

In Silico Design to Enhance the Barrier height for Magnetization Reversal in Dy(III) Sandwich Complexes by Stitching them Under the Umbrella of Corannulene

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Table S1. DFT optimized xyz coordinates for models **1-6**.[[η^5 -corannulene]Dy(Cp)] (**1**)

Gd	-1.234619000	0.002090000	-0.874692000
C	1.249057000	3.063831000	1.616429000
H	1.303390000	3.863909000	2.349123000
C	1.888057000	3.255058000	0.388365000
H	2.408384000	4.194670000	0.225845000
C	2.952646000	2.021476000	-1.662899000
H	3.557367000	2.863096000	-1.988455000
C	3.233212000	0.764470000	-2.204856000
H	4.042989000	0.689509000	-2.924994000
C	3.022058000	-1.813891000	-1.796806000
H	3.814507000	-2.093004000	-2.485344000
C	2.559668000	-2.782582000	-0.902599000
H	3.014653000	-3.768285000	-0.939144000
C	1.369147000	-3.140562000	1.402699000
H	1.730850000	-4.154218000	1.550040000
C	0.802329000	-2.481529000	2.497267000
H	0.751045000	-3.015065000	3.442101000
C	0.268023000	-0.126813000	3.509165000
H	0.173471000	-0.473311000	4.534412000
C	0.377629000	1.249477000	3.290349000
H	0.362933000	1.905592000	4.156038000
C	0.651865000	1.805162000	1.987829000
C	1.997106000	2.208147000	-0.598395000
C	2.588159000	-0.438953000	-1.739777000
C	1.614557000	-2.479392000	0.144634000
C	0.419995000	-1.092495000	2.448584000
C	0.475967000	-0.529364000	1.168223000
C	0.587129000	0.873391000	0.944651000
C	1.240256000	1.068135000	-0.305651000
C	1.523060000	-0.212586000	-0.860242000
C	1.054401000	-1.199843000	0.054038000
C	-3.120329000	0.309848000	0.881637000
C	-3.448230000	1.203327000	-0.176147000
C	-3.794510000	0.425690000	-1.318056000
C	-3.682735000	-0.947779000	-0.965152000
C	-3.261019000	-1.021407000	0.392437000
H	-2.855690000	0.590320000	1.894029000
H	-3.486962000	2.284954000	-0.107470000
H	-4.144302000	0.811982000	-2.269293000
H	-3.928671000	-1.790247000	-1.602593000
H	-3.133328000	-1.928571000	0.971687000

[[η^5 -corannulene]Dy(C₆H₆)] (**2**)

Gd	1.434798000	-0.133260000	-0.027496000
C	-2.134888000	1.688311000	2.805553000
H	-2.540670000	2.451150000	3.464569000
C	-2.128350000	0.360752000	3.253521000
H	-2.510287000	0.148885000	4.249193000

C	-2.194450000	-2.101097000	2.457592000
H	-2.639584000	-2.478235000	3.374773000
C	-2.215033000	-2.943496000	1.315788000
H	-2.664504000	-3.928317000	1.417493000
C	-2.251940000	-2.949649000	-1.264060000
H	-2.699562000	-3.936957000	-1.348788000
C	-2.267361000	-2.112268000	-2.407997000
H	-2.738346000	-2.493593000	-3.310364000
C	-2.223252000	0.347360000	-3.218613000
H	-2.629624000	0.129877000	-4.203278000
C	-2.216209000	1.674441000	-2.778392000
H	-2.635416000	2.435867000	-3.430545000
C	-2.149040000	3.211774000	-0.682062000
H	-2.528512000	4.087543000	-1.201490000
C	-2.126831000	3.215932000	0.702016000
H	-2.488247000	4.095316000	1.228267000
C	-1.759372000	2.032036000	1.467998000
C	-1.758923000	-0.747237000	2.379972000
C	-1.808399000	-2.472919000	0.020174000
C	-1.832114000	-0.757836000	-2.348337000
C	-1.805285000	2.025169000	-1.450466000
C	-1.204758000	0.982075000	-0.705843000
C	-1.181535000	0.985829000	0.711558000
C	-1.173749000	-0.365536000	1.159411000
C	-1.197643000	-1.209064000	0.008098000
C	-1.210563000	-0.370634000	-1.146866000
C	3.816062000	-0.550870000	-1.244484000
C	3.653403000	0.837597000	-1.224276000
C	3.779714000	-1.301985000	-0.025769000
H	3.692092000	1.403230000	-2.151565000
H	3.957407000	-2.372771000	-0.041544000
C	3.443982000	1.522662000	0.016535000
C	3.793375000	-0.590824000	1.216786000
H	3.371960000	2.605578000	0.033320000
H	3.938399000	-1.135767000	2.146044000
C	3.629642000	0.797709000	1.238436000
H	3.650530000	1.333059000	2.184046000
H	3.978389000	-1.065634000	-2.187998000

[(η^6 -corannulene)Dy(Cp)] (**3**)

Gd	-1.766900000	-0.416976000	-0.339676000
C	-0.587451000	-1.188944000	2.094190000
H	-1.079887000	-1.836102000	2.816439000
C	-0.795992000	0.203951000	2.217296000
H	-1.436162000	0.547663000	3.025311000
C	0.205183000	2.574114000	1.641427000
H	-0.359056000	3.119696000	2.391575000
C	1.277423000	3.205065000	1.017928000
H	1.507354000	4.225020000	1.313950000
C	3.519729000	2.835044000	-0.278557000
H	3.917879000	3.824749000	-0.076132000
C	4.380816000	1.861919000	-0.779615000
H	5.418720000	2.133696000	-0.949619000
C	4.773356000	-0.717749000	-0.998699000
H	5.840919000	-0.638369000	-1.183224000
C	4.251580000	-1.971803000	-0.689367000

H	4.929908000	-2.818464000	-0.644410000
C	2.247588000	-3.201133000	0.461197000
H	2.773277000	-4.143912000	0.586324000
C	1.049891000	-3.030238000	1.150370000
H	0.687677000	-3.838535000	1.778234000
C	0.369105000	-1.753239000	1.155120000
C	-0.071765000	1.172681000	1.411023000
C	2.161424000	2.522028000	0.094939000
C	3.969805000	0.485127000	-0.954257000
C	2.871332000	-2.141491000	-0.305029000
C	2.079873000	-1.009261000	-0.480716000
C	0.881869000	-0.817552000	0.243699000
C	0.665351000	0.597533000	0.365060000
C	1.733921000	1.253860000	-0.289125000
C	2.608247000	0.264595000	-0.796668000
C	-4.002827000	-0.151308000	-1.689115000
C	-4.392313000	-0.471114000	-0.357823000
C	-4.016250000	0.612359000	0.484024000
C	-3.398442000	1.607245000	-0.330008000
C	-3.393445000	1.135715000	-1.671926000
H	-4.197959000	-0.751772000	-2.571174000
H	-4.930661000	-1.360638000	-0.048874000
H	-4.229907000	0.698328000	1.542668000
H	-3.050595000	2.577426000	0.004130000
H	-3.037930000	1.683231000	-2.538173000

[[η^6 -corannulene]Dy(C₆H₆)] (**4**)

Gd	-1.545529000	-0.014354000	-0.279598000
C	-0.582913000	-0.724376000	2.140491000
H	-1.152228000	-1.226350000	2.919674000
C	-0.588913000	0.701560000	2.142674000
H	-1.163437000	1.195890000	2.922855000
C	0.745033000	2.849011000	1.383395000
H	0.267956000	3.534764000	2.077218000
C	1.903862000	3.259618000	0.724752000
H	2.281589000	4.255824000	0.940619000
C	4.066687000	2.455557000	-0.496335000
H	4.612303000	3.384603000	-0.359386000
C	4.776455000	1.322387000	-0.909403000
H	5.845068000	1.422986000	-1.079505000
C	4.786485000	-1.291928000	-0.915213000
H	5.855775000	-1.383606000	-1.086087000
C	4.085514000	-2.432243000	-0.507007000
H	4.638126000	-3.357791000	-0.374522000
C	1.929351000	-3.257632000	0.711537000
H	2.314684000	-4.251857000	0.923075000
C	0.767751000	-2.858493000	1.372578000
H	0.296120000	-3.550766000	2.063653000
C	0.283281000	-1.498289000	1.267893000
C	0.271027000	1.485482000	1.273072000
C	2.680991000	2.377869000	-0.122745000
C	4.164304000	0.013031000	-0.982651000
C	2.699394000	-2.366566000	-0.132537000

C	2.075440000	-1.144064000	-0.414735000
C	0.918846000	-0.724907000	0.273848000
C	0.913275000	0.720977000	0.276652000
C	2.066477000	1.151806000	-0.410175000
C	2.783499000	0.007472000	-0.827860000
C	-4.089436000	-1.349442000	-0.263489000
H	-4.189549000	-2.398863000	0.004406000
C	-4.211164000	-0.353354000	0.728983000
H	-4.406504000	-0.635240000	1.760473000
C	-4.148296000	1.011346000	0.370770000
H	-4.294986000	1.778540000	1.127168000
C	-3.963977000	1.378756000	-0.979304000
H	-3.966639000	2.429182000	-1.262392000
C	-3.836726000	0.382459000	-1.971661000
H	-3.742893000	0.665801000	-3.017954000
C	-3.900613000	-0.982040000	-1.613605000
H	-3.855353000	-1.748412000	-2.384566000

[(exo- η^5 -corannulene)Dy(endo- η^5 -corannulene)] (**5**)

Gd	-0.322959666	4.836565464	7.299124425
C	0.739356750	3.961052574	5.456582428
C	-1.693817250	4.117792574	5.211180428
C	2.282908750	5.767692574	5.198348428
C	3.080833750	5.216154574	6.191186428
C	3.090110750	3.592181574	8.253851428
C	2.295303750	2.755446574	9.012514428
C	-0.100116250	1.780827574	9.310847428
C	-1.371354250	1.813825574	8.797586428
C	-2.893769250	2.833227574	6.933810428
C	-2.896854250	3.699425574	5.847943428
C	-1.424046250	5.322219574	4.433269428
C	1.583849750	3.414228574	6.454232428
C	-0.156810250	5.823082574	4.280895428
C	0.775347750	2.544495574	7.220915428
C	-0.529687250	2.562172574	6.710862428
C	-0.551088250	3.450761574	5.612164428
C	0.988421750	5.193762574	4.872748428
C	2.669026750	4.044725574	6.935414428
C	1.036921750	2.282868574	8.542560428
C	-1.674412250	2.301724574	7.483961428
H	2.623766750	6.712849574	4.766889428
H	3.810354750	5.711124574	6.451024428
H	3.806192750	4.061224574	8.728617428
H	2.637086750	2.482034574	9.819295428
H	0.174496750	1.515664574	10.300477428
H	-2.092983250	1.492094574	9.370192428
H	-3.772137250	2.623454574	7.461505428
H	-3.858288250	3.978729574	5.649055428
H	-2.205449250	5.793619574	4.109274428
H	0.226054750	6.653924574	3.708289428
C	-0.025219974	7.163068703	8.044467849
C	-1.637766897	8.469347657	6.762220748
C	1.998038078	7.998536230	8.945457301
C	1.865194075	7.109754523	10.017786852
C	0.202648208	5.646537512	11.397296643
C	-1.135393331	5.284908255	11.493326780

C	-3.509869823	5.654681963	10.449240205
C	-4.214360419	6.289610457	9.458940270
C	-3.973155125	7.916627566	7.414469769
C	-3.049250844	8.664952094	6.665683635
C	-0.552904667	9.359892083	6.475134277
C	-0.136521649	6.272288896	9.145849967
C	0.695609565	9.197216125	7.064954383
C	-1.505246870	5.896659823	9.233147500
C	-2.220546840	6.558030765	8.191968624
C	-1.287053631	7.328279175	7.477682637
C	0.974656634	8.107746818	7.947643463
C	0.722960879	6.271814297	10.209403074
C	-2.080526197	5.529015041	10.437259527
C	-3.561749731	6.885333043	8.308214734
H	2.780063291	8.775291651	8.968183356
H	2.521058860	7.252259299	10.642577068
H	0.863136597	5.668400333	12.290180658
H	-1.478044543	4.983721684	12.348197167
H	-3.804476975	5.179835846	11.228696817
H	-5.172218201	6.483162732	9.321256534
H	-4.777584537	8.129780616	7.246389015
H	-3.456171981	9.461255988	6.216399843
H	-0.693351395	10.397300225	6.039505990
H	1.256458758	9.878637891	6.871452779

[(endo- η^5 -corannulene)Dy(endo- η^5 -corannulene)] (**6**)

Gd	0.000451000	-0.197035000	-0.000083000
C	-1.951186000	-1.062842000	-1.681633000
C	-0.075095000	0.280327000	-2.605907000
C	-1.908248000	-3.264863000	-0.757117000
C	-3.010425000	-2.954631000	0.043722000
C	-4.397163000	-0.940143000	1.104212000
C	-4.498709000	0.456937000	1.174288000
C	-3.424948000	2.750570000	0.332488000
C	-2.391923000	3.299390000	-0.434906000
C	-0.298767000	2.694100000	-1.965855000
C	0.435092000	1.643061000	-2.541384000
C	0.633115000	-0.991963000	-2.670055000
C	-3.013375000	-0.742941000	-0.807991000
C	0.071601000	-2.196800000	-2.194722000
C	-3.111106000	0.659762000	-0.731096000
C	-2.100626000	1.215008000	-1.543084000
C	-1.396418000	0.156442000	-2.170618000
C	-1.255648000	-2.268753000	-1.599434000
C	-3.552802000	-1.607812000	0.134646000
C	-3.763324000	1.337337000	0.285961000
C	-1.603717000	2.501141000	-1.355617000
H	-1.519043000	-4.278502000	-0.728507000
H	-3.428103000	-3.746636000	0.660078000
H	-4.942221000	-1.526459000	1.838748000
H	-5.117317000	0.879990000	1.961150000
H	-3.946112000	3.406710000	1.024675000
H	-2.160947000	4.352645000	-0.303850000
H	0.170118000	3.673617000	-1.934767000
H	1.426258000	1.862611000	-2.926625000
H	1.652201000	-1.021453000	-3.046021000
H	0.692424000	-3.087050000	-2.230772000
C	3.012203000	-0.743542000	0.807791000

C	1.254213000	-2.267894000	1.601264000
C	4.395877000	-0.942812000	-1.104190000
C	4.498310000	0.454203000	-1.175141000
C	3.426324000	2.749174000	-0.334202000
C	2.393950000	3.299133000	0.433337000
C	0.300691000	2.696158000	1.965282000
C	-0.433839000	1.645849000	2.541241000
C	-0.633720000	-0.989088000	2.671040000
C	-0.072956000	-2.194672000	2.196568000
C	1.906145000	-3.264953000	0.759521000
C	3.110651000	0.659018000	0.729866000
C	3.008271000	-2.955916000	-0.041902000
C	2.100972000	1.215360000	1.542039000
C	1.396365000	0.157687000	2.170551000
C	1.950349000	-1.062243000	1.682292000
C	3.551191000	-1.609417000	-0.134180000
C	3.763493000	1.335668000	-0.287400000
C	1.605217000	2.501919000	1.354497000
C	0.075224000	0.282702000	2.605992000
H	4.940629000	-1.529879000	-1.838353000
H	5.117255000	0.876306000	-1.962249000
H	3.947898000	3.404723000	-1.026641000
H	2.163944000	4.352569000	0.302006000
H	-0.167356000	3.676078000	1.934259000
H	-1.424715000	1.866313000	2.926707000
H	-1.652842000	-1.017753000	3.046976000
H	-0.694375000	-3.084475000	2.233334000
H	1.516492000	-4.278446000	0.731831000
H	3.425413000	-3.748677000	-0.657650000

Table S2: Frequencies of all the models 1-6.

Complex 1	Complex 2	Complex 3	Complex 4	Complex 5	Complex 6
6.9	-4.7	11.6	4.8	8.8	9.7
27.1	10.5	19.5	10.0	19.9	25.8
39.7	19.7	42.1	33.1	23.5	31.6
68.0	50.7	64.2	68.4	37.8	33.2
76.3	55.2	72.5	73.6	48.5	46.1
100.6	85.0	117.5	117.4	76.2	50.5
138.8	130.2	142.2	141.6	77.9	76.5
139.2	132.0	169.4	162.3	91.9	108.3
232.6	145.3	204.0	164.1	125.3	122.5
263.5	202.5	265.8	172.6	136.8	153.4
270.1	210.5	267.8	194.1	137.3	156.7
275.4	220.0	281.4	234.8	144.4	156.7
275.8	238.8	284.1	282.5	160.1	162.1
300.1	242.7	298.3	284.0	202.4	168.5
323.8	261.0	308.5	302.2	246.5	196.7
325.2	264.6	325.7	321.7	268.8	283.8
411.3	301.3	408.1	397.3	272.3	284.8
412.3	342.0	413.4	400.8	272.8	294.4
435.4	384.6	433.3	404.2	288.6	298.4

435.8	396.9	436.6	412.3	323.0	317.1
443.0	401.0	436.8	420.1	325.1	321.1
443.8	416.2	440.7	427.6	332.3	344.5
524.0	419.2	517.6	428.4	350.9	347.6
542.4	422.4	542.3	433.8	412.7	404.0
543.0	477.2	543.6	496.0	413.2	404.4
563.8	530.6	559.9	539.4	413.9	409.8
575.5	534.1	588.7	540.1	426.5	409.9
577.3	561.1	591.8	559.1	434.6	434.8
590.2	567.2	593.8	577.9	434.7	435.6
593.6	573.2	606.3	596.9	436.2	437.1
614.2	585.6	608.0	606.7	438.0	437.3
639.7	605.6	632.0	606.9	440.0	438.0
645.7	606.6	642.3	607.2	441.6	438.5
646.3	613.9	644.0	609.4	441.8	449.1
665.7	622.5	646.6	636.2	454.8	449.6
666.5	627.8	663.1	638.6	520.2	530.2
739.4	635.2	727.1	643.1	521.0	531.2
741.9	636.8	751.7	650.1	539.0	548.2
754.6	649.1	760.9	658.9	539.8	548.5
755.0	732.4	783.0	713.2	542.9	552.4
810.4	743.9	799.0	748.2	548.5	552.6
811.4	748.0	820.0	758.6	564.2	561.5
832.4	751.3	832.6	777.7	567.2	563.0
835.4	755.9	837.0	778.4	572.0	589.5
838.1	766.7	838.0	807.5	573.2	591.5
852.0	805.5	851.2	825.6	606.1	604.8
852.5	816.4	852.0	849.7	608.4	605.3
857.6	846.1	855.3	852.7	615.1	613.5
858.0	858.3	856.9	868.9	620.6	615.1
873.2	869.4	864.2	874.8	637.3	628.2
873.7	871.3	870.2	897.7	638.5	628.3
901.7	903.0	888.5	929.1	639.0	643.4
911.7	905.3	910.8	936.3	647.5	643.4
915.6	923.9	916.1	938.3	647.7	649.0
931.8	932.2	932.3	974.6	662.6	650.4
995.9	939.7	983.2	986.6	663.0	661.4
1005.1	957.5	993.4	999.4	664.0	662.0
1005.2	959.7	999.3	1006.8	668.0	676.6
1014.3	989.3	1005.1	1012.6	682.4	677.3
1014.6	990.4	1011.5	1012.7	730.4	753.9
1035.9	1001.1	1034.7	1020.6	731.1	754.0
1037.4	1004.1	1038.1	1030.5	753.8	756.3

1054.9	1013.5	1050.4	1031.9	753.9	756.6
1086.9	1014.8	1084.1	1040.5	757.1	780.8
1088.2	1022.0	1087.1	1045.5	762.0	781.3
1090.0	1027.2	1089.6	1046.4	790.0	783.4
1090.5	1039.2	1093.8	1048.7	798.5	784.4
1135.3	1058.6	1135.1	1082.6	815.5	811.3
1164.2	1076.2	1154.2	1092.7	815.6	812.4
1164.8	1081.7	1168.9	1138.7	816.8	819.9
1172.0	1110.6	1172.9	1160.3	827.7	823.8
1172.4	1125.5	1174.1	1168.8	854.2	857.3
1212.5	1138.7	1202.6	1172.6	854.9	859.3
1213.5	1174.5	1213.6	1192.2	855.4	861.2
1231.7	1182.5	1219.8	1201.9	859.3	861.4
1231.9	1187.8	1223.2	1202.2	874.5	866.3
1251.8	1193.8	1244.0	1207.8	878.1	871.8
1270.5	1212.0	1265.0	1212.2	878.4	872.5
1294.2	1221.6	1294.1	1221.8	880.1	875.6
1340.0	1230.6	1331.3	1226.2	905.1	894.6
1340.1	1235.4	1332.8	1244.9	907.5	899.7
1380.1	1257.7	1373.6	1262.4	929.3	938.7
1380.4	1270.7	1392.3	1323.5	934.1	939.0
1393.2	1325.4	1397.0	1326.0	993.8	976.3
1397.2	1332.2	1397.4	1336.2	1000.3	977.6
1429.0	1361.5	1431.7	1361.0	1001.5	989.8
1440.4	1364.2	1434.6	1379.9	1002.7	990.2
1440.7	1367.8	1439.0	1400.0	1009.3	1000.0
1446.8	1377.9	1448.1	1415.2	1009.7	1002.3
1447.4	1399.4	1452.0	1430.1	1009.8	1006.5
1455.4	1424.0	1463.9	1437.4	1016.1	1008.9
1457.2	1439.1	1469.5	1440.2	1019.0	1016.5
1470.5	1446.6	1472.6	1450.1	1019.1	1017.3
1472.2	1450.3	1473.0	1451.7	1052.8	1046.8
1482.0	1452.2	1475.0	1465.7	1056.1	1047.4
1482.3	1463.8	1485.3	1473.2	1087.3	1092.8
1523.9	1465.9	1511.9	1474.1	1087.9	1093.1
1623.6	1475.0	1609.9	1498.6	1089.9	1093.4
1625.4	1479.7	1624.9	1499.1	1091.1	1093.4
1626.0	1492.0	1641.2	1507.7	1156.5	1147.2
1635.6	1499.8	1649.0	1581.1	1165.0	1147.8
1636.5	1513.2	1653.1	1596.7	1165.5	1155.7
3204.2	1577.5	3194.2	1597.3	1165.8	1156.6
3204.8	1579.9	3203.5	1601.6	1170.1	1168.1
3205.0	1582.4	3204.3	1620.5	1172.4	1168.6

3205.2	1592.9	3205.7	1620.6	1172.9	1171.2
3205.4	1623.6	3206.2	1642.4	1173.2	1171.4
3215.6	3203.5	3208.7	3193.5	1195.0	1189.6
3216.2	3203.9	3216.6	3196.4	1214.1	1190.0
3216.3	3205.4	3217.3	3201.3	1214.4	1206.2
3216.4	3206.0	3218.2	3202.1	1215.9	1206.3
3216.6	3206.7	3218.3	3204.0	1220.5	1214.6
3227.2	3207.0	3226.9	3206.1	1221.5	1215.1
3232.2	3208.6	3232.4	3206.2	1232.2	1218.0
3241.8	3211.1	3241.7	3208.9	1232.5	1218.6
3243.6	3214.6	3245.2	3209.2	1245.0	1242.3
3255.4	3214.7	3256.4	3209.4	1252.7	1242.4
	3215.0		3210.3	1266.5	1259.1
	3216.3		3217.3	1272.1	1259.7
	3216.6		3218.3	1333.0	1329.0
	3218.5		3218.4	1336.1	1329.6
	3222.6		3220.0	1339.4	1331.5
	3224.7		3220.1	1339.8	1331.8
				1376.1	1379.0
				1377.3	1379.5
				1378.1	1393.2
				1398.4	1393.5
				1422.6	1427.4
				1432.9	1427.8
				1435.6	1429.1
				1438.2	1430.4
				1441.4	1436.8
				1441.8	1438.2
				1442.0	1442.4
				1443.4	1443.1
				1444.5	1449.9
				1450.7	1450.9
				1450.9	1461.7
				1452.1	1463.2
				1453.0	1464.0
				1469.4	1464.0
				1473.1	1468.0
				1481.8	1468.4
				1482.1	1493.5
				1483.3	1494.3
				1509.6	1500.2
				1523.9	1500.3
				1604.2	1630.4

1614.1	1630.8
1615.2	1640.9
1615.7	1642.5
1617.0	1656.9
1627.6	1658.0
1628.1	1665.8
1631.5	1666.2
1643.3	1674.1
1651.6	1674.3
3203.6	3203.3
3203.7	3203.5
3204.0	3204.3
3204.2	3204.4
3204.3	3205.9
3204.4	3205.9
3205.0	3207.8
3208.6	3207.8
3209.0	3209.7
3209.1	3209.9
3213.5	3215.3
3213.9	3215.5
3214.6	3215.7
3214.7	3216.1
3214.9	3216.3
3214.9	3216.4
3215.5	3220.0
3219.3	3220.1
3219.4	3220.3
3219.6	3220.5

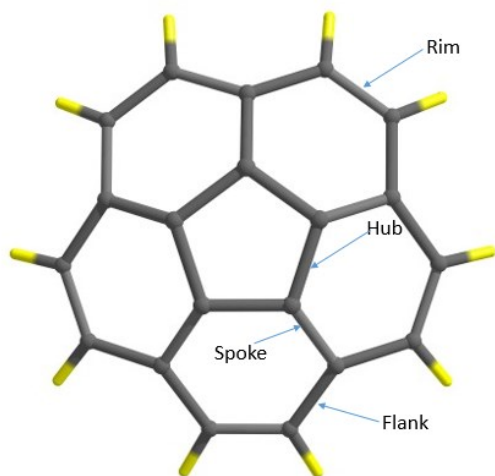


Figure S1: Four types of bonds in corannulene ligand.

Table S3. Bond critical point (BCP) properties for Models 1-6. ^aThe electron density at the bond critical density (BCP), ^b The Laplacian of the electron density at the BCP, ^cThe Virial Field function, ^dThe electronic kinetic energy density, ^eRatio of Virial field function to Electronic kinetic energy ^fThe total energy density at the BCP.

Model	Gd-C pairs	$\rho(r)^a$	$\nabla^2\rho(r)^b$	$ V(r)^c $	$G(r)^d$	$V(r)/G(r)^e$	$H(r)^f$
1	Gd-C31	0.0305	0.0234	0.0245	0.0247	0.9839	-0.0004
	Gd-C30	0.0284	0.0233	0.0232	0.0233	0.9968	7.5E-05
	Gd-C27	0.0317	0.0244	0.0259	0.0252	1.0272	0.0007
	Gd-C28	0.0319	0.0241	0.0258	0.0250	1.0333	0.0008
	Gd-C32	0.0445	0.0283	0.0376	0.0329	1.1415	0.0046
	Gd-C33	0.0433	0.0277	0.0361	0.0319	1.1322	0.0042
	Gd-C35	0.0418	0.0279	0.0351	0.0315	1.1322	0.0036
	Gd-C36	0.0445	0.0277	0.0372	0.0325	1.1465	0.0048
	Gd-C34	0.0412	0.0274	0.0346	0.0310	1.1165	0.0036
2	Gd-C29	0.0251	0.0161	0.0172	0.0167	1.0312	0.0005
	Gd-C31	0.0249	0.0161	0.0169	0.0166	1.0227	0.0004
	Gd-C30	0.0265	0.0165	0.0184	0.0175	1.0543	0.0009
	Gd-C34	0.0392	0.0263	0.0324	0.0294	1.1038	0.0030
	Gd-C37	0.0406	0.0271	0.0341	0.0306	1.1147	0.0035
3	Gd-C28	0.0288	0.0248	0.0232	0.0240	0.9685	-0.0008
	Gd-C34	0.0427	0.0287	0.0362	0.0324	1.1161	0.0038
	Gd-C35	0.0429	0.0293	0.0369	0.0331	1.1136	0.0038
	Gd-C29	0.0301	0.0234	0.0241	0.0237	1.0158	0.0004
	Gd-C2	0.0274	0.0205	0.0207	0.0206	1.0036	7.6E-05
	Gd-C4	0.0285	0.0189	0.0203	0.0196	1.0371	0.0007
	Gd-C33	0.0408	0.0285	0.0346	0.0315	1.0979	0.0031
	Gd-C32	0.0416	0.0274	0.0347	0.0311	1.1173	0.0036
	Gd-C36	0.0418	0.0292	0.0360	0.0326	1.1039	0.0034

4	Gd-C28	0.0393	0.0267	0.0328	0.0297	1.1028	0.0031
	Gd-C2	0.0366	0.0229	0.0260	0.0244	1.0627	0.0015
	Gd-C29	0.0392	0.0267	0.0326	0.0297	1.0993	0.0029
	Gd-C42	0.0249	0.0170	0.0169	0.0170	0.9968	-5.3E-05
	Gd-C34	0.0248	0.0173	0.0169	0.0171	0.9882	-0.0002
	Gd-C36	0.0250	0.0170	0.0169	0.0170	0.9950	-8.4E-05
	Gd-C38	0.0249	0.0169	0.0168	0.0169	0.9976	-4E-05
	Gd-C40	0.0246	0.0171	0.0169	0.0170	0.9952	-8E-05
	Gd-C32	0.0252	0.0169	0.0169	0.0169	0.9995	-8E-06
5	Gd-C27	0.0485	0.0343	0.0464	0.0404	1.1496	0.0060
	Gd-C46	0.0325	0.0239	0.0262	0.0250	1.0458	0.0011
	Gd-C45	0.0318	0.0237	0.0255	0.0246	1.0381	0.0009
	Gd-C32	0.0312	0.0232	0.0249	0.0241	1.0354	0.0008
	Gd-C43	0.0308	0.0235	0.0247	0.0241	1.0268	0.0006
	Gd-C47	0.0318	0.0238	0.0255	0.0247	1.0348	0.0009
6	Gd-C17	0.0418	0.0293	0.0365	0.0329	1.1095	0.0036
	Gd-C46	0.0419	0.0293	0.0366	0.0330	1.1098	0.0036

Table S4.Energy Decomposition Analysis of model 1-6.

Model	Total interaction energy(kJ/mol)	Orbital energy(kJ/mol)	Steric energy(kJ/mol)
1	-2513.9	-1495.1	-1018.8
2	-1192.3	-1496.8	304.4
3	-2488.8	-1682.9	-805.8
4	-1256.4	-1580.9	324.4
5	-1383.9	-1935.8	551.8
6	-1310.0	-1907.8	597.8

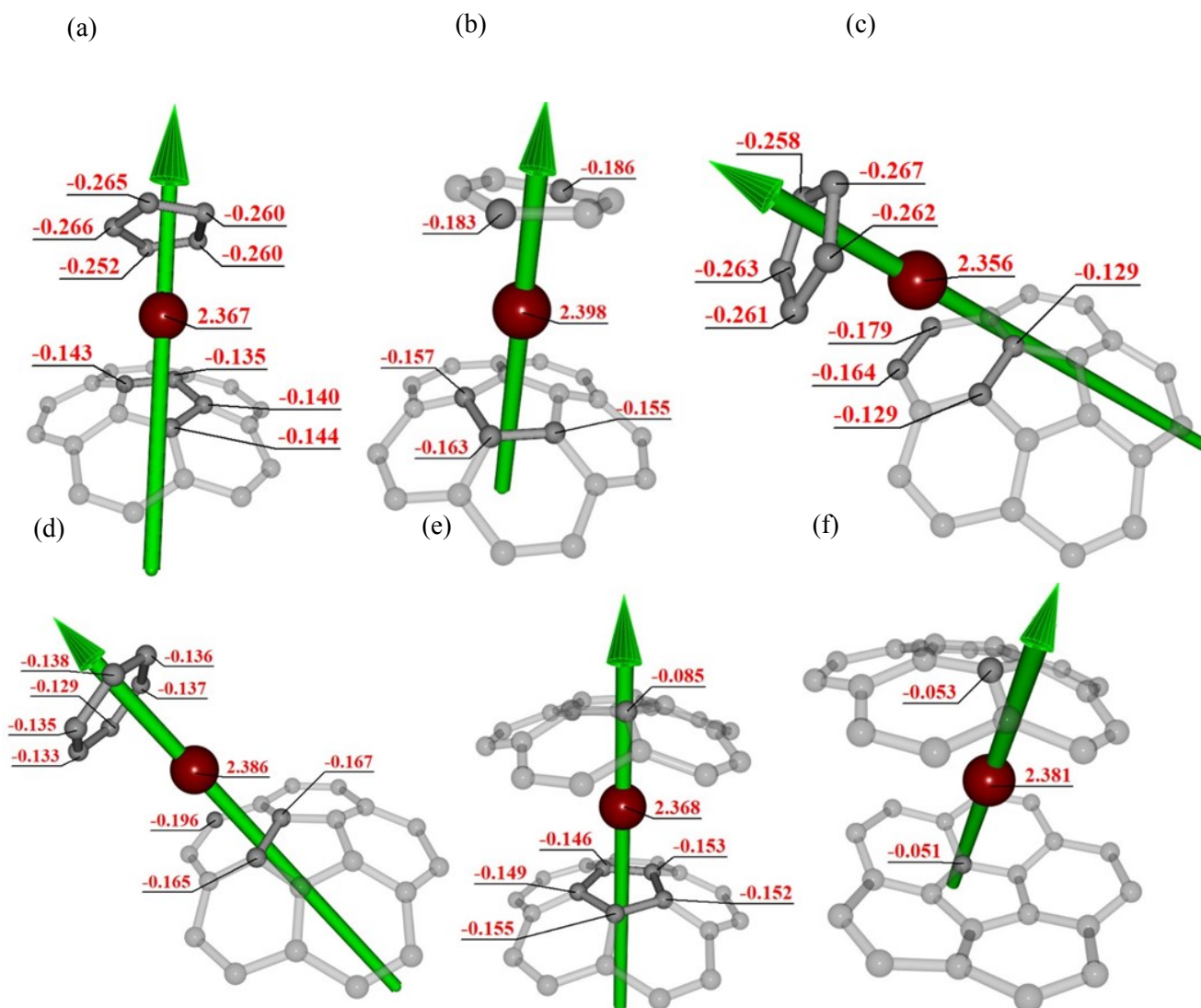


Fig. S2. *Ab initio* SINGLE_ANISO computed ground state KD orientation for (a-f) Models 1-6 respectively along with the computed LoProp charges on the important atoms.

Table S5: Thermally accessible structures at different time steps (in fs) for models **3,5** and **6**, along with their relative energies (ΔE), U_{cal} and magnetic relaxation mode. It is important to mention here that for model **6**, 128 structures are possible, and we have selected some representing structures from each potential well. See the text in the main manuscript for more information.

	t (fs)	ΔE (kJ/mol)	U_{cal} cm ⁻¹	Relaxation Via
5-1	<i>f1</i>	0.0	651.8	7 th KD (Orbach)
5-2	<i>f2</i>	8.5	647.3	7 th KD (Orbach)
5-3	<i>f3</i>	32.7	643.4	7 th KD (Orbach)
5-4	<i>f4</i>	63.9	640.7	7 th KD (Orbach)
5-5	<i>f60</i>	80.5	506.0	6 th KD (Orbach)
5-6	<i>f61</i>	81.4	510.2	6 th KD (Orbach)
6-1	<i>f1</i>	0.0	593.9	6 th KD (TA-QTM)

6-2	<i>f</i> ₂	8.5	598.3	6 th KD (TA-QTM)
6-3	<i>f</i> ₃	33.6	602.2	6 th KD (TA-QTM)
6-4	<i>f</i> ₂₁	75.4	595.3	6 th KD (TA-QTM)
6-5	<i>f</i> ₂₃	68.7	594.4	6 th KD (TA-QTM)
6-6	<i>f</i> ₂₅	81.4	583.5	6 th KD (TA-QTM)
6-7	<i>f</i> ₄₄	71.6	512.5	5 th KD (TA-QTM)
6-8	<i>f</i> ₆₀	58.8	491.0	5 th KD (TA-QTM)
6-9	<i>f</i> ₇₂	81.4	471.3	5 th KD (TA-QTM)
6-10	<i>f</i> ₈₅	82.0	424.1	5 th KD (TA-QTM)
6-11	<i>f</i> ₁₂₉	71.9	438.8	5 th KD (TA-QTM)
6-12	<i>f</i> ₁₅₆	73.9	500.0	5 th KD (TA-QTM)
6-13	<i>f</i> ₄₃₈	81.0	664.3	6 th KD (TA-QTM)
6-14	<i>f</i> ₄₈₁	73.8	517.5	6 th KD (Orbach)
6-15	<i>f</i> ₁₀₀₈	72.5	497.1	5 th KD (Orbach)
6-16	<i>f</i> ₁₀₃₀	73.9	483.2	5 th KD (Orbach)
6-17	<i>f</i> ₁₀₅₃	67.4	751.4	7 th KD (TA-QTM)
6-18	<i>f</i> ₁₀₇₂	82.1	720.1	7 th KD (Orbach)
6-19	<i>f</i> ₁₁₈₂	83.0	68.9	2 nd KD (Orbach)
6-20	<i>f</i> ₁₂₈₉	79.8	98.8	2 nd KD (Orbach)
6-21	<i>f</i> ₁₄₈₆	81.0	106.7	2 nd KD (Orbach)
6-22	<i>f</i> ₁₅₁₀	75.8	104.7	2 nd KD (Orbach)
6-23	<i>f</i> ₁₅₇₂	81.6	168.3	2 nd KD (Orbach)
6-24	<i>f</i> ₁₈₀₃	77.2	563.6	5 th KD (Orbach)
6-25	<i>f</i> ₁₈₁₈	77.6	506.8	5 th KD (TA-QTM)
6-26	<i>f</i> ₁₈₂₉	78.9	470.8	5 th KD (TA-QTM)
3-1	<i>f</i> ₁	7.2	891.9	6 th KD (TA-QTM)
3-2	<i>f</i> ₂	24.5	892.2	6 th KD (TA-QTM)
3-3	<i>f</i> ₃	42.7	892.6	6 th KD (TA-QTM)
3-4	<i>f</i> ₁₄	67.8	882.1	6 th KD (TA-QTM)
3-5	<i>f</i> ₂₂	53.1	897.5	6 th KD (TA-QTM)
3-6	<i>f</i> ₂₈	62.9	924.5	6 th KD (TA-QTM)
3-7	<i>f</i> ₃₃	62.5	936.7	6 th KD (TA-QTM)
3-8	<i>f</i> ₆₄	48.6	881.2	6 th KD (Orbach)
3-9	<i>f</i> ₁₂₇	71.9	878.8	6 th KD (TA-QTM)
3-10	<i>f</i> ₂₄₈	78.0	784.2	6 th KD (Orbach)

Table S6: CASSCF+RASSI-SO computed relative energies of eight low lying KDs and g tensors of eight low lying KDs for thermally accessible structures of Models 3,5 and 6, along with the matrix element of the transverse moment for QTM (quantum tunnelling of the magnetisation), TA-QTM (thermally assisted QTM) and Orbach process. We have also given the U_{cal} values for all the possible structures.

	KD (l)	E_{KD} (cm ⁻¹)	g_{xx}, g_{yy}, g_{zz}	QTM/TA-QTM	Orbach [$l \rightarrow (l+1)$]	U_{cal} (cm ⁻¹)
5-1	1	0.0	0.001,0.001,19.879	2.1E-04	4.0E-04	651.8
	2	164.9	0.001,0.005,17.395	4.8E-04	1.9E-03	

	3	291.1	0.027,0.030,14.542	9.8E-03	2.5E-02	
	4	411.2	0.187,0.247,12.055	7.5E-02	7.5E-02	
	5	501.1	0.123,0.234,9.750	7.1E-02	1.2E-01	
	6	580.3	0.461,0.862,6.875	2.5E-01	2.3	
	7	651.8	3.987,3.046,1.361	1.3	2.4	
	8	695.2	12.671,8.446,1.231	3.6		
5-2	1	0.0	0.001,0.001,19.877	2.2E-04	4.1E-04	647.3
	2	163.1	0.001,0.001,17.406	4.7E-04	1.9E-03	
	3	287.9	0.027,0.033,14.548	1.1E-02	2.5E-02	
	4	407.5	0.181,0.245,12.044	7.4E-02	6.8E-02	
	5	497.4	0.110,0.248,9.718	7.1E-02	1.2E-01	
	6	576.3	0.449,0.707,6.865	2.2E-01	9.0E-01	
	7	647.3	0.705,2.399,4.101	5.9E-01	5.3E-01	
	8	690.1	12.113,8.985,1.244	3.6		
5-3	1	0.0	0.001,0.001,19.875	2.2E-04	4.3E-04	643.4
	2	163.1	0.001,0.001,17.406	4.9E-04	2.0E-03	
	3	285.3	0.029,0.034,14.551	1.1E-02	2.5E-02	
	4	404.4	0.177,0.241,12.031	7.3E-02	6.2E-02	
	5	494.4	0.037,0.319,9.678	8.2E-02	1.4E-01	
	6	573.1	0.404,0.589,6.855	1.9E-01	1.9	
	7	643.4	4.229,2.727,1.041	1.4	2.0	
	8	686.5	12.592,8.415,1.208	3.6		
5-4	1	0.0	0.001,0.001,19.873	2.2E-04	4.4E-04	640.7
	2	161.0	0.001,0.001,17.417	4.8E-04	2.0E-03	
	3	283.4	0.030,0.036,14.553	1.2E-02	2.5E-02	
	4	402.0	0.178,0.241,12.018	7.2E-02	5.7E-02	
	5	492.2	0.029,0.389,9.637	9.7E-02	1.6E-01	
	6	570.9	0.359,0.566,6.845	1.8E-01	1.7	
	7	640.7	4.370,3.260,1.521	1.6	1.8	
	8	684.4	13.188,7.720,1.179	3.6		
5-60	1	0.0	0.002,0.002,19.768	5.9E-04	1.4E-03	506.0
	2	143.3	0.009,0.010,17.475	3.7E-03	6.1E-03	
	3	248.6	0.012,0.037,14.503	8.8E-03	4.2E-02	
	4	361.0	0.280,0.331,12.128	1.1E-01	1.7E-01	
	5	437.6	0.493,0.940,10.260	3.0E-01	3.2	
	6	506.0	2.870,3.449,7.283	1.3	2.1	
	7	577.9	2.627,4.915,10.645	1.3	7.7E-01	
	8	652.6	0.512,1.920,17.760	4.4E-01		
5-61	1	0.0	0.002,0.002,19.761	5.7E-04	1.4E-03	510.2
	2	148.2	0.009,0.010,17.476	3.6E-03	6.0E-03	
	3	252.0	0.015,0.041,14.506	1.0E-02	4.2E-02	
	4	364.7	0.263,0.310,12.109	1.0E-01	1.7E-01	
	5	441.6	0.617,1.010,10.213	3.3E-01	3.2	
	6	510.2	3.120,3.592,7.386	1.4	2.1	
	7	583.9	2.509,4.830,11.183	1.6	6.9E-01	
	8	664.7	0.454,1.629,18.015	3.9E-01		
6-1	1	0.0	0.000,0.000,19.982	2.5E-05	1.3E-04	593.9
	2	135.1	0.004,0.004,17.312	1.5E-03	1.5E-03	
	3	294.7	0.023,0.283,14.661	9.2E-03	8.6E-03	
	4	436.5	0.005,0.077,11.856	1.4E-02	3.4E-02	

	5	539.3	0.150,0.650,9.929	1.4E-01	2.1E-01	
	6	593.9	8.793,7.664,4.612	2.8	1.6	
	7	631.6	0.699,1.224,18.849	3.6E-01	3.9E-01	
	8	706.2	0.007,0.055,19.460	1.3E-02		
6-2	1	0.0	0.000,0.000,19.842	2.7E-05	1.3E-04	598.3
	2	136.8	0.004,0.004,17.306	1.4E-03	1.5E-03	
	3	298.1	0.021,0.026,14.660	8.6E-03	8.3E-03	
	4	440.5	0.003,0.064,11.856	1.3E-02	4.0E-02	
	5	543.6	0.198,0.675,8.937	1.5E-01	2.5E-01	
	6	598.3	8.669,7.724,4.252	2.8	1.6	
	7	635.3	0.692,1.249,18.731	3.9E-01	3.1E-01	
	8	711.8	0.015,0.073,19.465	2.0E-02		
6-3	1	0.0	0.000,0.000,19.844	3.1E-05	1.4E-04	602.2
	2	138.6	0.004,0.004,17.309	1.4E-03	1.4E-03	
	3	301.3	0.020,0.025,14.658	8.1E-03	8.0E-03	
	4	444.2	0.009,0.052,11.857	1.2E-02	4.9E-02	
	5	547.7	0.310,0.767,8.952	1.9E-01	3.0E-01	
	6	602.2	8.583,7.771,4.224	2.9	1.6	
	7	638.8	0.677,1.257,18.587	4.1E-01	2.5E-01	
	8	717.5	0.023,0.093,19.461	2.7E-02		
6-21	1	0.0	0.000,0.000,19.828	5.4E-05	3.1E-04	595.3
	2	148.6	0.004,0.004,17.446	1.7E-03	2.6E-03	
	3	303.6	0.032,0.038,14.737	1.3E-02	1.2E-02	
	4	443.5	0.030,0.118,11.899	2.6E-02	3.7E-02	
	5	544.1	0.148,0.624,9.385	1.5E-01	1.8	
	6	595.3	3.852,6.956,10.095	2.2	2.0	
	7	632.7	0.829,1.495,18.222	4.0E-01	6.3E-01	
	8	716.3	0.078,0.237,19.308	5.7E-02		
6-23	1	0.0	0.000,0.000,19.835	5.2E-05	3.5E-04	594.4
	2	148.8	0.005,0.005,17.497	2.0E-03	3.1E-03	
	3	302.5	0.036,0.042,14.730	1.5E-02	1.6E-02	
	4	442.7	0.037,0.131,11.910	2.9E-02	1.0E-01	
	5	543.2	0.619,1.178,9.474	3.4E-01	1.9	
	6	594.4	3.754,6.947,10.404	2.0	2.1	
	7	637.9	0.731,1.227,18.178	3.6E-01	6.5E-01	
	8	714.1	0.112,0.343,19.221	7.9E-02		
6-25	1	0.0	0.000,0.000,19.841	4.3E-05	5.0E-04	583.5
	2	147.7	0.006,0.007,17.572	2.5E-03	3.9E-03	
	3	297.1	0.037,0.046,14.738	1.6E-02	2.1E-02	
	4	436.3	0.056,0.156,11.906	3.7E-02	2.2E-01	
	5	534.1	1.421,2.129,9.513	6.8E-01	2.0	
	6	583.5	3.452,6.784,10.706	2.1	2.2	
	7	632.5	0.654,1.086,17.957	3.4E-01	6.6E-01	
	8	704.2	0.142,0.456,19.144	1.0E-01		
6-44	1	0.0	0.000,0.000,19.753	7.0E-05	7.0E-04	512.5
	2	160.7	0.010,0.011,14.927	3.9E-03	8.0E-03	
	3	299.7	0.097,0.098,14.927	3.6E-02	4.0E-02	
	4	415.9	0.203,0.437,11.833	1.2E-01	2.4E-01	
	5	512.5	1.863,3.108,8.989	9.2E-01	2.1	
	6	569.7	3.524,6.268,11.792	2.2	2.1	
	7	620.7	0.330,0.339,19.254	1.5E-01	5.7E-01	
	8	690.1	0.078,0.235,19.163	6.9E-02		
6-60	1	0.0	0.001,0.001,19.545	4.0E-04	1.4E-03	491.0
	2	140.2	0.014,0.017,17.175	5.5E-03	1.4E-02	
	3	297.2	0.124,0.131,11.818	4.7E-02	3.8E-02	
	4	402.4	0.023,0.311,11.818	5.7E-02	1.9E-01	

	5	491.0	1.045,2.474,8.879	9.5E-01	4.8E-01	
	6	532.9	11.706,7.585,2.879	3.5	1.1	
	7	579.8	0.483,0.633,19.073	1.9E-01	7.9E-01	
	8	672.7	0.021,0.211,19.324	4.3E-02		
6-72	1	0.0	0.000,0.001,19.330	2.1E-04	1.8E-03	471.3
	2	122.2	0.011,0.014,17.132	4.5E-03	1.7E-02	
	3	285.7	0.173,0.182,15.325	6.7E-02	5.6E-02	
	4	390.0	0.030,0.506,11.779	9.3E-02	5.0E-01	
	5	471.3	1.845,4.755,8.446	1.3	2.2	
	6	503.1	1.420,6.874,12.596	1.7	1.5	
	7	535.9	0.749,0.867,18.297	2.9E-01	1.0	
	8	641.8	0.144,0.462,19.236	1.1E-01		
6-85	1	0.0	0.009,0.020,19.027	4.8E-03	1.3E-02	424.1
	2	92.9	0.030,0.058,17.391	1.6E-02	3.7E-02	
	3	239.5	0.156,0.208,15.745	6.9E-02	7.2E-02	
	4	351.1	0.149,0.275,12.176	7.4E-02	4.7E-01	
	5	424.1	0.654,2.977,9.582	9.2E-01	6.5E-01	
	6	447.9	12.552,7.302,1.764	3.6	9.0E-01	
	7	493.3	0.253,0.878,18.054	2.2E-01	7.2E-01	
	8	635.5	0.139,0.349,19.361	8.4E-02		
6-129	1	0.0	0.001,0.004,19.766	8.9E-04	6.0E-03	438.8
	2	66.5	0.022,0.032,18.044	1.0E-02	1.8E-02	
	3	209.2	0.135,0.186,14.719	6.0E-02	9.5E-02	
	4	353.8	0.541,0.993,11.716	2.8E-01	7.0E-01	
	5	438.8	3.032,4.501,8.795	1.5	2.2	
	6	490.9	2.353,3.503,13.747	1.2	1.9	
	7	531.8	0.890,1.413,16.139	4.3E-01	1.6	
	8	592.0	0.439,2.000,17.996	4.2E-01		
6-156	1	0.0	0.004,0.006,19.782	1.7E-03	2.7E-03	500.0
	2	89.3	0.003,0.009,17.436	2.3E-03	5.7E-03	
	3	253.5	0.055,0.072,14.597	2.3E-02	6.5E-02	
	4	410.6	0.679,0.826,11.802	2.7E-01	3.2E-01	
	5	500.0	0.940,2.079,9.746	9.5E-01	9.1E-01	
	6	559.8	0.162,2.328,6.328	6.7E-01	7.7E-01	
	7	606.7	10.888,6.678,2.160	3.3	1.3	
	8	668.4	0.149,0.820,18.148	1.8E-01		
6-438	1	0.0	0.000,0.000,19.987	5.2E-05	1.4E-04	664.3
	2	154.1	0.000,0.005,17.576	1.7E-04	6.5E-04	
	3	322.3	0.029,0.029,14.530	1.0E-02	1.5E-02	
	4	483.1	0.051,0.101,11.962	2.6E-02	1.9E-01	
	5	592.5	1.092,1.345,10.451	4.7E-01	6.2E-01	
	6	664.3	1.071,3.477,7.667	1.0	5.8E-01	
	7	713.4	9.377,6.364,2.162	2.8	2.0	
	8	763.7	0.394,1.198,17.190	2.9E-01		
6-481	1	0.0	0.001,0.002,19.809	4.2E-04	1.0E-03	517.5
	2	96.9	0.025,0.003,18.966	1.1E-03	2.5E-03	
	3	223.4	0.086,0.100,14.561	3.5E-02	6.5E-02	
	4	383.5	0.631,0.735,11.700	2.5E-01	3.5E-01	
	5	479.2	0.827,1.059,11.803	3.7E-01	1.4	
	6	517.5	1.459,5.750,11.803	1.3	1.3	
	7	565.2	0.577,2.725,10.028	7.4E-01	1.8	
	8	603.4	1.164,6.134,14.447	1.5		
6-1008	1	0.0	0.000,0.000,19.816	2.2E-04	1.8E-03	572.9
	2	214.7	0.014,0.015,18.100	5.7E-03	1.1E-02	
	3	303.6	0.079,0.108,14.667	3.6E-02	3.9E-02	
	4	423.7	0.108,0.255,12.328	6.8E-02	3.0	

	5	497.1	0.576,1.218,11.807	3.6E-01	5.6E-01	
	6	572.9	1.826,4.399,7.288	1.3	1.9	
	7	661.9	0.462,3.420,7.335	7.3E-01	2.1	
	8	718.5	1.118,6.632,14.180	1.7		
6-1030	1	0.0	0.000,0.001,19.884	6.7E-05	8.7E-04	483.2
	2	222.7	0.009,0.010,17.711	3.7E-03	6.2E-03	
	3	307.9	0.053,0.068,14.744	2.3E-02	4.0E-02	
	4	404.5	0.246,0.352,12.706	1.1E-01	3.0	
	5	483.2	0.538,1.254,10.299	3.5E-01	4.3E-01	
	6	574.5	1.853,3.759,6.778	1.1	2.2	
	7	662.7	2.965,3.866,10.274	1.3	2.1	
	8	738.4	0.718,3.149,16.948	7.4E-01		
6-1053	1	0.0	0.000,0.000,19.934	4.5E-05	4.1E-04	751.4
	2	253.1	0.005,0.006,17.424	2.2E-03	5.1E-03	
	3	373.4	0.078,0.089,14.659	3.1E-02	3.1E-02	
	4	477.5	0.060,0.211,12.338	5.1E-02	8.8E-02	
	5	567.6	0.416,0.597,9.847	1.9E-01	2.3E-01	
	6	665.8	0.288,0.686,6.722	1.8E-01	3.4E-01	
	7	751.4	6.921,6.133,3.199	2.3	2.2	
	8	824.2	0.767,3.518,16.440	8.1E-01		
6-1072	1	0.0	0.000,0.001,19.939	2.8E-05	3.6E-04	720.1
	2	223.8	0.003,0.003,17.445	1.2E-03	3.4E-03	
	3	350.3	0.130,0.142,14.543	4.9E-02	4.7E-02	
	4	457.2	0.099,0.332,12.458	9.0E-02	1.1E-01	
	5	547.4	0.408,0.811,9.742	2.3E-01	4.1E-01	
	6	641.3	1.158,2.260,6.718	6.7E-01	2.3	
	7	720.1	3.083,4.163,7.959	1.5	1.8	
	8	779.7	0.838,4.018,15.783	9.0E-01		
6-1182	1	0.0	0.003,0.003,19.942	9.4E-04	1.2	68.9
	2	68.9	0.011,0.019,18.724	6.0E-03	1.0E-01	
	3	227.4	0.127,0.144,14.650	5.1E-02	6.6E-02	
	4	389.9	0.581,0.716,11.492	2.4E-01	2.0	
	5	475.2	3.413,5.259,11.830	1.7	2.2	
	6	517.9	0.159,3.031,10.199	8.2E-01	9.6E-01	
	7	569.5	1.250,2.436,15.029	7.8E-01	4.8E-01	
	8	638.2	0.250,0.560,19.466	1.5E-01		
6-1289	1	0.0	0.003,0.004,19.807	1.2E-03	1.8	98.8
	2	98.8	0.008,0.012,17.215	3.4E-03	2.4	
	3	272.5	0.077,0.095,14.620	2.9E-02	5.0E-02	
	4	423.4	0.850,1.019,11.578	3.2E-01	4.0E-01	
	5	510.5	2.581,5.094,7.639	1.4	2.1	
	6	563.4	2.203,3.439,8.502	1.1	1.1	
	7	616.4	0.881,2.406,14.070	6.1E-01	3.1E-01	
	8	708.1	0.184,0.568,19.108	1.4E-01		
6-1486	1	0.0	0.001,0.002,19.776	3.9E-04	1.6	106.7
	2	106.7	0.012,0.016,17.881	5.2E-03	2.4	
	3	266.9	0.048,0.067,14.905	2.2E-02	2.9	
	4	402.3	0.070,0.265,11.832	6.9E-02	2.9	
	5	493.9	2.094,4.291,8.930	1.3	2.3	
	6	529.0	1.292,6.600,12.049	1.9	1.3	
	7	559.3	0.692,0.879,18.262	3.0E-01	9.1E-01	
	8	671.6	0.171,0.484,19.336	1.2E-01		
6-1510	1	0.0	0.000,0.000,19.653	5.7E-05	1.8	104.7
	2	104.7	0.005,0.006,17.445	2.0E-03	2.3	
	3	269.6	0.068,0.075,14.962	2.7E-02	2.9	
	4	404.6	0.165,0.380,11.785	1.0E-01	3.2E-01	

	5	501.0	2.326,4.569,7.935	1.3	2.1	
	6	539.4	1.250,5.835,13.750	1.3	1.5	
	7	554.2	0.562,0.927,17.200	2.8E-01	4.7E-01	
	8	658.7	0.108,0.417,19.314	1.1E-01		
6-1572	1	0.0	0.000,0.002,19.799	5.1E-04	1.7	168.3
	2	168.3	0.013,0.005,17.615	5.2E-03	2.4	
	3	308.4	0.063,0.080,4.846	2.6E-02	1.4E-01	
	4	415.5	0.733,0.961,12.733	3.3E-01	3.4E-01	
	5	476.8	0.162,1.531,10.729	3.6E-01	2.4	
	6	558.7	6.187,4.420,2.514	1.9	2.2	
	7	635.9	2.805,5.433,11.150	1.4	2.1	
	8	715.9	0.447,1.538,18.385	3.7E-01		
6-1803	1	0.0	0.001,0.001,19.868	4.4E-04	8.4E-04	563.6
	2	116.1	0.005,0.007,17.326	2.2E-03	3.9E-03	
	3	295.9	0.078,0.096,14.549	3.1E-02	3.8E-02	
	4	451.4	0.135,0.255,11.577	6.8E-02	3.1	
	5	563.6	2.293,3.214,8.173	1.1	3.1	
	6	610.0	9.541,7.135,2.475	3.0	1.6	
	7	655.2	0.951,2.077,14.590	6.3E-01	4.0E-01	
	8	730.4	0.052,0.457,18.812	1.0E-01		
6-1818	1	0.0	0.001,0.002,19.806	5.9E-04	1.0E-03	506.8
	2	90.6	0.005,0.008,17.257	2.3E-03	3.4E-03	
	3	259.8	0.039,0.051,14.608	1.6E-02	2.4E-02	
	4	406.3	0.181,0.293,11.599	8.1E-02	1.9	
	5	506.8	7.440,6.212,3.939	2.6	7.2E-01	
	6	551.5	1.046,4.802,10.771	1.3	7.9E-01	
	7	603.1	0.979,1.869,15.678	6.0E-01	3.0E-01	
	8	684.4	0.035,0.274,19.155	6.3E-02		
6-1829	1	0.0	0.002,0.002,19.818	6.8E-04	1.2E-03	470.8
	2	86.0	0.007,0.011,17.293	3.1E-03	4.0E-03	
	3	241.1	0.040,0.056,14.647	1.6E-02	2.5E-02	
	4	376.8	0.307,0.397,11.782	1.2E-01	7.1E-01	
	5	470.8	3.844,4.795,8.253	1.7	2.5	
	6	512.3	1.320,5.299,11.210	1.5	1.1	
	7	553.2	1.202,2.842,14.638	8.3E-01	1.9E-01	
	8	646.0	0.018,0.112,19.299	2.7E-01		
3-1	1	0.0	0.000,0.000,20.027	3.5E-06	1.4E-05	891.9
	2	295.9	0.000,0.000,17.235	1.6E-04	3.2E-04	
	3	497.8	0.008,0.009,14.524	3.0E-03	4.3E-03	
	4	652.5	0.037,0.053,11.834	1.5E-02	1.5E-02	
	5	784.1	0.219,0.291,9.253	9.2E-02	4.3E-01	
	6	891.9	3.241,3.369,6.488	1.3	2.5	
	7	972.9	2.654,4.770,10.958	1.5	2.5	
	8	1050.6	0.459,1.698,17.692	4.3E-01		
3-2	1	0.0	0.000,0.000,20.028	3.2E-06	1.3E-05	892.2
	2	295.7	0.000,0.000,17.239	1.5E-04	3.4E-04	
	3	497.3	0.009,0.009,14.519	3.2E-03	4.6E-03	
	4	652.4	0.035,0.052,11.831	1.5E-02	1.4E-02	
	5	784.1	0.158,0.224,9.268	6.9E-02	4.2E-01	
	6	892.3	3.150,3.358,6.539	1.3	2.6	
	7	974.2	2.746,4.520,10.670	1.5	2.6	
	8	1047.1	0.528,2.048,17.450	5.4E-01		
3-3	1	0.0	0.000,0.000,20.028	2.7E-06	1.1E-05	892.6
	2	295.4	0.000,0.000,17.244	1.4E-04	3.4E-04	
	3	497.0	0.009,0.009,14.517	3.2E-03	4.7E-03	
	4	652.5	0.038,0.054,11.831	1.6E-02	1.3E-02	

	5	784.2	0.152,0.219,9.278	6.8E-02	4.2E-01	
	6	892.7	3.146,3.360,6.577	1.2	2.6	
	7	975.4	2.812,4.243,10.438	1.4	2.6	
	8	1044.5	0.588,2.375,17.228	6.3E-01		
3-14	1	0.0	0.000,0.000,20.017	7.1E-06	3.8E-05	882.1
	2	290.7	0.000,0.001,17.238	3.5E-04	5.5E-04	
	3	495.2	0.008,0.009,14.516	2.9E-03	4.6E-03	
	4	654.7	0.007,0.025,11.857	6.3E-03	3.9E-02	
	5	781.6	0.625,0.705,9.339	2.4E-01	5.6E-01	
	6	882.2	2.706,3.214,6.532	1.1	2.5	
	7	954.5	2.305,6.155,11.823	1.8	1.9	
	8	1066.2	0.199,0.577,18.839	1.3E-01		
3-22	1	0.0	0.000,0.000,20.026	3.3E-06	2.7E-05	897.5
	2	297.2	0.000,0.000,17.259	2.8E-04	4.2E-04	
	3	502.8	0.008,0.009,14.533	3.0E-03	4.4E-03	
	4	663.4	0.016,0.033,11.919	8.7E-03	2.6E-02	
	5	792.2	0.294,0.365,9.472	1.2E-01	2.7E-01	
	6	897.5	1.929,2.228,6.737	8.0E-01	2.4	
	7	972.9	2.754,5.767,11.359	1.7	1.8	
	8	1059.8	0.389,1.350,18.160	3.1E-01		
3-28	1	0.0	0.000,0.000,20.039	1.9E-06	1.5E-05	924.5
	2	307.5	0.000,0.000,17.290	4.1E-05	3.9E-04	
	3	514.2	0.013,0.015,14.492	5.1E-03	9.3E-03	
	4	676.8	0.052,0.075,11.991	2.4E-02	3.4E-02	
	5	809.9	0.226,0.362,9.511	1.1E-01	2.8E-01	
	6	924.5	2.168,2.946,6.830	9.8E-01	2.6	
	7	1016.5	4.909,3.343,0.887	1.5	2.5:	
	8	1066.1	12.328,8.724,1.257	3.6		
3-33	1	0.0	0.000,0.000,20.039	1.8E-06	1.6E-05	936.7
	2	317.9	0.000,0.000,17.295	1.3E-05	4.6E-04	
	3	524.6	0.014,0.017,14.492	5.6E-03	1.0E-2	
	4	686.4	0.053,0.799,12.022	2.4E-02	3.5E-02	
	5	819.9	0.217,0.365,9.534	1.1E-01	2.4E-01	
	6	936.7	1.932,2.696,6.886	8.8E-01	2.2	
	7	1030.3	5.597,3.502,0.618	1.6	2.3	
	8	1083.9	13.426,7.426,1.190	3.5		
3-64	1	0.0	0.000,0.000,20.005	2.8E-05	1.5E-04	881.2
	2	309.5	0.003,0.003,17.279	1.1E-03	1.7E-03	
	3	510.3	0.023,0.029,14.582	9.5E-03	1.4E-02	
	4	660.8	0.056,0.112,11.905	3.1E-02	7.9E-01	
	5	783.5	0.736,0.879,9.458	2.9E-01	3.2	
	6	881.2	3.214,4.504,6.863	1.5	2.1	
	7	956.4	2.212,4.702,12.415	1.5	2.1	
	8	1056.5	0.258,0.822,18.352	1.9E-01		
3-127	1	0.0	0.000,0.000,20.004	8.5E-06	9.1E-05	878.8
	2	255.6	0.001,0.001,17.445	4.4E-04	6.9E-04	
	3	483.2	0.009,0.011,14.550	3.5E-03	6.8E-03	
	4	671.7	0.065,0.073,11.854	2.4E-02	3.1	
	5	805.6	0.029,0.228,10.285	6.2E-02	8.1E-01	
	6	878.8	2.332,3.740,9.940	1.2E-01	1.9	
	7	944.1	2.472,4.352,13.255	1.3	1.8	
	8	1028.9	0.402,1.374,18.482	3.0E-01		
3-248	1	0.0	0.000,0.000,19.979	1.9E-05	5.1E-05	784.2
	2	251.8	0.001,0.001,17.274	3.3E-04	8.3E-04	
	3	431.2	0.016,0.020,14.550	6.4E-03	1.1E-02	
	4	566.8	0.186,0.228,11.753	7.1E-02	9.6E-02	

5	689.5	0.702,0.987,9.193	3.0E-01	2.9
6	784.2	4.378,5.337,7.659	1.9	2.6
7	864.1	1.798,2.692,13.687	9.2E-01	6.9E-01
8	939.1	0.318,1.029,17.893	2.5E-01	

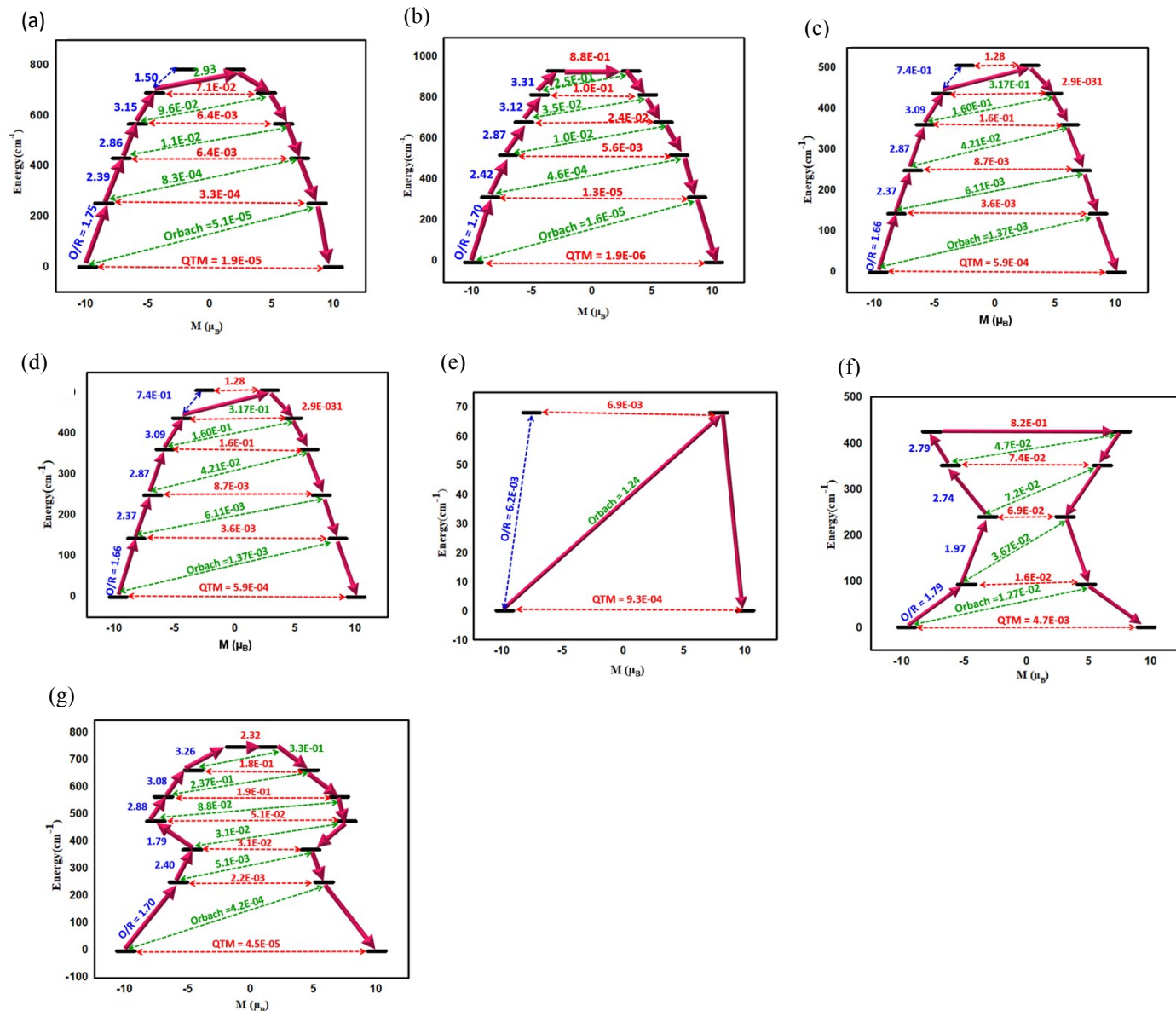


Figure S3. Magnetic blockade diagrams for, (a) 3-10 (b) 3-7 (c) 5-5, (d) 5-1, (e) 6-19, (f) 6-10, (g) 6-17

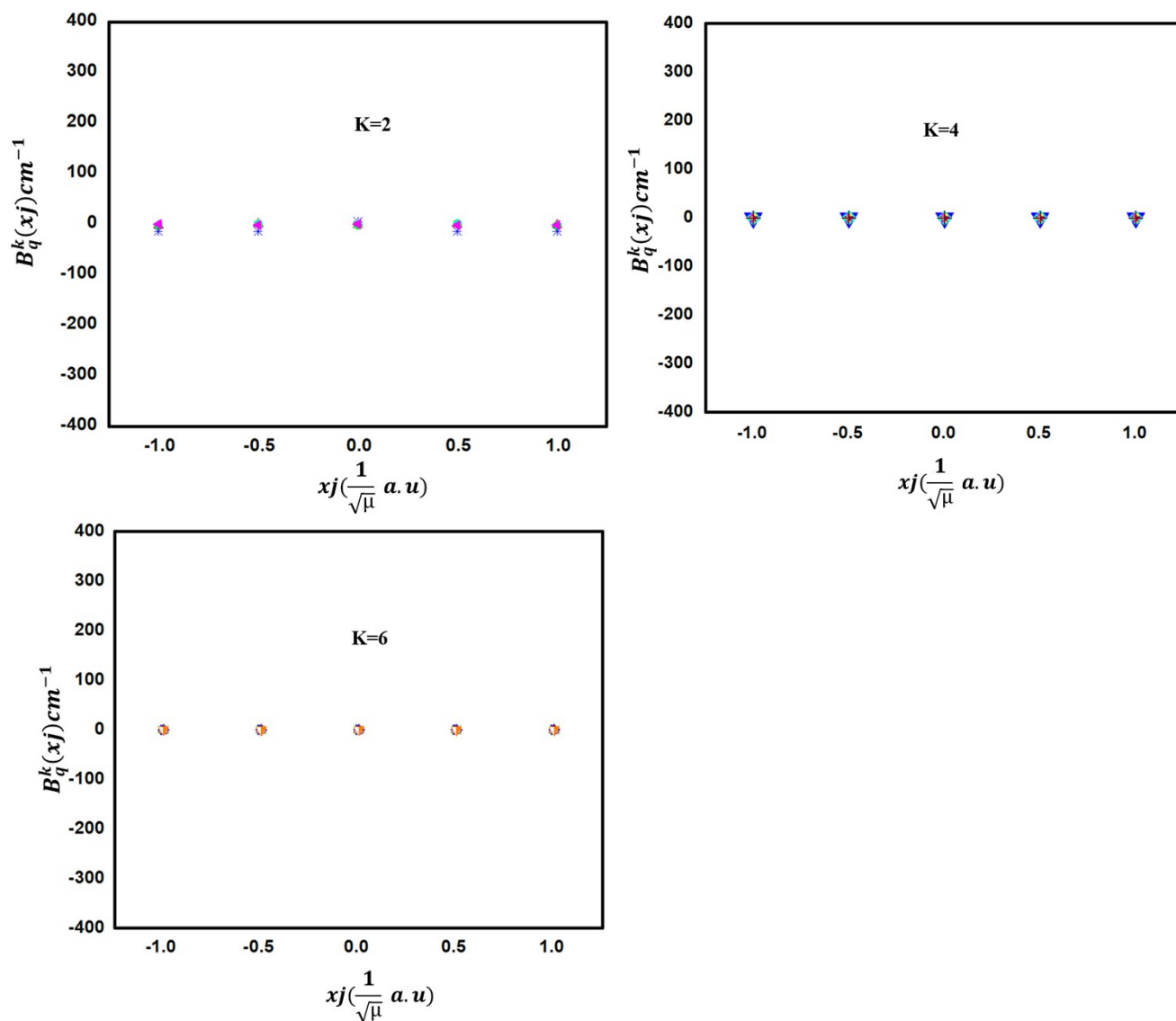


Figure S4. Plots showing the crystal field parameters for the complex **3**.

Table S7. CASSCF+RASSI-SO computed energies of all low-lying KDs, and SINGLE_ANISO computed g -tensors of of **3** at the

displacement, $\chi_j\left(\frac{1}{\sqrt{\mu_j}}a.u.\right) = 0.00$, **0.5, 1.0, (-0.5) and (-1.0)** (Note: Red highlighted KD are those from where relaxation is occurring)

KDs	$E(\text{cm}^{-1})$	g_{xx}	g_{yy}	g_{zz}
$\chi_j\left(\frac{1}{\sqrt{\mu_j}}a.u.\right) = 0.00$				

1	0.0	0.000	0.000	19.983
2	301.6	0.000	0.000	17.201
3	509.3	0.007	0.008	14.504
4	668.3	0.042	0.058	11.814
5	803.1	0.334	0.416	9.204
6	912.9	3.319	3.372	6.397
7	994.2	2.549	5.026	11.217
8	1505.7	0.389	1.373	17.938

$$\chi_j\left(\frac{1}{\sqrt{\mu_j}}a.u.\right) = 0.5$$

1	0.0	0.000	0.000	19.976
2	286.9	0.002	0.002	17.189
3	477.4	0.043	0.047	14.386
4	625.2	0.226	0.292	11.766
5	754.6	0.802	1.331	9.091
6	868.7	5.976	5.155	3.021
7	958.6	2.428	4.755	12.209
8	1055.4	0.351	1.134	18.479

$$\chi_j\left(\frac{1}{\sqrt{\mu_j}}a.u.\right) = 1$$

1	0.0	0.000	0.000	19.962
2	274.9	0.015	0.023	16.955
3	431.1	0.184	0.209	13.926
4	571.6	0.477	0.771	11.276

5	718.5	1.362	2.528	8.714
6	848.7	3.823	5.168	7.796
7	960.2	2.033	3.812	13.842
8	1070.1	0.332	0.979	18.870
$\chi_j\left(\frac{1}{\sqrt{\mu_j}}a.u.\right) = (-0.5)$				
1	0.0	0.000	0.000	19.955
2	285.9	0.004	0.005	17.079
3	473.6	0.047	0.055	14.248
4	618.4	0.454	0.563	11.431
5	743.6	2.849	3.397	8.250
6	851.3	4.043	4.975	9.332
7	969.7	1.107	1.822	15.085
8	1101.2	0.121	0.313	19.213
$\chi_j\left(\frac{1}{\sqrt{\mu_j}}a.u.\right) = (-1.0)$				
1	0.0	0.000	0.000	19.929
2	271.6	0.022	0.033	16.798
3	428.9	0.210	0.244	13.772
4	568.3	0.861	1.162	11.040
5	706.6	3.121	4.544	7.865
6	835.5	3.919	4.200	10.459
7	976.0	1.089	1.672	15.667
8	1121.4	0.141	0.341	19.415

Input for optimisation, Molcas and BOMD

Optimisation input

%mem=8000mb

%NProcShared=8

%NProLinda=2

%chk=/home/rajaraman/Tanu/Orca/opti_orca/opt-Cor6-5.chk

#p UB3LYP/gen opt freq scfcyc=500 gfinput gfoldprinT pseudo=cards

optimisation of opt-Cor6-5

2,8

Gd

	-1.766900000	-0.416976000	-0.339676000
C	-0.587451000	-1.188944000	2.094190000
H	-1.079887000	-1.836102000	2.816439000
C	-0.795992000	0.203951000	2.217296000
H	-1.436162000	0.547663000	3.025311000
C	0.205183000	2.574114000	1.641427000
H	-0.359056000	3.119696000	2.391575000
C	1.277423000	3.205065000	1.017928000
H	1.507354000	4.225020000	1.313950000
C	3.519729000	2.835044000	-0.278557000
H	3.917879000	3.824749000	-0.076132000
C	4.380816000	1.861919000	-0.779615000
H	5.418720000	2.133696000	-0.949619000
C	4.773356000	-0.717749000	-0.998699000
H	5.840919000	-0.638369000	-1.183224000
C	4.251580000	-1.971803000	-0.689367000
H	4.929908000	-2.818464000	-0.644410000
C	2.247588000	-3.201133000	0.461197000
H	2.773277000	-4.143912000	0.586324000
C	1.049891000	-3.030238000	1.150370000
H	0.687677000	-3.838535000	1.778234000

C	0.369105000	-1.753239000	1.155120000
C	-0.071765000	1.172681000	1.411023000
C	2.161424000	2.522028000	0.094939000
C	3.969805000	0.485127000	-0.954257000
C	2.871332000	-2.141491000	-0.305029000
C	2.079873000	-1.009261000	-0.480716000
C	0.881869000	-0.817552000	0.243699000
C	0.665351000	0.597533000	0.365060000
C	1.733921000	1.253860000	-0.289125000
C	2.608247000	0.264595000	-0.796668000
C	-4.002827000	-0.151308000	-1.689115000
C	-4.392313000	-0.471114000	-0.357823000
C	-4.016250000	0.612359000	0.484024000
C	-3.398442000	1.607245000	-0.330008000
C	-3.393445000	1.135715000	-1.671926000
H	-4.197959000	-0.751772000	-2.571174000
H	-4.930661000	-1.360638000	-0.048874000
H	-4.229907000	0.698328000	1.542668000
H	-3.050595000	2.577426000	0.004130000
H	-3.037930000	1.683231000	-2.538173000

CH 0

6-31G*

Gd 0

SP 3 1.00

17.24000000000000 3.607000091537422E-003 -2.072870013100241E-002

3.346000000000000 0.737570618717857 0.519148703280945

2.429000000000000 -1.71492784352095 -1.48838220940636

SP 1 1.00

0.934900000000000 1.000000000000000 1.000000000000000

SP 1 1.00

0.358800000000000 1.000000000000000 1.000000000000000

SP 1 1.00

8.105000000000000E-002 1.000000000000000 1.000000000000000

D 2 1.00

0.857300000000000 0.305193173183232

0.412800000000000 0.739945149015201

D 1 1.00

0.151900000000000 1.000000000000000

F 6 1.00

77.6000000000000 1.583755898700157E-002

28.6100000000000 9.647586944747537E-002

12.1300000000000 0.235859801924552

5.23900000000000 0.380304259854489

2.30500000000000 0.373451413617453

0.994200000000000 0.241992063517626

F 1 1.00

0.403100000000000 1.000000000000000

Gd 0

Gd1-ECP 3 46

component 1

2

1 13.095090800 -15.786726000

1 2.569738560 -6.127778140

component 2

3

2 2.702265230 -137.902125000

2 2.933477410 208.964540000

0 9.850809640 16.858693600

component 3

3

0 10.256201200 11.130834300

2 2.452732130 131.651321000

2 2.196934270 -77.444300800

component 4

2

2 2.247169230 31.466411800

0 6.430643690 8.345072860

Molcas inputs

Guess orbital

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  Charge
    2
  Coord
    3-Cor-TZVP.xyz
  Group
  NoSym
  Basis set
  C.ANO-RCC...4s3p2d1f.,H.ANO-RCC...3s2p1d.,Dy.ANO-RCC...8s7p5d3f2g1h.
  ANGM
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  SDIPolar
  AMFI
  Douglas-Kroll
&SEWARD
  Cholesky
&GUESSORB
  PRMO
    3
  PRPopulation
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Spin  
6  
Inactive  
110  
Nactel  
9 0 0  
Ras2  
7  
Alter  
7  
1 111 101  
1 112 102  
1 113 103  
1 114 104  
1 115 105  
1 116 106  
1 117 107  
CiRoot  
21 21 1
```

RASSI

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Nr of JobIph  
1 21  
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21  
Spin  
MEES  
Properties  
3  
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SOProperties  
3  
'AngMom' 1 'AngMom' 2 'AngMom' 3
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SINGLE_ANISO

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8  
2 2 2 2 2 2 2 2  
CRYS  
Dy  
UBAR  
TINT  
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BOMD input

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METHOD Quickstep

&DFT

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POTENTIAL_FILE_NAME /opt/cp2k-2.4.0/cp2k-2.4.0/tests/QS/GTH_POTENTIALS
WFN_RESTART_FILE_NAME /home/rajaraman/Tanu/MD-cp2k/Y-Cor6-5-RESTART.wfn
UKS T
CHARGE 3
MULTIPLICITY 1
&MGRID
  NGRIDS 5
  CUTOFF 400
  REL_CUTOFF 60
&END MGRID
&QS
METHOD GAPW
EXTRAPOLATION PS
EXTRAPOLATION_ORDER 4
EPS_DEFAULT 1.0E-8
&END QS
&SCF
  SCF_GUESS RESTART
  EPS_SCF 1.0E-8
  MAX_SCF 300
&MIXING T
  METHOD BROYDEN_MIXING
  ALPHA 0.1
  BETA 1.5
  NBROYDEN 8
&END MIXING
&OUTER_SCF
  EPS_SCF 1.0E-8
  MAX_SCF 100
  OPTIMIZER DIIS
&END OUTER_SCF
&OT ON
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N_HISTORY_VEC       7
ENERGY_GAP          1.0000000000000000E-04
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&PRINT
&RESTART
LOG_PRINT_KEY       T
&END RESTART
&END PRINT
&END SCF
&PRINT
&END PRINT
&XC
&XC_GRID
XC_SMOOTH_RHO       NN50
XC_DERIV             NN50_SMOOTH
&END XC_GRID
&XC_FUNCTIONAL      NO_SHORTCUT
&PBE T
PARAMETRIZATION     PBESOL
&END PBE
&END XC_FUNCTIONAL
&VDW_POTENTIAL
POTENTIAL_TYPE      PAIR_POTENTIAL
&PAIR_POTENTIAL
R_CUTOFF            1.6000000000000000E+01
TYPE                DFTD2
SCALING              1.0000000000000000E+00
&END PAIR_POTENTIAL
&END VDW_POTENTIAL
DENSITY_CUTOFF      1.0E-9
GRADIENT_CUTOFF     1.0E-9

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&END PRINT
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C 0.000000000 0.000000000 x
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&END CELL
&COORD
M x y z
&END COORD
&KIND H
BASIS_SET TZVP-MOLOPT-GTH
POTENTIAL GTH-PBE-q1
&END KIND
&KIND C
BASIS_SET TZVP-MOLOPT-GTH
POTENTIAL GTH-PBE-q4
&END KIND
&KIND Y
BASIS_SET DZVP-MOLOPT-SR-GTH
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  &FORCES OFF
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  &END EACH
&END FORCES
&DISTRIBUTION SILENT
&END DISTRIBUTION
&END PRINT
&END FORCE_EVAL
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PROJECT Y-Cor6-5
RUN_TYPE MD
PRINT_LEVEL LOW
&END GLOBAL
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&MD
ENSEMBLE NVT
STEPS 3000
TIMESTEP 1.00
TEMPERATURE 300
&THERMOSTAT
  &NOSE
    TIMECON 50
    LENGTH 3
    YOSHIDA 3
    MTS 2
  &END NOSE
&END THERMOSTAT
&END MD
&PRINT
```

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LOG_PRINT_KEY T
  &EACH
    MD 50
  &END EACH
ADD_LAST NUMERIC
&END RESTART
&TRAJECTORY
LOG_PRINT_KEY T
  &EACH
    MD 1
  &END EACH
ADD_LAST NUMERIC
&END TRAJECTORY
&VELOCITIES
LOG_PRINT_KEY T
  &EACH
    MD 1
  &END EACH
ADD_LAST NUMERIC
&END VELOCITIES
&END PRINT
&END MOTION
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