.742449
251.52	2.744052
254.55	2.745656
257.58	2.747261
260.61	2.748866
263.64	2.750471
266.67	2.752076
269.70	2.753683
272.73	2.755289
275.76	2.756896
278.79	2.758504
281.82	2.760112
284.85	2.761721
287.88	2.763330
290.91	2.764939
293.94	2.766549
296.97	2.768160
300.00	2.769771

Table S210. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex A4 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	2.350467
6.06	2.384771
9.09	2.416495
12.12	2.447835
15.15	2.479060
18.18	2.510204
21.21	2.541202
24.24	2.571903
27.27	2.602097
30.30	2.631546
33.33	2.660019
36.36	2.687316
39.39	2.713280
42.42	2.737802
45.45	2.760817
48.48	2.782303
51.52	2.802268

54.55	2.820750
57.58	2.837805
60.61	2.853503
63.64	2.867922
66.67	2.881147
69.70	2.893264
72.73	2.904356
75.76	2.914507
78.79	2.923796
81.82	2.932299
84.85	2.940084
87.88	2.947218
90.91	2.953761
93.94	2.959769
96.97	2.965292
100.00	2.970378
103.03	2.975068
106.06	2.979401
109.09	2.983413
112.12	2.987135
115.15	2.990595
118.18	2.993820
121.21	2.996834
124.24	2.999657
127.27	3.002308
130.30	3.004806
133.33	3.007166
136.36	3.009401
139.39	3.011524
142.42	3.013548
145.45	3.015483
148.48	3.017337
151.52	3.019120
154.55	3.020839
157.58	3.022501
160.61	3.024112
163.64	3.025678
166.67	3.027204
169.70	3.028695
172.73	3.030154
175.76	3.031586
178.79	3.032994
181.82	3.034381
184.85	3.035749
187.88	3.037102
190.91	3.038441
193.94	3.039768
196.97	3.041086
200.00	3.042395
203.03	3.043697
206.06	3.044994
209.09	3.046286
212.12	3.047575
215.15	3.048862
218.18	3.050146
221.21	3.051429
224.24	3.052712

227.27	3.053995
230.30	3.055278
233.33	3.056562
236.36	3.057847
239.39	3.059134
242.42	3.060422
245.45	3.061712
248.48	3.063003
251.52	3.064297
254.55	3.065592
257.58	3.066890
260.61	3.068189
263.64	3.069491
266.67	3.070794
269.70	3.072099
272.73	3.073406
275.76	3.074714
278.79	3.076024
281.82	3.077335
284.85	3.078648
287.88	3.079961
290.91	3.081275
293.94	3.082590
296.97	3.083905
300.00	3.085221

Table S211. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex B4 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	1.941486
6.06	2.011680
9.09	2.080200
12.12	2.147920
15.15	2.213627
18.18	2.275604
21.21	2.332454
24.24	2.383415
27.27	2.428323
30.30	2.467429
33.33	2.501225
36.36	2.530309
39.39	2.555297
42.42	2.576769
45.45	2.595251
48.48	2.611201
51.52	2.625014
54.55	2.637025
57.58	2.647516
60.61	2.656723
63.64	2.664844
66.67	2.672045
69.70	2.678464
72.73	2.684217
75.76	2.689401

78.79	2.694099
81.82	2.698378
84.85	2.702299
87.88	2.705910
90.91	2.709253
93.94	2.712364
96.97	2.715273
100.00	2.718008
103.03	2.720590
106.06	2.723038
109.09	2.725371
112.12	2.727601
115.15	2.729743
118.18	2.731806
121.21	2.733800
124.24	2.735733
127.27	2.737614
130.30	2.739447
133.33	2.741239
136.36	2.742995
139.39	2.744719
142.42	2.746415
145.45	2.748086
148.48	2.749735
151.52	2.751365
154.55	2.752978
157.58	2.754577
160.61	2.756163
163.64	2.757737
166.67	2.759302
169.70	2.760858
172.73	2.762407
175.76	2.763950
178.79	2.765488
181.82	2.767021
184.85	2.768551
187.88	2.770077
190.91	2.771601
193.94	2.773123
196.97	2.774643
200.00	2.776163
203.03	2.777682
206.06	2.779200
209.09	2.780718
212.12	2.782237
215.15	2.783756
218.18	2.785276
221.21	2.786796
224.24	2.788318
227.27	2.789841
230.30	2.791365
233.33	2.792890
236.36	2.794417
239.39	2.795946
242.42	2.797476
245.45	2.799008
248.48	2.800541

251.52	2.802077
254.55	2.803614
257.58	2.805153
260.61	2.806694
263.64	2.808236
266.67	2.809781
269.70	2.811327
272.73	2.812876
275.76	2.814426
278.79	2.815978
281.82	2.817532
284.85	2.819087
287.88	2.820645
290.91	2.822204
293.94	2.823765
296.97	2.825327
300.00	2.826892

Table S212. Ab initio calculated temperature-dependent magnetic susceptibility for S=3/2 ground state of Complex C4 measured at 1000 Oe with the def2-TZVP basis set.

Temperature (K)	chi*T (cm3*K/mol)
3.03	1.855632
6.06	1.986006
9.09	2.109712
12.12	2.218373
15.15	2.307027
18.18	2.376349
21.21	2.429596
24.24	2.470386
27.27	2.501820
30.30	2.526299
33.33	2.545609
36.36	2.561055
39.39	2.573586
42.42	2.583898
45.45	2.592502
48.48	2.599779
51.52	2.606015
54.55	2.611426
57.58	2.616178
60.61	2.620399
63.64	2.624190
66.67	2.627628
69.70	2.630777
72.73	2.633687
75.76	2.636397
78.79	2.638940
81.82	2.641344
84.85	2.643629
87.88	2.645814
90.91	2.647914
93.94	2.649941
96.97	2.651905
100.00	2.653817

103.03	2.655682
106.06	2.657508
109.09	2.659299
112.12	2.661060
115.15	2.662796
118.18	2.664509
121.21	2.666203
124.24	2.667880
127.27	2.669542
130.30	2.671191
133.33	2.672829
136.36	2.674457
139.39	2.676076
142.42	2.677688
145.45	2.679293
148.48	2.680893
151.52	2.682488
154.55	2.684079
157.58	2.685666
160.61	2.687249
163.64	2.688830
166.67	2.690409
169.70	2.691986
172.73	2.693561
175.76	2.695135
178.79	2.696707
181.82	2.698279
184.85	2.699850
187.88	2.701421
190.91	2.702991
193.94	2.704561
196.97	2.706130
200.00	2.707700
203.03	2.709270
206.06	2.710840
209.09	2.712410
212.12	2.713981
215.15	2.715552
218.18	2.717123
221.21	2.718695
224.24	2.720267
227.27	2.721840
230.30	2.723413
233.33	2.724987
236.36	2.726561
239.39	2.728136
242.42	2.729712
245.45	2.731289
248.48	2.732866
251.52	2.734443
254.55	2.736022
257.58	2.737601
260.61	2.739180
263.64	2.740761
266.67	2.742342
269.70	2.743923
272.73	2.745506

275.76	2.747089
278.79	2.748672
281.82	2.750257
284.85	2.751841
287.88	2.753427
290.91	2.755013
293.94	2.756600
296.97	2.758188
300.00	2.759776

Table S213. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex A0 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	0.000000
808.08	0.217611
1616.16	0.430705
2424.24	0.635199
3232.32	0.827786
4040.40	1.006128
4848.48	1.168880
5656.57	1.315596
6464.65	1.446548
7272.73	1.562526
8080.81	1.664650
8888.89	1.754208
9696.97	1.832542
10505.05	1.900966
11313.13	1.960713
12121.21	2.012909
12929.29	2.058563
13737.37	2.098565
14545.45	2.133691
15353.54	2.164614
16161.62	2.191912
16969.70	2.216083
17777.78	2.237553
18585.86	2.256686
19393.94	2.273793
20202.02	2.289140
21010.10	2.302954
21818.18	2.315430
22626.26	2.326735
23434.34	2.337013
24242.42	2.346387
25050.51	2.354964
25858.59	2.362835
26666.67	2.370079
27474.75	2.376767
28282.83	2.382958
29090.91	2.388704
29898.99	2.394052
30707.07	2.399041
31515.15	2.403707
32323.23	2.408081
33131.31	2.412191

33939.39	2.416060
34747.47	2.419710
35555.56	2.423162
36363.64	2.426430
37171.72	2.429532
37979.80	2.432480
38787.88	2.435288
39595.96	2.437965
40404.04	2.440523
41212.12	2.442969
42020.20	2.445313
42828.28	2.447562
43636.36	2.449722
44444.44	2.451799
45252.53	2.453800
46060.61	2.455730
46868.69	2.457592
47676.77	2.459392
48484.85	2.461133
49292.93	2.462820
50101.01	2.464455
50909.09	2.466041
51717.17	2.467582
52525.25	2.469080
53333.33	2.470538
54141.41	2.471958
54949.49	2.473341
55757.58	2.474691
56565.66	2.476009
57373.74	2.477296
58181.82	2.478555
58989.90	2.479786
59797.98	2.480991
60606.06	2.482173
61414.14	2.483331
62222.22	2.484466
63030.30	2.485581
63838.38	2.486676
64646.46	2.487753
65454.55	2.488811
66262.63	2.489852
67070.71	2.490876
67878.79	2.491885
68686.87	2.492879
69494.95	2.493859
70303.03	2.494826
71111.11	2.495780
71919.19	2.496721
72727.27	2.497651
73535.35	2.498569
74343.43	2.499477
75151.52	2.500374
75959.60	2.501261
76767.68	2.502139
77575.76	2.503009
78383.84	2.503869
79191.92	2.504721

80000.00	2.505565

Table S214. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex B0 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	0.000000
808.08	0.145450
1616.16	0.288951
2424.24	0.428676
3232.32	0.563032
4040.40	0.690730
4848.48	0.810827
5656.57	0.922724
6464.65	1.026143
7272.73	1.121076
8080.81	1.207734
8888.89	1.286487
9696.97	1.357813
10505.05	1.422254
11313.13	1.480383
12121.21	1.532771
12929.29	1.579976
13737.37	1.622524
14545.45	1.660907
15353.54	1.695575
16161.62	1.726936
16969.70	1.755359
17777.78	1.781172
18585.86	1.804670
19393.94	1.826113
20202.02	1.845730
21010.10	1.863727
21818.18	1.880282
22626.26	1.895553
23434.34	1.909680
24242.42	1.922785
25050.51	1.934978
25858.59	1.946353
26666.67	1.956994
27474.75	1.966977
28282.83	1.976367
29090.91	1.985222
29898.99	1.993594
30707.07	2.001528
31515.15	2.009067
32323.23	2.016244
33131.31	2.023095
33939.39	2.029646
34747.47	2.035924
35555.56	2.041953
36363.64	2.047752
37171.72	2.053341
37979.80	2.058736
38787.88	2.063954
39595.96	2.069006

40404.04	2.073906
41212.12	2.078666
42020.20	2.083294
42828.28	2.087802
43636.36	2.092196
44444.44	2.096485
45252.53	2.100676
46060.61	2.104775
46868.69	2.108788
47676.77	2.112721
48484.85	2.116578
49292.93	2.120364
50101.01	2.124084
50909.09	2.127741
51717.17	2.131339
52525.25	2.134881
53333.33	2.138370
54141.41	2.141809
54949.49	2.145201
55757.58	2.148548
56565.66	2.151853
57373.74	2.155117
58181.82	2.158343
58989.90	2.161533
59797.98	2.164687
60606.06	2.167809
61414.14	2.170899
62222.22	2.173959
63030.30	2.176989
63838.38	2.179993
64646.46	2.182970
65454.55	2.185921
66262.63	2.188848
67070.71	2.191752
67878.79	2.194634
68686.87	2.197494
69494.95	2.200334
70303.03	2.203153
71111.11	2.205954
71919.19	2.208736
72727.27	2.211501
73535.35	2.214248
74343.43	2.216979
75151.52	2.219694
75959.60	2.222393
76767.68	2.225078
77575.76	2.227748
78383.84	2.230404
79191.92	2.233047
80000.00	2.235677

Table S215. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex C0 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	-0.000000

808.08	0.130581
1616.16	0.259695
2424.24	0.385959
3232.32	0.508140
4040.40	0.625212
4848.48	0.736385
5656.57	0.841113
6464.65	0.939084
7272.73	1.030192
8080.81	1.114505
8888.89	1.192228
9696.97	1.263664
10505.05	1.329186
11313.13	1.389204
12121.21	1.444147
12929.29	1.494447
13737.37	1.540520
14545.45	1.582767
15353.54	1.621560
16161.62	1.657246
16969.70	1.690141
17777.78	1.720535
18585.86	1.748689
19393.94	1.774835
20202.02	1.799187
21010.10	1.821930
21818.18	1.843233
22626.26	1.863245
23434.34	1.882099
24242.42	1.899914
25050.51	1.916794
25858.59	1.932833
26666.67	1.948114
27474.75	1.962710
28282.83	1.976688
29090.91	1.990106
29898.99	2.003016
30707.07	2.015465
31515.15	2.027494
32323.23	2.039141
33131.31	2.050440
33939.39	2.061419
34747.47	2.072105
35555.56	2.082524
36363.64	2.092696
37171.72	2.102642
37979.80	2.112378
38787.88	2.121921
39595.96	2.131285
40404.04	2.140484
41212.12	2.149530
42020.20	2.158432
42828.28	2.167202
43636.36	2.175847
44444.44	2.184377
45252.53	2.192799
46060.61	2.201120

46868.69	2.209346
47676.77	2.217483
48484.85	2.225536
49292.93	2.233511
50101.01	2.241411
50909.09	2.249242
51717.17	2.257006
52525.25	2.264708
53333.33	2.272351
54141.41	2.279938
54949.49	2.287472
55757.58	2.294956
56565.66	2.302391
57373.74	2.309781
58181.82	2.317128
58989.90	2.324433
59797.98	2.331699
60606.06	2.338927
61414.14	2.346118
62222.22	2.353275
63030.30	2.360399
63838.38	2.367491
64646.46	2.374552
65454.55	2.381583
66262.63	2.388586
67070.71	2.395562
67878.79	2.402510
68686.87	2.409433
69494.95	2.416331
70303.03	2.423205
71111.11	2.430055
71919.19	2.436882
72727.27	2.443686
73535.35	2.450468
74343.43	2.457229
75151.52	2.463968
75959.60	2.470687
76767.68	2.477385
77575.76	2.484062
78383.84	2.490719
79191.92	2.497357
80000.00	2.503974

Table S216. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex A2 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	-0.000000
808.08	0.179728
1616.16	0.356393
2424.24	0.527178
3232.32	0.689709
4040.40	0.842185
4848.48	0.983418
5656.57	1.112811
6464.65	1.230268

7272.73	1.336095
8080.81	1.430882
8888.89	1.515402
9696.97	1.590529
10505.05	1.657169
11313.13	1.716215
12121.21	1.768516
12929.29	1.814861
13737.37	1.855967
14545.45	1.892477
15353.54	1.924965
16161.62	1.953934
16969.70	1.979828
17777.78	2.003033
18585.86	2.023885
19393.94	2.042676
20202.02	2.059660
21010.10	2.075058
21818.18	2.089059
22626.26	2.101830
23434.34	2.113514
24242.42	2.124236
25050.51	2.134106
25858.59	2.143218
26666.67	2.151654
27474.75	2.159487
28282.83	2.166781
29090.91	2.173591
29898.99	2.179966
30707.07	2.185948
31515.15	2.191577
32323.23	2.196885
33131.31	2.201903
33939.39	2.206656
34747.47	2.211168
35555.56	2.215461
36363.64	2.219553
37171.72	2.223461
37979.80	2.227199
38787.88	2.230783
39595.96	2.234222
40404.04	2.237530
41212.12	2.240715
42020.20	2.243787
42828.28	2.246753
43636.36	2.249622
44444.44	2.252400
45252.53	2.255093
46060.61	2.257707
46868.69	2.260247
47676.77	2.262719
48484.85	2.265125
49292.93	2.267470
50101.01	2.269759
50909.09	2.271994
51717.17	2.274178
52525.25	2.276315

53333.33	2.278408
54141.41	2.280457
54949.49	2.282467
55757.58	2.284439
56565.66	2.286376
57373.74	2.288278
58181.82	2.290148
58989.90	2.291988
59797.98	2.293799
60606.06	2.295583
61414.14	2.297340
62222.22	2.299073
63030.30	2.300781
63838.38	2.302468
64646.46	2.304133
65454.55	2.305777
66262.63	2.307402
67070.71	2.309008
67878.79	2.310597
68686.87	2.312168
69494.95	2.313723
70303.03	2.315263
71111.11	2.316788
71919.19	2.318298
72727.27	2.319795
73535.35	2.321279
74343.43	2.322750
75151.52	2.324209
75959.60	2.325656
76767.68	2.327092
77575.76	2.328518
78383.84	2.329934
79191.92	2.331339
80000.00	2.332735

Table S217. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex B2 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	0.000000
808.08	0.144004
1616.16	0.286092
2424.24	0.424469
3232.32	0.557566
4040.40	0.684114
4848.48	0.803180
5656.57	0.914171
6464.65	1.016807
7272.73	1.111076
8080.81	1.197178
8888.89	1.275476
9696.97	1.346436
10505.05	1.410590
11313.13	1.468500
12121.21	1.520728
12929.29	1.567824

13737.37	1.610307
14545.45	1.648662
15353.54	1.683333
16161.62	1.714725
16969.70	1.743202
17777.78	1.769090
18585.86	1.792680
19393.94	1.814231
20202.02	1.833969
21010.10	1.852098
21818.18	1.868796
22626.26	1.884219
23434.34	1.898507
24242.42	1.911781
25050.51	1.924148
25858.59	1.935704
26666.67	1.946533
27474.75	1.956708
28282.83	1.966295
29090.91	1.975351
29898.99	1.983929
30707.07	1.992073
31515.15	1.999825
32323.23	2.007220
33131.31	2.014291
33939.39	2.021066
34747.47	2.027571
35555.56	2.033829
36363.64	2.039861
37171.72	2.045684
37979.80	2.051317
38787.88	2.056774
39595.96	2.062069
40404.04	2.067213
41212.12	2.072219
42020.20	2.077096
42828.28	2.081853
43636.36	2.086499
44444.44	2.091042
45252.53	2.095488
46060.61	2.099844
46868.69	2.104115
47676.77	2.108308
48484.85	2.112426
49292.93	2.116476
50101.01	2.120459
50909.09	2.124382
51717.17	2.128246
52525.25	2.132056
53333.33	2.135814
54141.41	2.139524
54949.49	2.143187
55757.58	2.146806
56565.66	2.150385
57373.74	2.153923
58181.82	2.157425
58989.90	2.160891

59797.98	2.164323
60606.06	2.167723
61414.14	2.171092
62222.22	2.174431
63030.30	2.177743
63838.38	2.181028
64646.46	2.184288
65454.55	2.187523
66262.63	2.190735
67070.71	2.193924
67878.79	2.197092
68686.87	2.200239
69494.95	2.203366
70303.03	2.206474
71111.11	2.209563
71919.19	2.212635
72727.27	2.215691
73535.35	2.218729
74343.43	2.221752
75151.52	2.224760
75959.60	2.227753
76767.68	2.230732
77575.76	2.233697
78383.84	2.236649
79191.92	2.239588
80000.00	2.242515

Table S218. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex B2' at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	-0.000000
808.08	0.136738
1616.16	0.271875
2424.24	0.403901
3232.32	0.531477
4040.40	0.653489
4848.48	0.769088
5656.57	0.877690
6464.65	0.978969
7272.73	1.072824
8080.81	1.159342
8888.89	1.238754
9696.97	1.311400
10505.05	1.377688
11313.13	1.438070
12121.21	1.493012
12929.29	1.542979
13737.37	1.588423
14545.45	1.629773
15353.54	1.667431
16161.62	1.701766
16969.70	1.733118
17777.78	1.761795
18585.86	1.788073
19393.94	1.812202

20202.02	1.834407
21010.10	1.854885
21818.18	1.873816
22626.26	1.891357
23434.34	1.907649
24242.42	1.922818
25050.51	1.936974
25858.59	1.950218
26666.67	1.962636
27474.75	1.974307
28282.83	1.985302
29090.91	1.995682
29898.99	2.005504
30707.07	2.014815
31515.15	2.023663
32323.23	2.032085
33131.31	2.040119
33939.39	2.047795
34747.47	2.055144
35555.56	2.062191
36363.64	2.068959
37171.72	2.075471
37979.80	2.081745
38787.88	2.087800
39595.96	2.093650
40404.04	2.099311
41212.12	2.104796
42020.20	2.110116
42828.28	2.115284
43636.36	2.120308
44444.44	2.125199
45252.53	2.129965
46060.61	2.134614
46868.69	2.139152
47676.77	2.143587
48484.85	2.147925
49292.93	2.152172
50101.01	2.156333
50909.09	2.160412
51717.17	2.164414
52525.25	2.168345
53333.33	2.172206
54141.41	2.176003
54949.49	2.179739
55757.58	2.183417
56565.66	2.187039
57373.74	2.190609
58181.82	2.194129
58989.90	2.197602
59797.98	2.201030
60606.06	2.204415
61414.14	2.207760
62222.22	2.211065
63030.30	2.214334
63838.38	2.217567
64646.46	2.220766
65454.55	2.223933

66262.63	2.227069
67070.71	2.230176
67878.79	2.233255
68686.87	2.236306
69494.95	2.239332
70303.03	2.242332
71111.11	2.245309
71919.19	2.248263
72727.27	2.251195
73535.35	2.254106
74343.43	2.256996
75151.52	2.259867
75959.60	2.262720
76767.68	2.265554
77575.76	2.268370
78383.84	2.271170
79191.92	2.273954
80000.00	2.276722

Table S219. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex C2 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	0.000000
808.08	0.126418
1616.16	0.251745
2424.24	0.374937
3232.32	0.495039
4040.40	0.611215
4848.48	0.722779
5656.57	0.829198
6464.65	0.930098
7272.73	1.025251
8080.81	1.114567
8888.89	1.198066
9696.97	1.275864
10505.05	1.348150
11313.13	1.415166
12121.21	1.477192
12929.29	1.534529
13737.37	1.587488
14545.45	1.636384
15353.54	1.681523
16161.62	1.723203
16969.70	1.761707
17777.78	1.797302
18585.86	1.830235
19393.94	1.860740
20202.02	1.889029
21010.10	1.915299
21818.18	1.939730
22626.26	1.962485
23434.34	1.983715
24242.42	2.003556
25050.51	2.022132
25858.59	2.039554

26666.67	2.055925
27474.75	2.071338
28282.83	2.085876
29090.91	2.099615
29898.99	2.112623
30707.07	2.124964
31515.15	2.136694
32323.23	2.147865
33131.31	2.158522
33939.39	2.168708
34747.47	2.178462
35555.56	2.187819
36363.64	2.196810
37171.72	2.205464
37979.80	2.213809
38787.88	2.221866
39595.96	2.229660
40404.04	2.237209
41212.12	2.244532
42020.20	2.251645
42828.28	2.258564
43636.36	2.265303
44444.44	2.271874
45252.53	2.278289
46060.61	2.284559
46868.69	2.290694
47676.77	2.296702
48484.85	2.302593
49292.93	2.308372
50101.01	2.314049
50909.09	2.319628
51717.17	2.325117
52525.25	2.330520
53333.33	2.335842
54141.41	2.341088
54949.49	2.346263
55757.58	2.351370
56565.66	2.356414
57373.74	2.361396
58181.82	2.366322
58989.90	2.371192
59797.98	2.376011
60606.06	2.380781
61414.14	2.385503
62222.22	2.390181
63030.30	2.394816
63838.38	2.399409
64646.46	2.403964
65454.55	2.408480
66262.63	2.412961
67070.71	2.417407
67878.79	2.421819
68686.87	2.426198
69494.95	2.430547
70303.03	2.434865
71111.11	2.439155
71919.19	2.443416

72727.27	2.447650
73535.35	2.451857
74343.43	2.456038
75151.52	2.460195
75959.60	2.464327
76767.68	2.468435
77575.76	2.472520
78383.84	2.476583
79191.92	2.480623
80000.00	2.484642

Table S220. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex A4 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	0.000000
808.08	0.169124
1616.16	0.335541
2424.24	0.496748
3232.32	0.650614
4040.40	0.795492
4848.48	0.930260
5656.57	1.054306
6464.65	1.167467
7272.73	1.269942
8080.81	1.362195
8888.89	1.444873
9696.97	1.518725
10505.05	1.584548
11313.13	1.643137
12121.21	1.695262
12929.29	1.741643
13737.37	1.782945
14545.45	1.819768
15353.54	1.852651
16161.62	1.882072
16969.70	1.908455
17777.78	1.932170
18585.86	1.953543
19393.94	1.972858
20202.02	1.990362
21010.10	2.006272
21818.18	2.020776
22626.26	2.034037
23434.34	2.046199
24242.42	2.057386
25050.51	2.067707
25858.59	2.077257
26666.67	2.086119
27474.75	2.094366
28282.83	2.102062
29090.91	2.109263
29898.99	2.116019
30707.07	2.122374
31515.15	2.128366
32323.23	2.134030

33131.31	2.139395
33939.39	2.144490
34747.47	2.149338
35555.56	2.153960
36363.64	2.158375
37171.72	2.162602
37979.80	2.166655
38787.88	2.170548
39595.96	2.174294
40404.04	2.177904
41212.12	2.181389
42020.20	2.184757
42828.28	2.188016
43636.36	2.191176
44444.44	2.194242
45252.53	2.197221
46060.61	2.200118
46868.69	2.202940
47676.77	2.205691
48484.85	2.208375
49292.93	2.210997
50101.01	2.213560
50909.09	2.216067
51717.17	2.218523
52525.25	2.220930
53333.33	2.223291
54141.41	2.225608
54949.49	2.227884
55757.58	2.230122
56565.66	2.232322
57373.74	2.234487
58181.82	2.236620
58989.90	2.238720
59797.98	2.240791
60606.06	2.242834
61414.14	2.244850
62222.22	2.246840
63030.30	2.248805
63838.38	2.250747
64646.46	2.252667
65454.55	2.254566
66262.63	2.256444
67070.71	2.258304
67878.79	2.260144
68686.87	2.261967
69494.95	2.263773
70303.03	2.265563
71111.11	2.267337
71919.19	2.269097
72727.27	2.270842
73535.35	2.272574
74343.43	2.274292
75151.52	2.275998
75959.60	2.277692
76767.68	2.279374
77575.76	2.281045
78383.84	2.282705

79191.92	2.284355
80000.00	2.285996

Table S221. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex B4 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)
0.00	0.000000
808.08	0.138681
1616.16	0.275653
2424.24	0.409307
3232.32	0.538224
4040.40	0.661239
4848.48	0.777473
5656.57	0.886344
6464.65	0.987543
7272.73	1.081002
8080.81	1.166853
8888.89	1.245374
9696.97	1.316952
10505.05	1.382043
11313.13	1.441138
12121.21	1.494737
12929.29	1.543339
13737.37	1.587419
14545.45	1.627425
15353.54	1.663774
16161.62	1.696849
16969.70	1.726995
17777.78	1.754528
18585.86	1.779727
19393.94	1.802844
20202.02	1.824104
21010.10	1.843705
21818.18	1.861824
22626.26	1.878618
23434.34	1.894225
24242.42	1.908769
25050.51	1.922359
25858.59	1.935090
26666.67	1.947048
27474.75	1.958309
28282.83	1.968940
29090.91	1.979001
29898.99	1.988546
30707.07	1.997620
31515.15	2.006268
32323.23	2.014526
33131.31	2.022429
33939.39	2.030006
34747.47	2.037285
35555.56	2.044290
36363.64	2.051042
37171.72	2.057563
37979.80	2.063869
38787.88	2.069977

39595.96	2.075901
40404.04	2.081654
41212.12	2.087250
42020.20	2.092698
42828.28	2.098009
43636.36	2.103191
44444.44	2.108254
45252.53	2.113204
46060.61	2.118049
46868.69	2.122795
47676.77	2.127449
48484.85	2.132015
49292.93	2.136499
50101.01	2.140905
50909.09	2.145238
51717.17	2.149501
52525.25	2.153699
53333.33	2.157835
54141.41	2.161911
54949.49	2.165932
55757.58	2.169899
56565.66	2.173815
57373.74	2.177684
58181.82	2.181506
58989.90	2.185284
59797.98	2.189021
60606.06	2.192718
61414.14	2.196376
62222.22	2.199998
63030.30	2.203585
63838.38	2.207138
64646.46	2.210659
65454.55	2.214149
66262.63	2.217610
67070.71	2.221042
67878.79	2.224446
68686.87	2.227825
69494.95	2.231178
70303.03	2.234506
71111.11	2.237811
71919.19	2.241093
72727.27	2.244354
73535.35	2.247593
74343.43	2.250812
75151.52	2.254011
75959.60	2.257191
76767.68	2.260352
77575.76	2.263496
78383.84	2.266622
79191.92	2.269732
80000.00	2.272825

Table S222. Ab initio calculated field-dependent molar magnetization for S=3/2 ground state of Complex C4 at 2.0 K with the def2-TZVP basis set.

M. FIELD (Gauss)	M/N (\mu_B)

0.00	-0.000000
808.08	0.130988
1616.16	0.260465
2424.24	0.387007
3232.32	0.509349
4040.40	0.626440
4848.48	0.737476
5656.57	0.841905
6464.65	0.939416
7272.73	1.029915
8080.81	1.113480
8888.89	1.190333
9696.97	1.260793
10505.05	1.325248
11313.13	1.384126
12121.21	1.437870
12929.29	1.486921
13737.37	1.531709
14545.45	1.572643
15353.54	1.610103
16161.62	1.644441
16969.70	1.675980
17777.78	1.705013
18585.86	1.731803
19393.94	1.756587
20202.02	1.779578
21010.10	1.800965
21818.18	1.820916
22626.26	1.839582
23434.34	1.857096
24242.42	1.873577
25050.51	1.889129
25858.59	1.903847
26666.67	1.917812
27474.75	1.931100
28282.83	1.943775
29090.91	1.955896
29898.99	1.967514
30707.07	1.978677
31515.15	1.989426
32323.23	1.999797
33131.31	2.009823
33939.39	2.019536
34747.47	2.028960
35555.56	2.038120
36363.64	2.047038
37171.72	2.055733
37979.80	2.064223
38787.88	2.072522
39595.96	2.080647
40404.04	2.088610
41212.12	2.096422
42020.20	2.104094
42828.28	2.111637
43636.36	2.119058
44444.44	2.126367
45252.53	2.133571

46060.61	2.140677
46868.69	2.147690
47676.77	2.154617
48484.85	2.161463
49292.93	2.168233
50101.01	2.174931
50909.09	2.181562
51717.17	2.188130
52525.25	2.194637
53333.33	2.201088
54141.41	2.207486
54949.49	2.213832
55757.58	2.220131
56565.66	2.226385
57373.74	2.232595
58181.82	2.238765
58989.90	2.244896
59797.98	2.250989
60606.06	2.257048
61414.14	2.263073
62222.22	2.269066
63030.30	2.275028
63838.38	2.280962
64646.46	2.286867
65454.55	2.292746
66262.63	2.298600
67070.71	2.304429
67878.79	2.310235
68686.87	2.316019
69494.95	2.321781
70303.03	2.327522
71111.11	2.333243
71919.19	2.338946
72727.27	2.344630
73535.35	2.350296
74343.43	2.355945
75151.52	2.361577
75959.60	2.367193
76767.68	2.372794
77575.76	2.378380
78383.84	2.383951
79191.92	2.389508
80000.00	2.395051