Structural and Spectroscopic Characterization of Iron(II), Cobalt(II), and Nickel(II) *Ortho*-Dihalophenolate Complexes: Insights into Metal-Halogen Secondary Bonding

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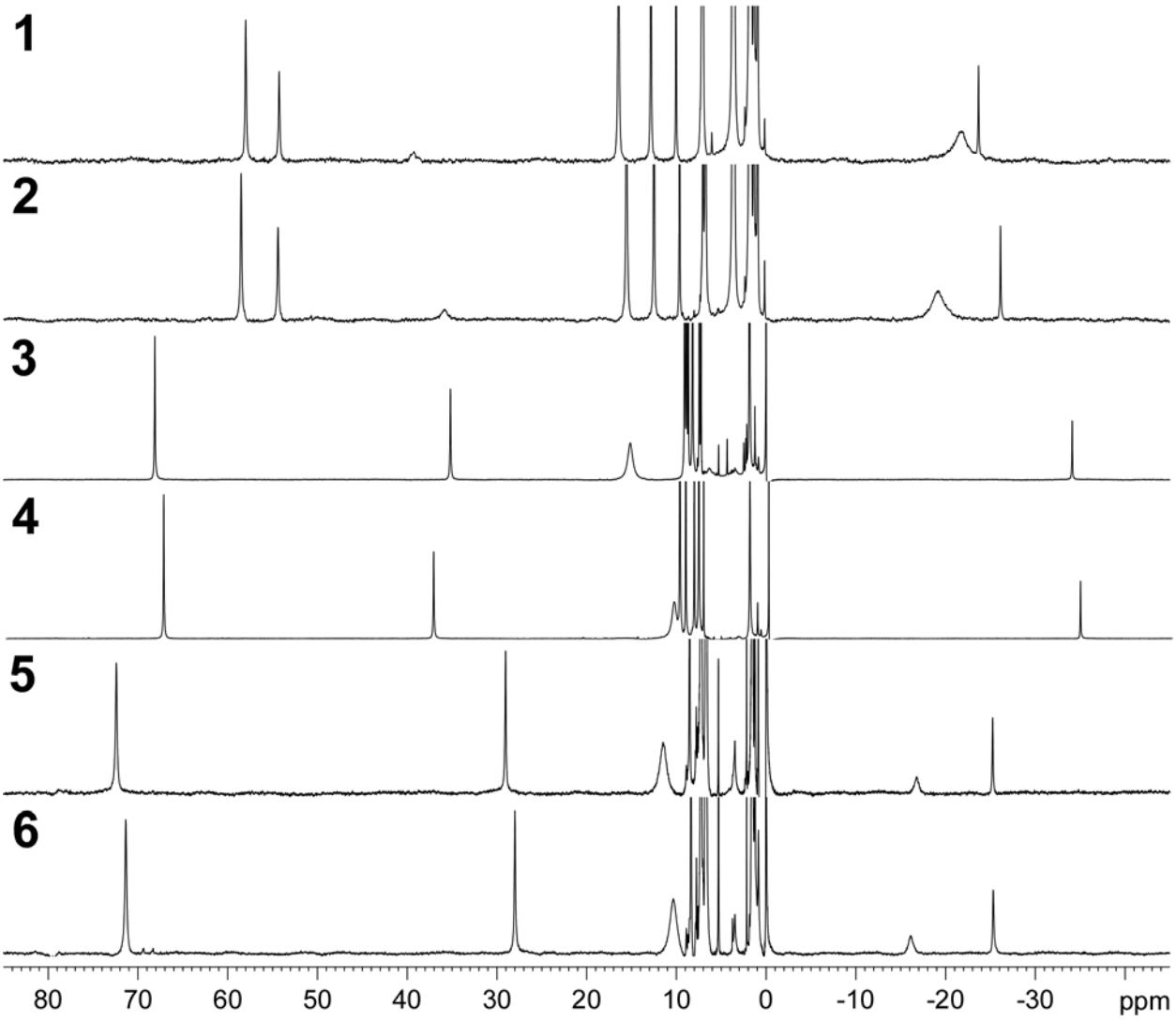

Figure S1. Room-temperature ^{1}H NMR spectra of complexes **1-6**. Complexes **1** and **2** are in d_8-THF, and complexes **3-6** are in $CDCl_3$.

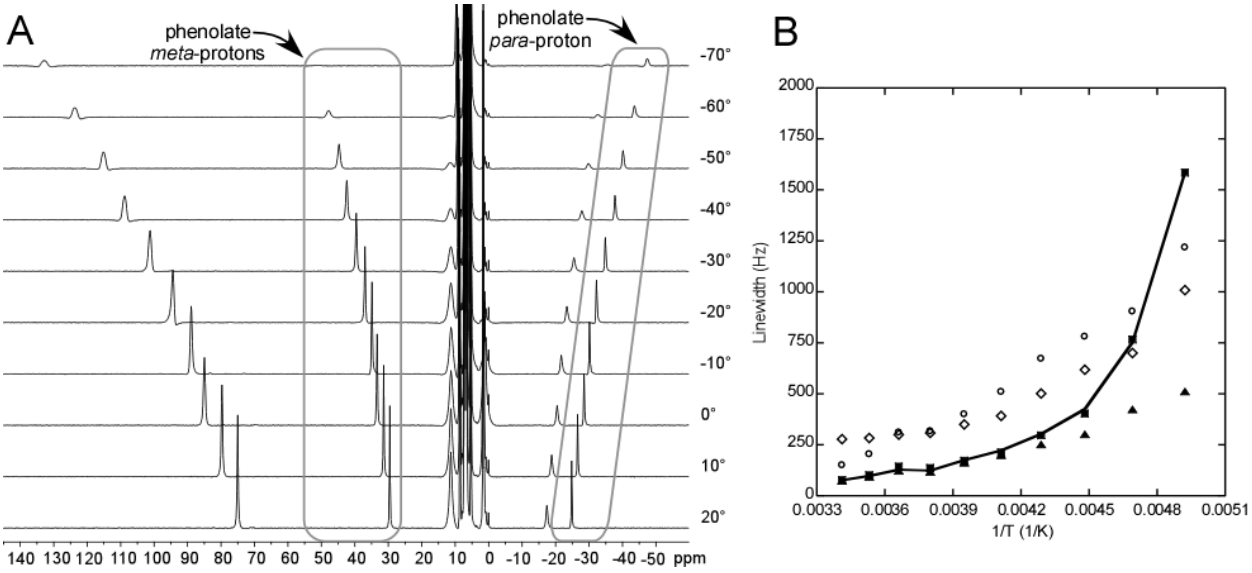

Figure S2. (A) Variable temperature ^{1}H NMR spectra of **5** in CD_2Cl_2. The phenolate *meta* and *para* protons are highlighted. (B) The temperature dependence of linewidth of the pyrazole H4 (○), phenolate *meta* (■), borate H (◇), and phenolate *para* (▲) proton signals. The fit to the temperature dependence of the linewidth of the phenolate *meta* protons due to exchange broadening as described in the text is shown as a solid line.

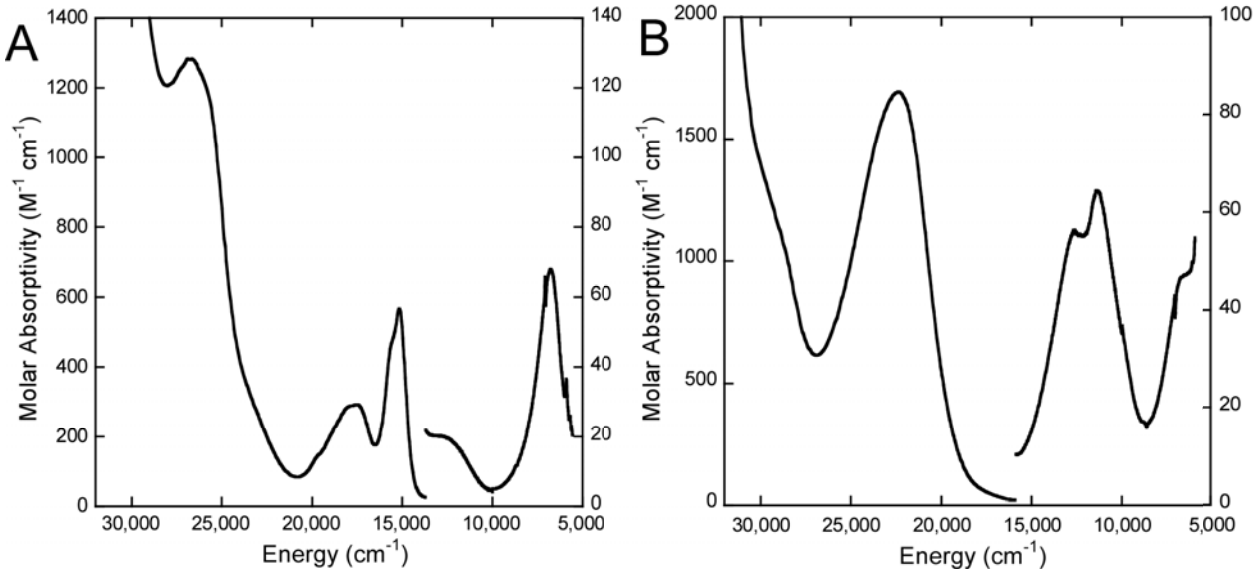

Figure S3. UV-vis-NIR absorption spectra of **4** (A) and **6** (B) in $CHCl_3$ at room temperature.

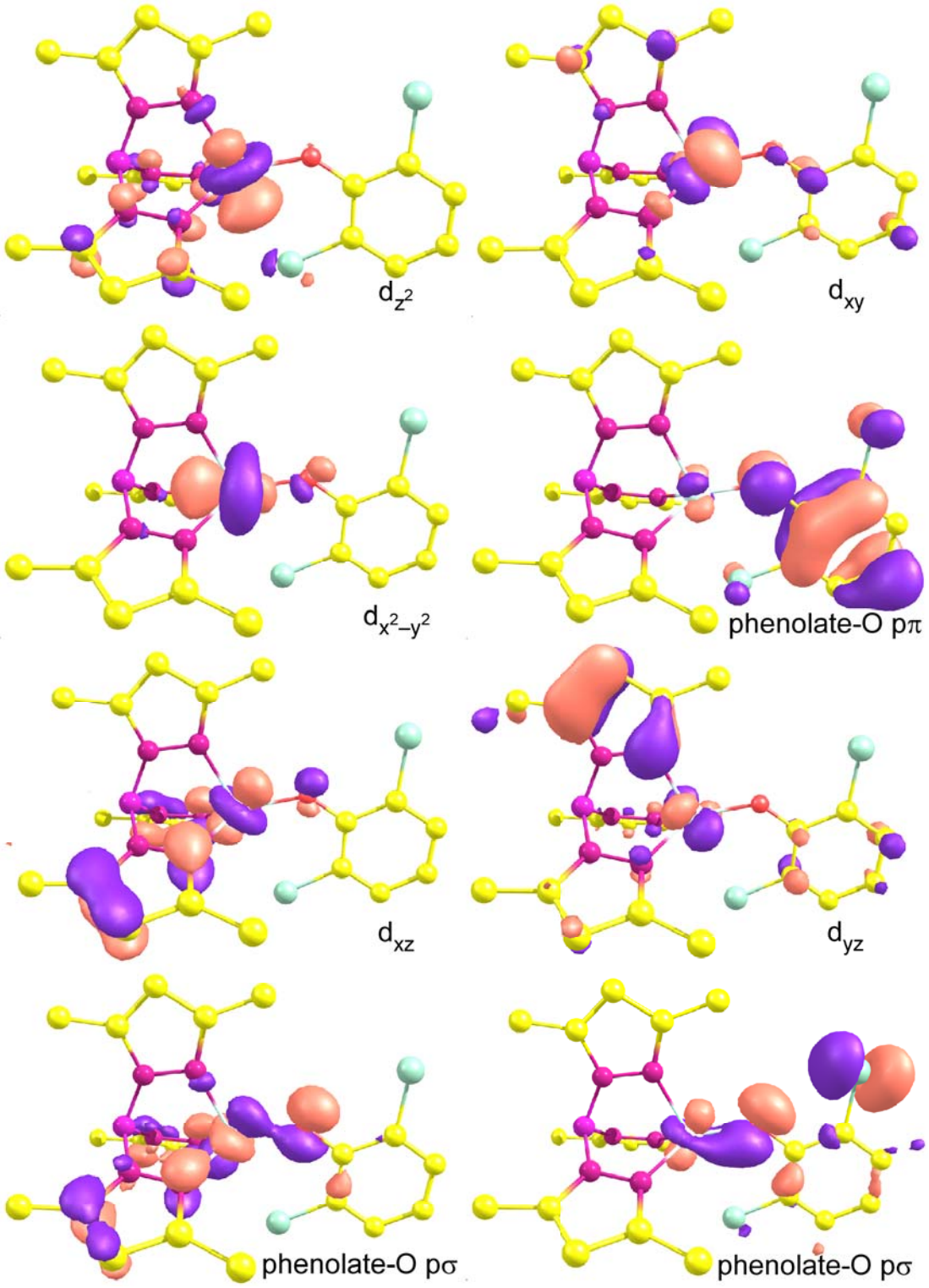

Figure S4. Contour surface of the MOs of Tp*Co(2,6-dcp) with predominantly metal d or phenolate O orbital character, calculated with PBE1PBE.

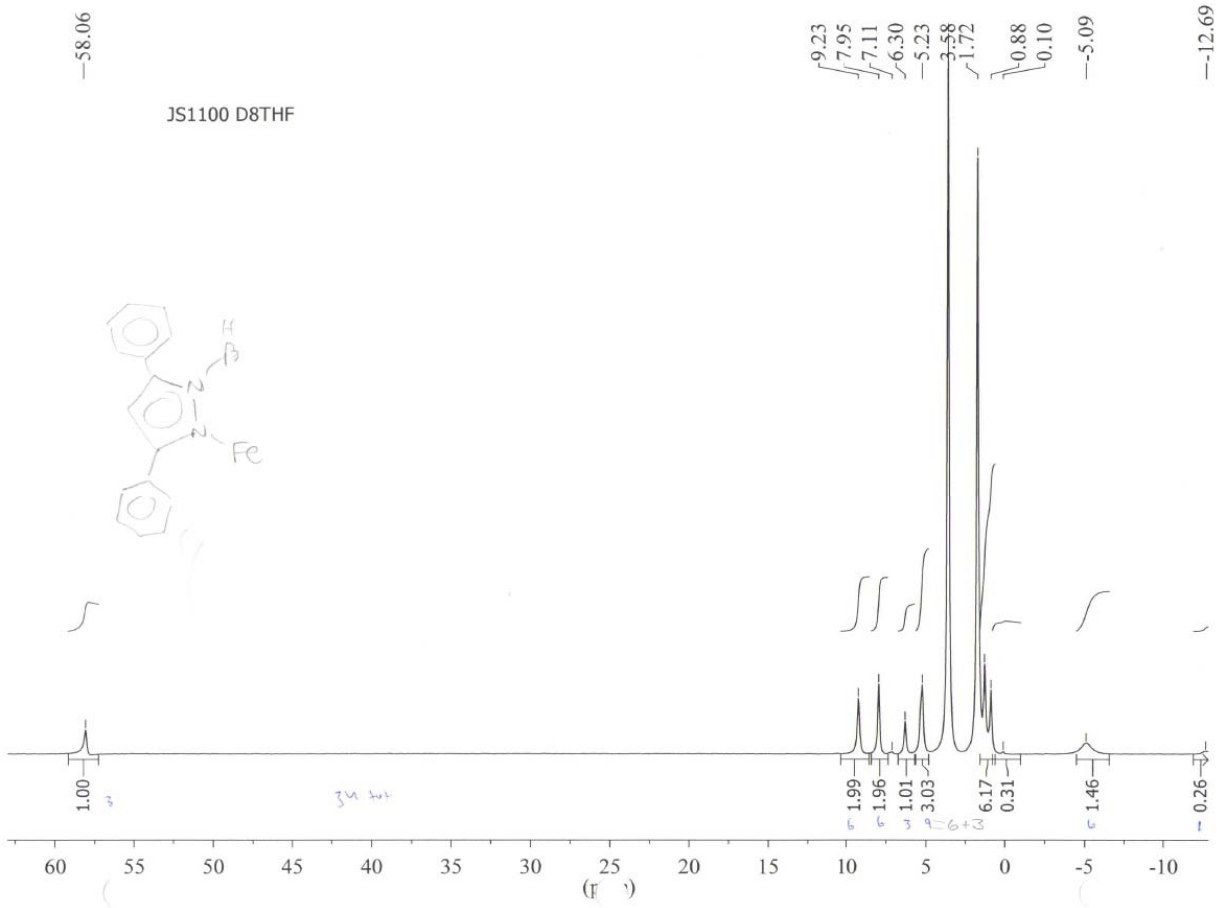

Figure S5. Room-temperature ^{1}H NMR spectra of $Tp^{Ph2}NiBr$ in d_8-THF.

Table S1. Comparison of selected experimentally determined geometric data of Tp^{Ph2}Co(2,6-dcp) (**3**) and Tp^{Ph2}Ni(2,6-dcp) (**5**) with the geometry optimized results from B3LYP and PBE1PBE.

Bond Lengths (Å)						
	3 (exp.)	**3** (B3LYP)	**3** (PBE1)	**5** (exp.)	**5** (B3LYP)	**5** (PBE1)
M-N1	2.038(3)	2.058	2.044	2.0319(16)	2.031	2.008
M-N3	2.088(3)	2.066	2.051	2.0387(15)	2.051	2.036
M-N5	2.036(3)	2.058	2.044	2.0348(15)	2.027	2.021
M-O1	1.885(3)	1.900	1.898	1.9035(13)	1.933	1.931
M-X1	2.8325(12)	3.035	2.908	2.5601(6)	2.849	2.695
Bond Angles (°)						
O1-M-N1	132.45(12)	128.78	129.12	116.67(6)	135.21	119.42
O1-M-N5	125.66(12)	128.58	129.14	149.52(6)	128.52	145.22
N1-M-N5	95.63(12)	95.15	95.06	93.50(6)	93.36	93.41
N3-M-O1	108.90(12)	110.31	109.26	93.95(6)	104.03	101.21
N3-M-N1	91.47(12)	91.20	91.05	93.48(6)	89.36	90.22
N3-M-N5	90.15(12)	91.22	91.05	88.05(6)	89.75	88.96
X1-M-O1	75.03(9)	71.13	73.18	80.14(4)	74.84	77.27
X1-M-N1	86.80(9)	87.79	87.31	96.82(4)	91.00	92.45
X1-M-N5	86.18(9)	87.83	87.31	92.74(4)	91.50	91.1
N3-M-X1	175.77(9)	178.55	177.56	169.60(5)	178.68	177.32
M-O1-$C46_{phen}$	130.1(3)	137.08	134.32	125.79(13)	132.00	128.70
$C47_{phen}$-X1-M	91.35(14)	89.67	91.24	94.92(7)	92.08	93.79
Torsion Angles (°)						
M-O1-$C46_{phen}$-$C47_{phen}$	15.4(5)	0.03	–0.03	–5.3(3)	–2.5	–4.8
N3-M-O1-$C46_{phen}$	163.5(3)	179.98	180.03	176.33(15)	–178.24	–177.37
Tau value	0.72	0.83	0.81	0.33	0.72	0.54

Table S2. Wiberg and Löwdin bond orders for Tp*M(2,6-dcp).

	Wiberg		Löwdin	
Bond	M = Co	M = Ni	M = Co	M = Ni
M-O	0.343	0.324	0.433	0.342
M-$N3_{(ax)}$	0.208	0.222	0.319	0.329
M-$N1_{(eq)}$	0.216	0.216	0.322	0.338
M-$N5_{(eq)}$	0.216	0.252	0.322	0.323
M-Cl	0.016	0.084	0.083	0.128

Table S3. Optimized energies for Tp*Co(2,6-dcp) model with different dihedral angles (Co-O-$C46_{phen}$-$C47_{phen}$) using either B3LYP or PBE1PBE and 6-311+G(d) basis set for all atoms and 6-311++G(d) for chlorine atoms.

	B3LYP		PBE1PBE	
Dihedral Angle (°)	Energy (Hartree)	ΔE (kJ/mol)	Energy (Hartree)	ΔE (kJ/mol)
0	-3547.5762605	0.000	-3545.5270556	0.000
15	-3547.5761091	0.398	-3545.5268928	0.428
30	-3547.5755996	1.735	-3545.5262123	1.787
45	-3547.5745839	4.402	-3545.5249411	5.552
60	-3547.5734826	7.293	-3545.5235114	9.305
75	-3547.5726485	9.483	-3545.5223390	12.384
90	-3547.5723506	10.263	-3545.5219622	13.373

Table S4. Optimized energies for Tp*Co(2,6-dmp) model with different dihedral angles (Co-O-$C46_{phen}$-$C47_{phen}$) using either B3LYP or PBE1PBE and 6-311+G(d) basis set for all atoms.

	B3LYP		PBE1PBE	
Dihedral Angle (°)	Energy (Hartree)	ΔE (kJ/mol)	Energy (Hartree)	ΔE (kJ/mol)
0	-2706.9702742	0.492	-2705.1398524	0.801
15	-2706.9703419	0.315	-2705.1399718	0.487
30	-2706.9704617	0.000		
32			-2705.1401573	0.000
45	-2706.9704237	0.100	-2705.1400192	0.363
60	-2706.9702302	0.608	-2705.1396372	1.366
75	-2706.9702302	0.608	-2705.1393886	2.018
90	-2706.9700756	1.014	-2705.1393611	2.091

Table S5. Coordinates of the B3LYP geometry-optimized Tp*Co(2,6-dcp) model.

Total number of atoms: 57, Charge = 0, and Spin=3/2, Energy=-3547.5762605 Hartree

Co	-0.173552000	0.121558000	-0.001974000
O	-1.994313000	0.667585000	-0.001875000
C	-3.167711000	0.089567000	-0.000927000
C	-3.372500000	-1.311042000	-0.000078000
Cl	-1.939073000	-2.348018000	-0.000548000
C	-4.626527000	-1.905976000	0.001039000
H	-4.705372000	-2.986958000	0.001534000
C	-5.764392000	-1.104879000	0.001422000
H	-6.750165000	-1.555624000	0.002301000
C	-5.625563000	0.282175000	0.000663000
H	-6.497574000	0.925801000	0.000987000
C	-4.362583000	0.855476000	-0.000516000
Cl	-4.222350000	2.607185000	-0.001471000
N	0.906591000	-0.745379000	1.520473000
C	0.703456000	-1.311513000	2.713940000
C	-0.663376000	-1.469288000	3.301217000
H	-0.630737000	-1.344966000	4.385940000
H	-1.074861000	-2.460926000	3.092860000
H	-1.359022000	-0.733717000	2.894543000
C	1.941717000	-1.695380000	3.255055000
H	2.116923000	-2.176978000	4.205387000
C	2.900972000	-1.323041000	2.323366000
C	4.385730000	-1.490132000	2.392984000
H	4.767764000	-2.097324000	1.568155000
H	4.655859000	-1.986370000	3.326309000
H	4.908797000	-0.530879000	2.360046000
N	2.255789000	-0.747615000	1.278469000
N	1.070658000	1.772113000	-0.004514000
C	0.979486000	3.104417000	-0.007196000
C	-0.342004000	3.804432000	-0.009994000
H	-0.442531000	4.445450000	-0.890879000
H	-0.445747000	4.446239000	0.869959000
H	-1.166977000	3.091790000	-0.010978000
C	2.276115000	3.650031000	-0.006540000
H	2.543599000	4.696161000	-0.008385000
C	3.148270000	2.571044000	-0.003341000
C	4.644138000	2.576086000	-0.001328000
H	5.056754000	2.073933000	-0.880406000
H	5.054333000	2.077061000	0.880701000
H	5.007884000	3.604616000	-0.002625000
N	2.399917000	1.438785000	-0.002186000
N	0.910386000	-0.751866000	-1.518201000
C	0.710093000	-1.322288000	-2.710142000
C	-0.655105000	-1.481056000	-3.300884000
H	-0.622577000	-1.340920000	-4.383760000
H	-1.356139000	-0.756286000	-2.884427000
H	-1.059739000	-2.478542000	-3.107433000
C	1.949594000	-1.709059000	-3.246394000
H	2.127180000	-2.194817000	-4.194165000
C	2.906533000	-1.333574000	-2.313602000
C	4.391440000	-1.501160000	-2.378520000
H	4.771860000	-2.100324000	-1.547158000
H	4.914165000	-0.541413000	-2.353510000
H	4.663685000	-2.006000000	-3.306594000
N	2.258888000	-0.753791000	-1.272671000
B	2.825956000	-0.058715000	0.001952000
H	4.015173000	-0.138787000	0.003555000

Table S6. Coordinates of the B3LYP geometry-optimized Tp*Ni(2,6-dcp) model.

Total number of atoms: 57, Charge = 0, and Spin = 1, Energy = -3673.10812841 Hartree

Ni	-0.181338000	0.001329000	-0.074761000	C	-0.540112000	3.634200000	-0.378489000
O	-1.990451000	0.683490000	-0.099699000	H	-0.695944000	4.376884000	0.409605000
C	-3.150245000	0.086378000	-0.043329000	H	-1.330453000	2.889271000	-0.309698000
C	-3.319301000	-1.319558000	0.004584000	H	-0.638701000	4.155275000	-1.335985000
Cl	-1.846898000	-2.304227000	-0.010881000	C	2.068555000	3.638009000	-0.234355000
C	-4.550606000	-1.955288000	0.060969000	H	2.265674000	4.697566000	-0.301675000
H	-4.597153000	-3.037626000	0.094423000	C	3.006512000	2.624905000	-0.109221000
C	-5.710893000	-1.186506000	0.073232000	C	4.497065000	2.730542000	-0.038563000
H	-6.682531000	-1.664938000	0.116944000	H	4.893885000	2.321679000	0.894486000
C	-5.613055000	0.203575000	0.028801000	H	4.793889000	3.778852000	-0.096681000
H	-6.504296000	0.820299000	0.037779000	H	4.985321000	2.198666000	-0.859632000
C	-4.369308000	0.815503000	-0.027223000	N	2.333325000	1.448630000	-0.057251000
Cl	-4.286554000	2.568915000	-0.080409000	N	1.045939000	-0.878973000	-1.432663000
N	0.894783000	-0.666811000	1.508990000	C	0.898840000	-1.500907000	-2.608556000
C	0.623373000	-1.106931000	2.743232000	C	-0.438109000	-1.730142000	-3.240175000
C	-0.773522000	-1.260299000	3.256416000	H	-0.359744000	-1.667214000	-4.327795000
H	-0.795418000	-1.130896000	4.340444000	H	-1.169622000	-0.991132000	-2.909754000
H	-1.177235000	-2.251381000	3.031748000	H	-0.835414000	-2.718785000	-2.993650000
H	-1.445522000	-0.523045000	2.813670000	C	2.166554000	-1.860832000	-3.094742000
C	1.832200000	-1.370679000	3.407914000	H	2.388101000	-2.376718000	-4.017015000
H	1.954104000	-1.738467000	4.415691000	C	3.082029000	-1.410773000	-2.152526000
C	2.842876000	-1.054325000	2.509494000	C	4.574093000	-1.513335000	-2.168251000
C	4.324769000	-1.132979000	2.696311000	H	4.957470000	-2.028138000	-1.283649000
H	4.797473000	-1.773294000	1.947155000	H	5.051326000	-0.530295000	-2.204492000
H	4.550349000	-1.545882000	3.680685000	H	4.895550000	-2.073236000	-3.047747000
H	4.798900000	-0.150050000	2.629521000	N	2.381543000	-0.819274000	-1.155490000
N	2.252368000	-0.629925000	1.366785000	B	2.856620000	-0.007440000	0.079613000
N	0.986600000	1.686451000	-0.145906000	H	4.047946000	-0.015258000	0.140871000
C	0.811083000	3.007702000	-0.254143000				

Table S7. Coordinates of the B3LYP geometry-optimized Tp*Co(2,6-dcp) model with Co-O-$C46_{Phen}$-$C47_{phen}$ dihedral angle of 90°.

Total number of atoms: 57, Charge = 0, and Spin=3/2, Energy=-3547.5723506 Hartree

Co	0.112143000	0.046915000	-0.415159000
O	1.922226000	0.037705000	-0.966159000
C	3.113252000	0.010089000	-0.421940000
C	3.794777000	-1.198991000	-0.132171000
Cl	2.958461000	-2.717766000	-0.438948000
C	5.079985000	-1.240743000	0.390777000
H	5.544786000	-2.200901000	0.582244000
C	5.754796000	-0.053638000	0.664049000
H	6.760375000	-0.077645000	1.068500000
C	5.127546000	1.164456000	0.415815000
H	5.629909000	2.101304000	0.626872000
C	3.841865000	1.184752000	-0.107844000
Cl	3.068894000	2.741621000	-0.386390000
N	-0.434095000	-0.087270000	1.555608000
C	0.131728000	-0.159562000	2.765321000
C	1.615842000	-0.157976000	2.952018000
H	1.864573000	-0.118377000	4.013718000
H	2.083257000	0.700660000	2.464315000
H	2.073839000	-1.058496000	2.534157000
C	-0.877297000	-0.239632000	3.737502000
H	-0.746637000	-0.307724000	4.807015000
C	-2.082451000	-0.212259000	3.047084000
C	-3.474318000	-0.269316000	3.591687000
H	-4.051288000	0.623448000	3.336523000
H	-3.439883000	-0.345179000	4.679478000
H	-4.026702000	-1.133263000	3.213113000
N	-1.793540000	-0.119492000	1.726487000
N	-1.215634000	-1.392121000	-1.034641000
C	-1.269129000	-2.438824000	-1.862930000
C	-0.087303000	-2.868811000	-2.671649000
H	-0.309244000	-2.817834000	-3.741717000
H	0.189601000	-3.902465000	-2.446211000
H	0.779314000	-2.239131000	-2.470476000
C	-2.563138000	-2.986541000	-1.823020000
H	-2.926913000	-3.841382000	-2.373240000
C	-3.284569000	-2.205741000	-0.931187000
C	-4.714792000	-2.340354000	-0.514773000
H	-5.303809000	-1.458642000	-0.780888000
H	-4.814359000	-2.484639000	0.564133000
H	-5.162305000	-3.203070000	-1.010440000
N	-2.452501000	-1.242286000	-0.461816000
N	-1.239790000	1.539677000	-0.829372000
C	-1.315654000	2.692548000	-1.500532000
C	-0.145446000	3.259891000	-2.238094000
H	-0.403749000	3.457401000	-3.282262000
H	0.704880000	2.578407000	-2.217660000
H	0.176797000	4.207932000	-1.797667000
C	-2.618493000	3.206006000	-1.381495000
H	-2.999189000	4.123306000	-1.805063000
C	-3.322407000	2.294338000	-0.607891000
C	-4.753681000	2.343517000	-0.176134000
H	-4.852938000	2.329692000	0.912299000
H	-5.328573000	1.499352000	-0.565959000
H	-5.216768000	3.260677000	-0.543013000
N	-2.472203000	1.289095000	-0.280707000
B	-2.735392000	-0.040815000	0.490889000
H	-3.871070000	-0.075708000	0.850614000

Table S8. Coordinates of the PBE1PBE geometry-optimized Tp*Co(2,6-dcp) structure.

Total number of atoms: 57, Charge = 0, and Spin=3/2, Energy=-3545.5270556 Hartree

Co	-0.179436000	0.123372000	-0.000362000
O	-1.986154000	0.704836000	-0.000724000
C	-3.135973000	0.097527000	-0.000335000
C	-3.293545000	-1.304708000	-0.000048000
Cl	-1.833137000	-2.268359000	-0.000280000
C	-4.523615000	-1.940710000	0.000394000
H	-4.565232000	-3.024651000	0.000587000
C	-5.683882000	-1.178801000	0.000575000
H	-6.654951000	-1.661612000	0.000922000
C	-5.590452000	0.208521000	0.000327000
H	-6.482974000	0.824979000	0.000472000
C	-4.350201000	0.823077000	-0.000114000
Cl	-4.258655000	2.557772000	-0.000411000
N	0.898100000	-0.738403000	1.507923000
C	0.690855000	-1.303001000	2.695670000
C	-0.673176000	-1.448994000	3.273751000
H	-0.661665000	-1.235024000	4.345216000
H	-1.054697000	-2.465857000	3.142592000
H	-1.380290000	-0.767518000	2.797144000
C	1.924529000	-1.689483000	3.236360000
H	2.100560000	-2.173206000	4.186149000
C	2.879470000	-1.316554000	2.305185000
C	4.357758000	-1.478398000	2.363875000
H	4.735996000	-2.072946000	1.527820000
H	4.635749000	-1.985501000	3.289205000
H	4.875418000	-0.515491000	2.339683000
N	2.232883000	-0.742280000	1.268841000
N	1.057737000	1.758995000	-0.000459000
C	0.960013000	3.086079000	-0.000762000
C	-0.360808000	3.771884000	-0.001166000
H	-0.467913000	4.411804000	-0.882086000
H	-0.468207000	4.412264000	0.879383000
H	-1.179265000	3.049972000	-0.001111000
C	2.251203000	3.634848000	-0.000608000
H	2.517634000	4.681851000	-0.000766000
C	3.121186000	2.557979000	-0.000245000
C	4.609611000	2.554753000	0.000011000
H	5.016860000	2.050684000	-0.880878000
H	5.016561000	2.051032000	0.881235000
H	4.979700000	3.581207000	-0.000130000
N	2.373993000	1.432945000	-0.000123000
N	0.898771000	-0.739041000	-1.507794000
C	0.692043000	-1.304288000	-2.695322000
C	-0.671726000	-1.450440000	-3.273984000
H	-0.659810000	-1.236342000	-4.345421000
H	-1.379138000	-0.769134000	-2.797585000
H	-1.053136000	-2.467381000	-3.143108000
C	1.925947000	-1.691151000	-3.235218000
H	2.102396000	-2.175394000	-4.184665000
C	2.880471000	-1.317811000	-2.303781000
C	4.358772000	-1.479827000	-2.361660000
H	4.736529000	-2.074024000	-1.525137000
H	4.876513000	-0.516960000	-2.337652000
H	4.637177000	-1.987388000	-3.286614000
N	2.233436000	-0.742916000	-1.268060000
B	2.800106000	-0.055503000	0.000341000
H	3.994806000	-0.135689000	0.000624000

Table S9. Coordinates of the PBE1PBE geometry-optimized Tp*Ni(2,6-dcp) structure.

Total number of atoms: 57, Charge = 0, and Spin = 1, Energy = -3671.04756870682 Hartree

Ni	-0.175271000	-0.056474000	-0.238141000	C	-0.547731000	3.438966000	-1.185724000
O	-1.955763000	0.689479000	-0.264232000	H	-0.720989000	4.410743000	-0.715844000
C	-3.092580000	0.080446000	-0.122042000	H	-1.353316000	2.763645000	-0.898342000
C	-3.226818000	-1.320566000	-0.010639000	H	-0.595610000	3.590505000	-2.269384000
Cl	-1.739040000	-2.245435000	-0.070782000	C	2.012069000	3.562064000	-0.725570000
C	-4.433808000	-1.981146000	0.134872000	H	2.202646000	4.603305000	-0.941923000
H	-4.451582000	-3.063039000	0.211443000	C	2.936727000	2.614011000	-0.325748000
C	-5.605817000	-1.238417000	0.179201000	C	4.398465000	2.768636000	-0.091326000
H	-6.563314000	-1.734713000	0.292555000	H	4.675569000	2.524964000	0.938100000
C	-5.541640000	0.147318000	0.076285000	H	4.693977000	3.801685000	-0.281920000
H	-6.445073000	0.746891000	0.108576000	H	4.988764000	2.124215000	-0.748848000
C	-4.320770000	0.783190000	-0.068943000	N	2.275510000	1.448666000	-0.163544000
Cl	-4.271398000	2.514168000	-0.194315000	N	1.211525000	-1.080023000	-1.293985000
N	0.705429000	-0.445406000	1.524035000	C	1.216047000	-1.877639000	-2.363029000
C	0.291195000	-0.714629000	2.761895000	C	-0.025024000	-2.233910000	-3.105221000
C	-1.149734000	-0.843458000	3.112315000	H	0.178087000	-2.295750000	-4.176838000
H	-1.317123000	-0.540848000	4.148174000	H	-0.811576000	-1.492684000	-2.951541000
H	-1.496233000	-1.875988000	3.008084000	H	-0.420690000	-3.203331000	-2.787849000
H	-1.773151000	-0.217621000	2.470785000	C	2.533483000	-2.270994000	-2.629932000
C	1.410250000	-0.836535000	3.596003000	H	2.874626000	-2.916128000	-3.426511000
H	1.415455000	-1.052583000	4.654480000	C	3.314829000	-1.654045000	-1.666206000
C	2.512602000	-0.613887000	2.786969000	C	4.789576000	-1.708171000	-1.474119000
C	3.956990000	-0.604677000	3.145466000	H	5.056047000	-2.065975000	-0.476062000
H	4.528160000	-1.326443000	2.555378000	H	5.253992000	-0.726503000	-1.603202000
H	4.076954000	-0.861961000	4.199092000	H	5.232264000	-2.387173000	-2.204631000
H	4.410108000	0.377877000	2.986315000	N	2.489043000	-0.941279000	-0.874926000
N	2.055453000	-0.380259000	1.540419000	B	2.798211000	0.059164000	0.261310000
N	0.959939000	1.621386000	-0.444115000	H	3.978691000	0.101795000	0.462476000
C	0.779211000	2.895890000	-0.788814000				

Table S10. Coordinates of the PBE1PBE geometry-optimized Tp*Co(2,6-dcp) model with Co-O-C46$_{Phen}$-C47$_{phen}$ dihedral angle of 90°.

Total number of atoms: 57, Charge = 0, and Spin=3/2, Energy=-3545.5219622 Hartree

Co	0.108270000	-0.018378000	0.447754000	C	-0.151514000	-3.123588000	2.375211000
O	1.899397000	-0.017319000	1.037416000	H	0.173067000	-4.098701000	2.000426000
C	3.067573000	-0.004055000	0.459676000	H	-0.414921000	-3.250234000	3.429152000
C	3.745950000	1.192918000	0.136833000	H	0.698588000	-2.442642000	2.311792000
Cl	2.932849000	2.699686000	0.450631000	C	-2.603627000	-3.137010000	1.473886000
C	5.009704000	1.218168000	-0.430255000	H	-2.987955000	-4.040248000	1.924927000
H	5.474366000	2.174149000	-0.646413000	C	-3.293210000	-2.261901000	0.651762000
C	5.661869000	0.025941000	-0.717096000	C	-4.705920000	-2.328804000	0.188418000
H	6.653292000	0.037327000	-1.156976000	H	-4.775807000	-2.358482000	-0.902328000
C	5.033074000	-1.180909000	-0.439811000	H	-5.288396000	-1.468394000	0.529356000
H	5.516268000	-2.125925000	-0.663386000	H	-5.179430000	-3.230462000	0.580031000
C	3.769048000	-1.184905000	0.127520000	N	-2.443230000	-1.270855000	0.308267000
Cl	2.986887000	-2.709852000	0.431141000	N	-0.384049000	0.035610000	-1.523601000
N	-1.227425000	1.427872000	0.968830000	C	0.212494000	0.065445000	-2.714836000
C	-1.298344000	2.504249000	1.748413000	C	1.694204000	0.065170000	-2.857180000
C	-0.134438000	2.965038000	2.552583000	H	2.146859000	-0.798494000	-2.362770000
H	-0.382336000	2.988297000	3.617748000	H	2.140378000	0.961152000	-2.416484000
H	0.167794000	3.976419000	2.265956000	H	1.973923000	0.034779000	-3.911526000
H	0.724916000	2.307379000	2.413066000	C	-0.768895000	0.099047000	-3.712382000
C	-2.589517000	3.043015000	1.660181000	H	-0.612940000	0.127521000	-4.780890000
H	-2.969476000	3.918664000	2.166015000	C	-1.986235000	0.087918000	-3.049866000
C	-3.284434000	2.221270000	0.788849000	C	-3.361966000	0.111708000	-3.617137000
C	-4.698032000	2.319803000	0.334126000	H	-3.927172000	0.984967000	-3.280134000
H	-4.770518000	2.410356000	-0.753039000	H	-3.935017000	-0.776250000	-3.336228000
H	-5.166788000	3.200153000	0.776621000	H	-3.309633000	0.146080000	-4.706469000
H	-5.283199000	1.444063000	0.628364000	N	-1.725115000	0.049324000	-1.727445000
N	-2.438458000	1.250313000	0.383355000	B	-2.693102000	0.016176000	-0.521091000
N	-1.234382000	-1.487026000	0.885949000	H	-3.824799000	0.029887000	-0.911543000
C	-1.311271000	-2.608740000	1.598418000				