

Supporting Information for:

DFT Study of Co-C Bond Cleavage in the Neutral and One-electron Reduced Alkyl-cobalt(III) Phthalocyanines

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Gaussian 03 full reference:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*; Gaussian, Inc.: Wallingford, CT, 2004.

Table S1. Axial bond lengths (Å), electronic energies (a.u.) and bond dissociation energies (kcal/mol) based on optimized structures calculated at BP86/6-31G(d) (5d) level of theory.

System	Co-C	Co-N(Py)	Total energy	Total energy +ZPE	Co-C BDE ^a	Co-N(Py) BDE ^a
Py-[Co ^{III} Pc]-Me	1.970	2.148	-3338.295666	-3337.766684	41.7(36.8)	14.4(12.7)
[Co ^{III} Pc]-Me	1.941	-	-3089.997759	-3089.557298	46.8(42.4)	-
Py-[Co ^{III} Pc]-Et	1.999	2.174	-3377.604041	-3377.046400	36.6(32.2)	12.7(11.2)
[Co ^{III} Pc]-Et	1.968	-	-3129.308855	-3128.840030	43.4(39.4)	-
Py-[Co ^{II} Pc]	-	2.099	-3298.398748	-3297.906219	-	19.5(18.4)
[Co ^{II} Pc]	-	-	-3050.092778	-3049.688409	-	-
Py-[Co ^{III} Pc ^{•-}]-Me ⁻	1.963	2.127	-3338.355009	-3337.830781	36.2(32.5)	10.7(9.2)
[Co ^{III} Pc ^{•-}]-Me ⁻	1.932	-	-3090.063001	-3089.627510	25.5(23.3)	-
[Co ^{III} Pc ^{•-}]-Et ⁻	1.956	-	-3129.373376	-3128.909874	21.6(20.0)	-
Pyridine	-	-	-248.274891	-248.188551	-	-
Me radical	-	-	-39.830409	-39.801268	-	-
Et radical	-	-	-79.146914	-79.088864	-	-

^a ZPE corrected in parenthesis

Table S2. Influence of the functional and the basis set on the DFT results for alkyl-cobalt(III) phthalocyanines (bond lengths in Å, energies in a.u., BDE in kcal/mol)

System	Co-C	Co-N(Py)	Total energy	Total energy + ZPE	Co-C BDE ^a
BP86/6-31G(d)					
Py-[Co ^{III} Pc]-Me	1.970	2.148	-3338.295666	-3337.7666684	41.7(36.8)
[Co ^{III} Pc]-Et	1.968	-	3129.308855	-3128.840030	43.4(39.4)
Py-[Co ^{II} Pc]	-	2.099	-3298.398748	-3297.906219	-
[Co ^{II} Pc]	-	-	-3050.092778	-3049.688409	-
Me radical	-	-	-39.830409	-39.801268	-
Et radical	-	-	-79.146914	-79.088864	-
BP86/6-311G(d,p)					
Py-[Co ^{III} Pc]-Me	1.981	2.185	-3338.891441	-	39.2(34.5) ^b
[Co ^{III} Pc]-Et	1.984	-	-3129.851735	-	41.5(37.7) ^b
Py-[Co ^{II} Pc]	-	2.142	-3298.982640	-	-
[Co ^{II} Pc]	-	-	-3050.611621	-	-
Me radical	-	-	-39.846260	-	-
Et radical	-	-	-79.173957	-	-
B3LYP/6-31G(d)					
Py-[Co ^{III} Pc]-Me	1.952	2.227	-3338.050847	-3337.505058	29.0(23.8)
[Co ^{III} Pc]-Et	1.952	-	-3129.064746	-3128.581416	26.8(22.6)
Py-[Co ^{II} Pc]	-	2.210	-3298.167171	-3297.659499	-
[Co ^{II} Pc]	-	-	-3049.865627	-3049.448668	-
Me radical	-	-	-39.837517	-39.807697	-
Et radical	-	-	-79.156387	-79.096722	-
B3LYP/6-311G(d,p)					
Py-[Co ^{III} Pc]-Me	1.963	2.271	-3338.050847	-	25.4(20.5) ^b
[Co ^{III} Pc]-Et	1.967	-	-3129.602359	-	24.6(20.6) ^b
Py-[Co ^{II} Pc]	-	2.262	-3298.747587	-	-
[Co ^{II} Pc]	-	-	-3050.379452	-	-
Me radical	-	-	-39.853757	-	-
Et radical	-	-	-79.183653	-	-
Experiment					
Py-[Co ^{III} Pc]-Me	1.993(4)	2.177(3)	-	-	30±1
[Co ^{III} Pc]-Et	2.031(3)	-	-	-	-

^a ZPE corrected in parenthesis

^b ZPE corrected BDE for 6-311G(d,p) basis set were estimated on the basis of results obtained with 6-31G(d) basis set

Table S3. Comparison of DFT computed geometry of Pc macrocycle^a with experiment

	Co ^I Pc ⁻		Co ^{II} Pc		Py-[Co ^{III} Pc]-Me		[Co ^{III} Pc]-Et	
	BP86 ^b	exper. ¹	BP86 ^b	exper. ²	BP86 ^b	exper. ³	BP86 ^b	exper. ³
Distances (Å)								
Co-N _{eq}	1.892	1.894 ^c	1.912	1.911(1)	1.928	1.922(3)	1.915	1.914(3)
N _{eq} -C _a	1.400	1.385	1.396	1.380(3)	1.389	1.373(4)	1.395	1.376(5)
C _a -N _{aza}	1.326	1.314	1.327	1.325(1)	1.330	1.322(5)	1.327	1.327(3)
C _a -C _b	1.455	1.452	1.457	1.457(3)	1.460	1.453(4)	1.457	1.449(6)
C _b -C _b	1.412	1.392	1.411	1.398(1)	1.412	1.391(6)	1.411	1.387(5)
C _b -C _c	1.404	1.375	1.404	1.397(2)	1.403	1.389(4)	1.404	1.391(3)
C _c -C _d	1.403	1.386	1.403	1.396(1)	1.403	1.381(5)	1.403	1.378(4)
C _d -C _d	1.418	1.411	1.417	1.410(1)	1.416	1.394(6)	1.417	1.395(5)
Co-C _t ^d	-	-	-	-	-0.0062	-0.005(1)	0.129	0.086(1)
Angles (°)								
C _a -N _{eq} -C _a	105.4	106.4	106.2	107.0(1)	106.9	107.2(2)	106.1	106.4(1)
C _a -N _{aza} -C _a	120.2	?	121.0	121.0(3)	121.3	121.5(1)	121.0	122.1(2)
N _{aza} -C _a -C _b	121.4	?	121.9	121.9(4)	122.0	122.2(4)	121.8	121.8(2)
N _{eq} -C _a -C _b	111.0	110.4	110.5	110.1(2)	110.2	110.0(3)	110.6	110.5(1)
C _a -C _b -C _b	106.3	106.3	106.4	106.4(1)	106.4	106.4(3)	106.4	106.3(3)
C _b -C _b -C _c	121.1	121.0	121.4	121.6(5)	121.3	121.3(6)	121.3	121.1(2)
C _b -C _c -C _d	117.8	118.9	117.4	117.1(2)	117.5	117.4(4)	117.4	117.4(4)
C _c -C _d -C _d	121.0	120.0	121.2	121.4(3)	121.2	121.4(3)	121.2	121.4(4)

^a C_a, C_b - carbon atoms of pyrrole rings; C_c and C_d - carbon atoms of benzo groups.

^b Computed using 6-31G(d) basis set. ^c Average value of 1.88(1) and 1.92(1) Å.

^d Displacement of the cobalt atom from the mean plane of the four N_{eq} atoms toward the alkyl group.

¹ Hückstadt, H.; Homborg, H. *Z. Anorg. Allg. Chem.* **1998**, *624*, 715-720.

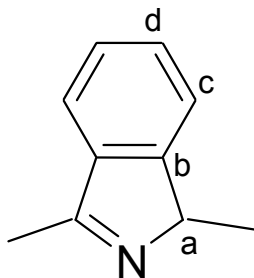
² Figgis, B.N.; Kucharski, E.S.; Reynolds, P.A. *J. Am. Chem. Soc.* **1989**, *111*, 1683-1692.

³ Galezowski, W.; Kubicki, M. *Inorg. Chem.* **2005**, *44*, 9902-9913.

Table S4 BP86/6-31G(d) computed Mulliken charges on some atoms and groups of cobalt phthalocyanine complexes and spin density on cobalt

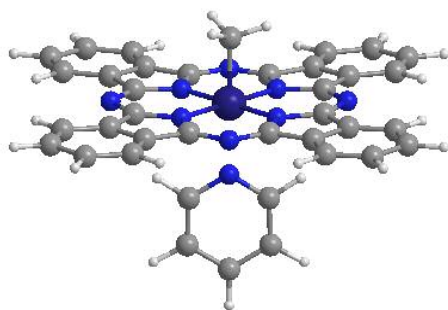
	Co	CH ₃	Pc ring	4×N _{eq}	4×N _{aza}	benzo-groups ^a	Py	spin on Co
[Co ^I Pc] ⁻	0.61	–	–1.61	–2.34	–1.66	–0.93	–	
[Co ^{II} Pc]	0.89	–	–0.89	–2.46	–1.60	–0.31	–	1.21
Py-[Co ^{II} Pc]	0.81	–	–0.96	–2.28	–1.62	–0.40	0.14	1.05
[Co ^{III} Pc]-Me	0.69	0.030	–0.72	–2.25	–1.59	–0.04	–	
Py-[Co ^{III} Pc]-Me	0.60	–0.007	–0.76	–2.07	–1.62	–0.39	0.16	
Py-[Co ^{III} Pc]-Me ^b	0.68	–0.038	–0.79	–2.24	–1.72	–0.35	0.14	
[Co ^{III} Pc ^{•-}]-Me ⁻	0.68	–0.016	–1.66	–2.28	–1.69	–0.93	–	0.08
Py-[Co ^{III} Pc ^{•-}]-Me ⁻	0.60	–0.042	–1.67	–2.11	–1.72	–0.99	0.12	0.08

^a outer C₁₆H₁₆ (carbons c and d). ^b B3LYP 6-31 G(d)



Labeling of carbon atoms in the Pc ring

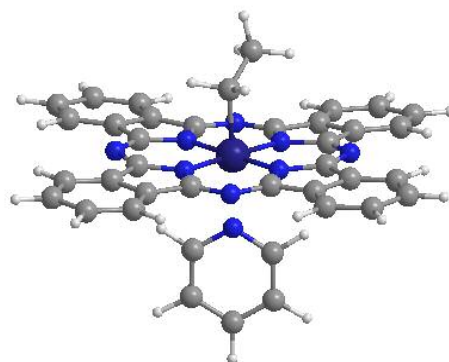
Table S5: BP86/6-31G(d) (5d) optimized xyz coordinates of Py-[Co^{III}Pc]-Me



	X	Y	Z
C	4.131245	-5.137741	-0.395138
C	2.769990	-4.800517	-0.344842
C	2.439055	-3.437220	-0.360423
C	3.437488	-2.441074	-0.426996
C	4.799121	-2.775619	-0.478101
C	5.132518	-4.138642	-0.461168
C	2.737996	-1.159546	-0.422146
N	1.365026	-1.361499	-0.352811
C	1.159227	-2.735041	-0.327778
Co	0.000063	0.000016	-0.347053
N	1.365085	1.361475	-0.352728
C	2.738037	1.159470	-0.422193
C	3.437574	2.440978	-0.427203
C	2.439177	3.437161	-0.360604
C	1.159329	2.735022	-0.327774
C	2.770164	4.800445	-0.345111
C	4.131430	5.137618	-0.395529
C	5.132662	4.138482	-0.461582
C	4.799216	2.775469	-0.478418
N	0.000841	-3.387026	-0.299499
C	-1.157919	-2.736158	-0.327332
N	-1.363363	-1.363108	-0.353835
C	-2.736134	-1.160085	-0.424914
C	-3.436105	-2.441368	-0.426746
C	-2.438012	-3.437887	-0.358167
C	-2.769596	-4.800949	-0.338928
C	-4.131046	-5.137732	-0.387435
C	-5.131883	-4.138374	-0.455401
C	-4.797893	-2.775528	-0.476199
N	3.390655	-0.000049	-0.457732
N	-3.387892	0.000075	-0.461247
C	-2.736100	1.160215	-0.424760
N	-1.363319	1.363171	-0.353638
C	-1.157820	2.736218	-0.327082
C	-2.437888	3.437996	-0.357803
C	-3.436019	2.441516	-0.426448
C	-4.797792	2.775742	-0.475872
C	-5.131727	4.138599	-0.454967
C	-4.130851	5.137914	-0.386934
C	-2.769416	4.801072	-0.338466
N	0.000966	3.387045	-0.299358
C	-0.035087	0.000232	-2.316530
N	0.004115	-0.000108	1.800954
C	-1.153957	-0.000141	2.503307

C	-1.200005	-0.000176	3.902735
C	0.003916	-0.000178	4.621280
C	1.207970	-0.000147	3.902839
C	1.162110	-0.000111	2.503482
H	-1.082984	-0.000677	-2.659364
H	0.477673	-0.899335	-2.695412
H	0.476067	0.900802	-2.695191
H	-2.074017	-0.000139	1.912630
H	-2.168854	-0.000195	4.411640
H	0.003873	-0.000205	5.716569
H	2.176763	-0.000155	4.411864
H	2.082379	-0.000082	1.913073
H	1.988020	-5.564854	-0.295992
H	4.427789	-6.192627	-0.384839
H	6.185794	-4.438320	-0.501567
H	5.565079	-1.995484	-0.531850
H	-5.563602	-1.995236	-0.531261
H	-6.185334	-4.437665	-0.494096
H	-4.428042	-6.192453	-0.374050
H	-1.987986	-5.565554	-0.288485
H	-1.987765	5.565633	-0.287976
H	-4.427807	6.192644	-0.373470
H	-6.185168	4.437929	-0.493635
H	-5.563542	1.995491	-0.530994
H	5.565139	1.995301	-0.532178
H	6.185945	4.438121	-0.502070
H	4.428008	6.192495	-0.385312
H	1.988231	5.564819	-0.296234

Table S6: BP86/6-31G(d) (5d) optimized xyz coordinates of Py-[Co^{III}Pc]-Et

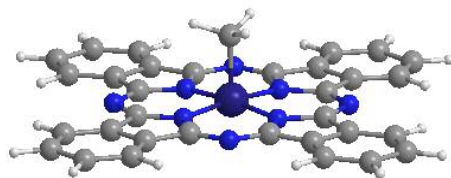


	X	Y	Z
C	4.215462	-5.030765	-0.116315
C	2.847439	-4.718022	-0.100591
C	2.491472	-3.363213	-0.174310
C	3.471797	-2.351031	-0.263195
C	4.840310	-2.661060	-0.278885
C	5.198763	-4.015780	-0.204575
C	2.747258	-1.084551	-0.321482
N	1.377607	-1.310787	-0.272608
C	1.198387	-2.685674	-0.194508
Co	-0.012831	0.023510	-0.305043
N	1.327429	1.408608	-0.315359
C	2.704087	1.232547	-0.391099

C	3.378191	2.527241	-0.417984
C	2.361504	3.504822	-0.348286
C	1.095806	2.778602	-0.294066
C	2.667179	4.874378	-0.344725
C	4.021182	5.236750	-0.411414
C	5.040465	4.256199	-0.479992
C	4.732606	2.887045	-0.483460
N	0.052309	-3.360016	-0.175635
C	-1.117886	-2.733214	-0.251345
N	-1.348361	-1.364167	-0.304807
C	-2.724564	-1.187888	-0.390239
C	-3.399161	-2.482583	-0.395506
C	-2.383771	-3.459462	-0.298423
C	-2.690761	-4.828438	-0.268674
C	-4.044527	-5.191155	-0.337900
C	-5.062347	-4.211486	-0.434529
C	-4.753329	-2.842899	-0.463649
N	3.378651	0.085179	-0.394885
N	-3.398467	-0.039918	-0.417152
C	-2.770311	1.132173	-0.356234
N	-1.401726	1.361003	-0.285239
C	-1.221516	2.737063	-0.252509
C	-2.515108	3.414494	-0.265511
C	-3.494752	2.399909	-0.338901
C	-4.862783	2.709562	-0.380166
C	-5.221798	4.065740	-0.345707
C	-4.239407	5.082792	-0.273013
C	-2.871703	4.770682	-0.233360
N	-0.074220	3.408748	-0.244615
C	-0.109958	0.083331	-2.300605
N	-0.007663	0.029834	1.868566
C	-1.158580	-0.105786	2.568911
C	-1.208743	-0.101015	3.968380
C	-0.015700	0.050864	4.689037
C	1.181430	0.191918	3.972958
C	1.139256	0.175818	2.573272
H	-1.191860	0.125446	-2.516259
H	0.333955	1.054944	-2.580213
H	-2.070802	-0.219308	1.976646
H	-2.171845	-0.214698	4.475592
H	-0.018855	0.059245	5.784330
H	2.141614	0.313280	4.483908
H	2.054971	0.281197	1.984850
H	2.079169	-5.494861	-0.034756
H	4.531491	-6.078545	-0.060629
H	6.258055	-4.296216	-0.216472
H	5.592566	-1.869003	-0.350075
H	-5.532397	-2.077691	-0.538929
H	-6.109192	-4.530875	-0.488615
H	-4.321965	-6.251102	-0.317983
H	-1.896306	-5.577765	-0.194185
H	-2.104106	5.549173	-0.180486
H	-4.555785	6.131678	-0.249408
H	-6.280805	4.345652	-0.377821
H	-5.614342	1.915915	-0.440038
H	5.512719	2.121089	-0.537383
H	6.087467	4.575323	-0.532588
H	4.297706	6.297128	-0.411559
H	1.871577	5.624314	-0.291966
C	0.536887	-1.046491	-3.092646
H	1.636076	-1.061499	-2.996162

H	0.155503	-2.041522	-2.803664
H	0.306253	-0.913973	-4.170361

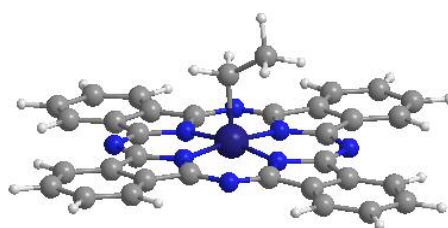
Table S7: BP86/6-31G(d) (5d) optimized xyz coordinates of [Co^{III}Pc]-Me



	X	Y	Z
C	-1.553265	-2.525012	-0.055105
N	-0.314009	-1.883338	-0.055834
C	0.647912	-2.893840	-0.068992
C	0.011832	-4.204250	-0.101340
C	-1.379580	-3.971271	-0.091316
C	-2.297238	-5.033080	-0.117410
C	-1.777845	-6.335570	-0.150726
C	-0.380551	-6.569373	-0.161048
C	0.534290	-5.506487	-0.137987
Co	0.000512	-0.001322	0.061233
N	1.885098	-0.313074	-0.046351
C	2.896360	0.648416	-0.038231
C	4.207153	0.012553	-0.049975
C	3.974069	-1.378719	-0.057930
C	2.527453	-1.552496	-0.049679
C	5.036194	-2.296331	-0.074000
C	6.338985	-1.776833	-0.078116
C	6.572934	-0.379451	-0.070178
C	5.509857	0.535261	-0.058034
N	2.758954	1.967787	-0.036623
C	1.556122	2.527168	-0.052779
N	0.317465	1.883959	-0.049785
C	-0.644636	2.895223	-0.064485
C	-0.009099	4.205872	-0.095445
C	1.382125	3.973358	-0.086946
C	2.299619	5.035388	-0.113089
C	1.779822	6.337661	-0.144989
C	0.382341	6.571076	-0.153781
C	-0.532150	5.508003	-0.130588
N	-1.964356	2.759183	-0.057352
C	-2.525636	1.557264	-0.051735
N	-1.883155	0.318937	-0.048064
C	-2.893541	-0.643693	-0.037774
C	-4.204740	-0.008543	-0.050735
C	-3.972212	1.382897	-0.061070
C	-5.034632	2.300029	-0.079387
C	-6.337289	1.780062	-0.083386
C	-6.570703	0.382670	-0.073115
C	-5.507257	-0.531654	-0.058622
N	-2.755095	-1.963293	-0.036026
N	1.967128	-2.755264	-0.058418
C	-0.034766	-0.038258	2.001841
H	-0.926529	-0.599931	2.321059

H	0.881524	-0.533650	2.359035
H	-5.675806	-1.613051	-0.052276
H	-7.602042	0.012695	-0.076874
H	-7.192554	2.464885	-0.094857
H	-4.843743	3.377656	-0.088623
H	-1.613555	5.676399	-0.138234
H	0.012548	7.602173	-0.179338
H	2.464749	7.192716	-0.163726
H	3.377243	4.844370	-0.107342
H	5.678704	1.616612	-0.053426
H	7.604424	-0.009898	-0.073857
H	7.194029	-2.461963	-0.087843
H	4.844867	-3.373892	-0.081627
H	1.615622	-5.675326	-0.146671
H	-0.011013	-7.600530	-0.187658
H	-2.463099	-7.190363	-0.169339
H	-3.374829	-4.841893	-0.110340
H	-0.080165	0.996187	2.374724

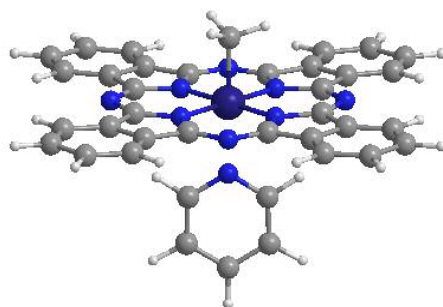
Table S8: BP86/6-31G(d) (5d) optimized xyz coordinates of [Co^{III}Pc]-Et



	X	Y	Z
C	-2.173623	2.047861	-0.139249
N	-1.805312	0.702466	-0.134429
C	-2.993774	-0.027740	-0.154359
C	-4.141848	0.867634	-0.216115
C	-3.623451	2.179964	-0.204569
C	-4.469360	3.299053	-0.250005
C	-5.850962	3.063347	-0.305569
C	-6.371373	1.745774	-0.317438
C	-5.523802	0.629030	-0.273635
Co	-0.030231	0.002585	0.020218
N	-0.728144	-1.776931	-0.079102
C	0.000612	-2.966302	-0.069818
C	-0.895191	-4.115647	-0.053603
C	-2.207177	-3.596801	-0.059203
C	-2.074425	-2.145760	-0.077028
C	-3.326668	-4.443556	-0.056950
C	-3.091411	-5.826213	-0.042442
C	-1.773908	-6.347095	-0.036819
C	-0.656909	-5.498843	-0.045660
N	1.319482	-3.107518	-0.106923
C	2.116492	-2.047790	-0.160499
N	1.747348	-0.702591	-0.132836
C	2.935497	0.026850	-0.188965
C	4.082018	-0.867580	-0.280315
C	3.564283	-2.179747	-0.260191
C	4.408458	-3.298829	-0.333840

C	5.787914	-3.062865	-0.425909
C	6.307897	-1.745027	-0.446552
C	5.462016	-0.628590	-0.375105
N	3.078654	1.345818	-0.156900
C	2.021127	2.146140	-0.105579
N	0.675840	1.776982	-0.089155
C	-0.054188	2.966119	-0.072577
C	0.841157	4.115790	-0.068957
C	2.153275	3.597417	-0.092243
C	3.272277	4.444675	-0.106442
C	3.036709	5.827275	-0.089926
C	1.719250	6.347674	-0.065919
C	0.602600	5.498964	-0.058466
N	-1.373755	3.105885	-0.092304
N	-3.133262	-1.346460	-0.113486
C	-0.181682	0.089747	1.980812
C	1.108213	-0.099211	2.760081
H	-0.620447	1.083302	2.174706
H	-0.923729	-0.685684	2.235976
H	0.886441	0.028495	3.840593
H	1.878301	0.646075	2.498232
H	1.540598	-1.105604	2.632222
H	-0.419539	5.890170	-0.043272
H	1.573305	7.433635	-0.054669
H	3.885415	6.520396	-0.096388
H	4.286109	4.032704	-0.128476
H	5.852944	0.393650	-0.391288
H	7.391418	-1.598785	-0.519915
H	6.478982	-3.911291	-0.483437
H	3.996248	-4.312679	-0.319001
H	0.365183	-5.890453	-0.045391
H	-1.628202	-7.433081	-0.026149
H	-3.940414	-6.519027	-0.036577
H	-4.340474	-4.031140	-0.064993
H	-5.915206	-0.393123	-0.281878
H	-7.456475	1.599679	-0.361138
H	-6.543179	3.912110	-0.340157
H	-4.057239	4.313003	-0.240640

Table S9: BP86/6-31G(d) (5d) optimized xyz coordinates of Py-[Co^{III}Pc]-Me⁻

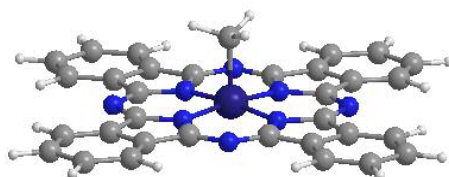


	X	Y	Z
C	-4.144105	5.141881	-0.390056
C	-2.783016	4.809234	-0.360729
C	-2.436275	3.445507	-0.368826
C	-3.438456	2.442975	-0.408117

C	-4.801848	2.777497	-0.437835
C	-5.146254	4.137303	-0.428171
C	-2.743564	1.160375	-0.405107
N	-1.377827	1.363275	-0.359888
C	-1.162561	2.752563	-0.348137
Co	-0.000247	0.000007	-0.358766
N	-1.377822	-1.363269	-0.359897
C	-2.743559	-1.160379	-0.405091
C	-3.438443	-2.442984	-0.408070
C	-2.436254	-3.445508	-0.368792
C	-1.162544	-2.752555	-0.348141
C	-2.782985	-4.809236	-0.360676
C	-4.144073	-5.141893	-0.389969
C	-5.146230	-4.137323	-0.428071
C	-4.801833	-2.777515	-0.437755
N	-0.000960	3.397403	-0.331992
C	1.160975	2.753735	-0.347190
N	1.375871	1.364966	-0.361962
C	2.741398	1.161014	-0.409752
C	3.436731	2.443367	-0.408721
C	2.434919	3.446290	-0.365891
C	2.782273	4.809793	-0.353158
C	4.143518	5.142006	-0.380992
C	5.145219	4.137145	-0.422294
C	4.800265	2.777511	-0.436927
N	-3.414369	-0.000004	-0.423244
N	3.411372	0.000020	-0.429985
C	2.741408	-1.160979	-0.409782
N	1.375883	-1.364940	-0.361995
C	1.160995	-2.753711	-0.347241
C	2.434943	-3.446257	-0.365961
C	3.436749	-2.443327	-0.408778
C	4.800284	-2.777463	-0.436992
C	5.145246	-4.137096	-0.422380
C	4.143551	-5.141963	-0.381091
C	2.782305	-4.809759	-0.353249
N	-0.000937	-3.397386	-0.332024
C	0.033171	-0.000085	-2.321953
N	-0.003419	-0.000017	1.768040
C	1.155497	-0.000039	2.469253
C	1.201149	-0.000057	3.869183
C	-0.002141	-0.000050	4.589052
C	-1.206135	-0.000027	3.870181
C	-1.161730	-0.000011	2.470313
H	1.080737	0.000701	-2.667772
H	-0.481049	0.899422	-2.701532
H	-0.479664	-0.900444	-2.701383
H	2.073178	-0.000044	1.874827
H	2.171145	-0.000075	4.377045
H	-0.001687	-0.000062	5.685137
H	-2.175687	-0.000021	4.378907
H	-2.080076	0.000007	1.876837
H	-2.003072	5.578003	-0.332786
H	-4.443796	6.197479	-0.384603
H	-6.202659	4.432062	-0.452024
H	-5.562343	1.989514	-0.469462
H	5.560497	1.989370	-0.470900
H	6.201767	4.431523	-0.444566
H	4.443643	6.197451	-0.371657
H	2.002694	5.578838	-0.322636
H	2.002730	-5.578808	-0.322734

H	4.443683	-6.197406	-0.371771
H	6.201796	-4.431467	-0.444658
H	5.560512	-1.989318	-0.470953
H	-5.562334	-1.989537	-0.469374
H	-6.202633	-4.432090	-0.451898
H	-4.443757	-6.197494	-0.384499
H	-2.003035	-5.578001	-0.332744

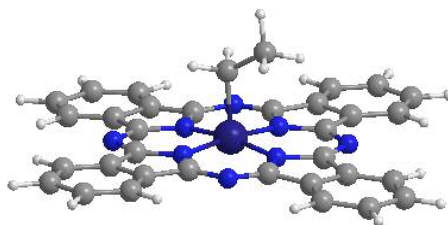
Table S10: BP86/6-31G(d) (5d) optimized xyz coordinates of [Co^{III}Pc⁻]-Me⁻



	X	Y	Z
C	-0.043361	-0.006783	1.994675
H	-1.092315	0.072905	2.323674
H	0.398533	-0.949065	2.357809
H	0.538275	0.851715	2.368564
Co	0.000875	-0.000388	0.063101
C	-4.730285	2.869864	-0.102569
C	-3.372832	2.509727	-0.080785
C	-2.351867	3.491716	-0.074592
C	-2.670881	4.862884	-0.091241
C	-4.024890	5.221077	-0.109717
C	-5.047318	4.235550	-0.115349
C	-1.094437	2.775081	-0.052209
N	-1.329110	1.382327	-0.055979
C	-2.706334	1.215199	-0.059748
N	0.076863	3.395469	-0.043867
C	1.219006	2.722026	-0.048425
N	1.392312	1.319708	-0.055268
C	2.761509	1.093612	-0.062086
C	3.483938	2.357879	-0.078808
C	2.506539	3.382953	-0.068433
C	4.855803	2.659345	-0.099931
C	5.231308	4.010107	-0.108182
C	4.252250	5.038753	-0.098826
C	2.884103	4.739092	-0.080895
N	3.407586	-0.074756	-0.060028
C	2.710692	-1.213742	-0.064020
N	1.333135	-1.379310	-0.056082
C	1.097877	-2.772668	-0.048626
C	2.354870	-3.489863	-0.070394
C	3.376395	-2.508586	-0.082124
C	2.673230	-4.861340	-0.083090
C	4.026983	-5.220201	-0.102611
C	5.050008	-4.235250	-0.113224
C	4.733645	-2.869408	-0.104724
N	-1.389846	-1.321382	-0.055809
C	-2.758199	-1.093887	-0.059450
C	-3.481101	-2.357985	-0.079558
C	-2.504026	-3.383641	-0.072677

C	-1.216194	-2.723014	-0.050899
C	-4.853026	-2.659061	-0.101192
C	-5.228979	-4.009727	-0.113108
C	-4.250403	-5.038720	-0.106762
C	-2.882078	-4.739477	-0.088485
N	-3.402948	0.075558	-0.053960
N	-0.073398	-3.394383	-0.042820
H	-5.505900	2.096355	-0.107622
H	-6.097748	4.551042	-0.130184
H	-4.304048	6.282143	-0.120023
H	-1.875844	5.616449	-0.087561
H	2.122048	5.525931	-0.074444
H	4.576935	6.086807	-0.105694
H	6.294371	4.280029	-0.122392
H	5.597494	1.853234	-0.108011
H	5.509592	-2.096265	-0.113628
H	6.100236	-4.551367	-0.128567
H	4.305597	-6.281444	-0.109717
H	1.877807	-5.614463	-0.075564
H	-2.120344	-5.526652	-0.084295
H	-4.575415	-6.086644	-0.116343
H	-6.292159	-4.279183	-0.127805
H	-5.594549	-1.852770	-0.106799

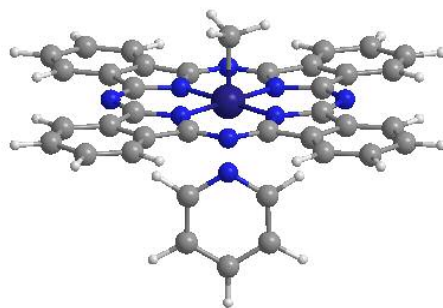
Table S11: BP86/6-31G(d) (5d) optimized xyz coordinates of [Co^{III}Pc⁻]-Et⁻



	X	Y	Z
C	-1.963866	2.272847	-0.138655
N	-1.736438	0.879397	-0.135626
C	-2.984085	0.274583	-0.153215
C	-4.033135	1.283734	-0.213516
C	-3.385269	2.543468	-0.200771
C	-4.130100	3.737145	-0.244195
C	-5.526411	3.637962	-0.297034
C	-6.174521	2.374723	-0.308549
C	-5.433056	1.185315	-0.267347
Co	-0.030005	0.006058	0.021665
N	-0.914071	-1.698182	-0.081915
C	-0.296473	-2.967958	-0.071423
C	-1.301017	-4.009880	-0.056082
C	-2.557609	-3.355393	-0.061920
C	-2.282821	-1.925796	-0.079107
C	-3.758482	-4.084263	-0.058380
C	-3.677899	-5.483763	-0.044334
C	-2.418944	-6.141108	-0.039893
C	-1.221047	-5.415523	-0.048567
N	1.002126	-3.234388	-0.110385
C	1.906080	-2.266306	-0.162405

N	1.677282	-0.872917	-0.137424
C	2.925163	-0.269055	-0.193338
C	3.972651	-1.277182	-0.281132
C	3.325438	-2.536679	-0.257631
C	4.068827	-3.730264	-0.326700
C	5.463258	-3.630629	-0.413893
C	6.111021	-2.367177	-0.435375
C	5.370830	-1.178144	-0.370323
N	3.217393	1.033340	-0.157944
C	2.229195	1.932165	-0.111043
N	0.861476	1.703562	-0.094567
C	0.242505	2.973203	-0.072961
C	1.246442	4.015607	-0.070519
C	2.503398	3.361878	-0.096744
C	3.703725	4.091479	-0.109119
C	3.622611	5.490949	-0.090695
C	2.363522	6.147494	-0.066026
C	1.166005	5.421248	-0.058663
N	-1.057146	3.238427	-0.093757
N	-3.272560	-1.028157	-0.111611
C	-0.168000	0.105079	1.970602
C	1.099979	-0.215062	2.748232
H	-0.501907	1.137271	2.174637
H	-0.983381	-0.590772	2.234126
H	0.912067	-0.058278	3.832878
H	1.942798	0.438140	2.464550
H	1.420725	-1.262477	2.616026
H	0.190555	5.919527	-0.042500
H	2.331692	7.244148	-0.052860
H	4.541349	6.090079	-0.096508
H	4.666412	3.569170	-0.131843
H	5.854190	-0.195222	-0.385991
H	7.204881	-2.324925	-0.504367
H	6.069078	-4.543883	-0.466341
H	3.560601	-4.700540	-0.309660
H	-0.245717	-5.914302	-0.048150
H	-2.387595	-7.237810	-0.029940
H	-4.596949	-6.082422	-0.037914
H	-4.720995	-3.561215	-0.065683
H	-5.916921	0.202547	-0.274664
H	-7.269772	2.332722	-0.350200
H	-6.133225	4.551480	-0.329495
H	-3.621675	4.707424	-0.234143

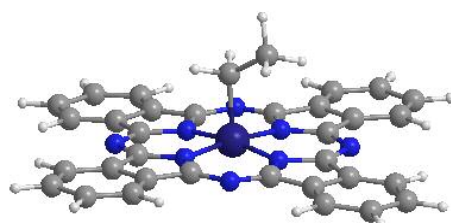
Table S12: BP86/6-311G(d,p) (5d) optimized xyz coordinates of Py-[Co^{III}Pc]-Me



	X	Y	Z
C	4.129353	-5.132085	-0.391157
C	2.770887	-4.796056	-0.346163
C	2.439252	-3.435643	-0.363547
C	3.436042	-2.440750	-0.426602
C	4.795173	-2.775173	-0.472818
C	5.128201	-4.135002	-0.454068
C	2.738163	-1.159208	-0.425408
N	1.368636	-1.365642	-0.361738
C	1.158992	-2.735713	-0.336110
Co	-0.001001	0.000003	-0.362088
N	1.368641	1.365640	-0.361726
C	2.738169	1.159212	-0.425384
C	3.436048	2.440753	-0.426542
C	2.439250	3.435637	-0.363475
C	1.158991	2.735710	-0.336072
C	2.770867	4.796050	-0.346070
C	4.129330	5.132098	-0.391055
C	5.128189	4.135026	-0.453977
C	4.795179	2.775195	-0.472747
N	0.000746	-3.382494	-0.309924
C	-1.157838	-2.736678	-0.335623
N	-1.367384	-1.367211	-0.361505
C	-2.736687	-1.159858	-0.426597
C	-3.434926	-2.441204	-0.424807
C	-2.438277	-3.436322	-0.360901
C	-2.770302	-4.796538	-0.340296
C	-4.128956	-5.132313	-0.382538
C	-5.127581	-4.135103	-0.446000
C	-4.794186	-2.775388	-0.468264
N	3.385869	0.000002	-0.458578
N	-3.383605	0.000002	-0.460354
C	-2.736684	1.159861	-0.426598
N	-1.367385	1.367218	-0.361491
C	-1.157841	2.736685	-0.335623
C	-2.438281	3.436333	-0.360923
C	-3.434924	2.441207	-0.424828
C	-4.794182	2.775374	-0.468299
C	-5.127594	4.135087	-0.446049
C	-4.128980	5.132307	-0.382588
C	-2.770324	4.796549	-0.340333
N	0.000745	3.382495	-0.309902
C	-0.039520	0.000127	-2.342640
N	0.005064	-0.000031	1.823270
C	-1.149976	-0.000064	2.524177
C	-1.193971	-0.000072	3.920733
C	0.007911	-0.000049	4.635945
C	1.208374	-0.000016	3.918276
C	1.161511	-0.000006	2.521872
H	-1.087419	-0.000847	-2.673847
H	0.472480	-0.899869	-2.711248
H	0.470761	0.901174	-2.711066
H	-2.071389	-0.000080	1.938831
H	-2.159513	-0.000094	4.430426
H	0.009038	-0.000057	5.728623
H	2.175002	-0.000001	4.425915
H	2.081728	0.000020	1.934673
H	1.990733	-5.558777	-0.300061
H	4.426103	-6.184133	-0.379557
H	6.178951	-4.434290	-0.490868

H	5.559145	-1.996525	-0.524398
H	-5.558074	-1.996674	-0.520165
H	-6.178489	-4.434142	-0.480278
H	-4.425978	-6.184247	-0.368093
H	-1.990345	-5.559420	-0.293518
H	-1.990374	5.559440	-0.293556
H	-4.426011	6.184239	-0.368156
H	-6.178504	4.434117	-0.480338
H	-5.558062	1.996653	-0.520201
H	5.559159	1.996556	-0.524338
H	6.178937	4.434325	-0.490771
H	4.426070	6.184148	-0.379439
H	1.990705	5.558762	-0.299961

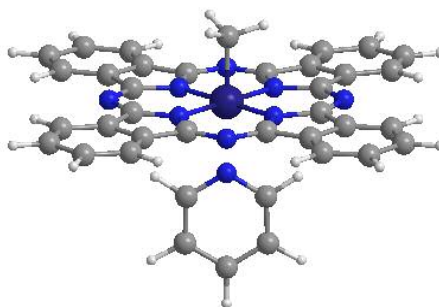
Table S13: BP86/6-311G(d,p) (5d) optimized xyz coordinates of [Co^{III}Pc]-Et



	X	Y	Z
C	-2.104384	2.121457	-0.132765
N	-1.787849	0.766451	-0.126294
C	-2.994300	0.074007	-0.148349
C	-4.109988	1.008515	-0.210596
C	-3.548517	2.300635	-0.199041
C	-4.355557	3.444726	-0.247288
C	-5.741036	3.256065	-0.305210
C	-6.304207	1.959752	-0.316948
C	-5.496504	0.817791	-0.270788
Co	-0.030743	0.004321	0.025764
N	-0.791720	-1.757738	-0.081447
C	-0.100729	-2.965543	-0.073648
C	-1.035867	-4.082275	-0.060985
C	-2.327558	-3.520151	-0.065385
C	-2.147658	-2.074687	-0.078908
C	-3.472255	-4.327964	-0.064274
C	-3.284332	-5.714612	-0.052354
C	-1.988182	-6.278497	-0.047979
C	-0.845795	-5.470254	-0.055498
N	1.210893	-3.145471	-0.107734
C	2.045040	-2.117664	-0.157262
N	1.727614	-0.762812	-0.126973
C	2.934253	-0.071502	-0.185086
C	4.048126	-1.005183	-0.277750
C	3.487065	-2.296909	-0.257739
C	4.291997	-3.441112	-0.334156
C	5.675354	-3.252402	-0.428661
C	6.238370	-1.955970	-0.449274
C	5.432645	-0.814186	-0.375304
N	3.117763	1.239990	-0.154071
C	2.092810	2.077786	-0.105249

N	0.738179	1.759868	-0.087589
C	0.045370	2.967453	-0.070806
C	0.979820	4.084679	-0.072872
C	2.271794	3.523440	-0.096977
C	3.415697	4.332087	-0.116544
C	3.226989	5.718675	-0.104167
C	1.930730	6.281652	-0.079053
C	0.788977	5.472557	-0.066538
N	-1.266951	3.146906	-0.087734
N	-3.173898	-1.237689	-0.110775
C	-0.162938	0.090441	2.003845
C	1.123154	-0.148105	2.768846
H	-0.564897	1.096497	2.191273
H	-0.929176	-0.661381	2.241689
H	0.910015	-0.035900	3.850834
H	1.910089	0.580542	2.521984
H	1.527510	-1.160489	2.622994
H	-0.217262	5.896309	-0.051138
H	1.822167	7.369275	-0.070646
H	4.095824	6.381885	-0.115120
H	4.412791	3.887614	-0.139796
H	5.856420	0.192029	-0.391888
H	7.323424	-1.847381	-0.524587
H	6.335972	-4.121205	-0.488624
H	3.846902	-4.438086	-0.319924
H	0.160264	-5.894708	-0.055515
H	-1.880281	-7.366188	-0.039409
H	-4.153662	-6.377245	-0.047065
H	-4.469224	-3.882667	-0.070949
H	-5.920521	-0.188416	-0.279570
H	-7.390909	1.851208	-0.362563
H	-6.403137	4.125025	-0.342129
H	-3.910763	4.441901	-0.238599

Table S14: B3LYP/6-31G(d) (5d) optimized xyz coordinates of Py-[Co^{III}Pc]-Me

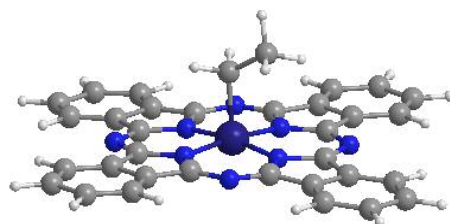


	X	Y	Z
C	4.118368	-5.119720	-0.402893
C	2.765541	-4.784181	-0.358451
C	2.435834	-3.428164	-0.369993
C	3.428736	-2.437638	-0.426644
C	4.783233	-2.771084	-0.471947
C	5.114859	-4.125543	-0.459162
C	2.729069	-1.159272	-0.421022
N	1.372300	-1.368237	-0.360795

C	1.159169	-2.725691	-0.340302
Co	-0.000827	0.000004	-0.372037
N	1.372302	1.368240	-0.360776
C	2.729069	1.159278	-0.421001
C	3.428735	2.437645	-0.426598
C	2.435831	3.428169	-0.369942
C	1.159166	2.725694	-0.340274
C	2.765536	4.784187	-0.358382
C	4.118363	5.119727	-0.402808
C	5.114856	4.125553	-0.459081
C	4.783231	2.771094	-0.471886
N	0.000909	-3.364516	-0.316798
C	-1.158005	-2.726541	-0.339848
N	-1.371111	-1.369822	-0.359654
C	-2.727971	-1.159842	-0.420274
C	-3.427676	-2.438092	-0.423974
C	-2.434734	-3.428823	-0.367657
C	-2.764704	-4.784761	-0.354301
C	-4.117628	-5.120157	-0.396432
C	-5.114059	-4.125896	-0.452352
C	-4.782283	-2.771513	-0.467117
N	3.369026	0.000003	-0.449956
N	-3.367099	-0.000003	-0.448403
C	-2.727974	1.159837	-0.420287
N	-1.371116	1.369820	-0.359658
C	-1.158010	2.726540	-0.339853
C	-2.434740	3.428819	-0.367677
C	-3.427680	2.438086	-0.424000
C	-4.782288	2.771506	-0.467155
C	-5.114066	4.125888	-0.452397
C	-4.117636	5.120150	-0.396471
C	-2.764712	4.784756	-0.354327
N	0.000903	3.364515	-0.316783
C	-0.038235	0.000109	-2.324089
N	0.005072	-0.000024	1.854632
C	-1.143806	-0.000012	2.551203
C	-1.191008	-0.000017	3.943367
C	0.006934	-0.000034	4.655884
C	1.203940	-0.000045	3.941732
C	1.154892	-0.000039	2.549681
H	-1.076090	-0.000752	-2.670801
H	0.467570	-0.890326	-2.709771
H	0.466049	0.891478	-2.709605
H	-2.057940	0.000000	1.968826
H	-2.151013	-0.000007	4.449541
H	0.007684	-0.000038	5.742241
H	2.164628	-0.000058	4.446617
H	2.068332	-0.000047	1.966177
H	1.990649	-5.543151	-0.317204
H	4.412704	-6.165779	-0.395644
H	6.159450	-4.423014	-0.494901
H	5.544006	-1.998161	-0.517952
H	-5.543067	-1.998569	-0.512678
H	-6.158747	-4.423256	-0.486132
H	-4.412102	-6.166164	-0.387548
H	-1.989910	-5.543844	-0.313281
H	-1.989919	5.543841	-0.313302
H	-4.412112	6.166157	-0.387592
H	-6.158754	4.423246	-0.486187
H	-5.543070	1.998561	-0.512720
H	5.544006	1.998172	-0.517895

H	6.159446	4.423025	-0.494807
H	4.412697	6.165787	-0.395543
H	1.990642	5.543155	-0.317132

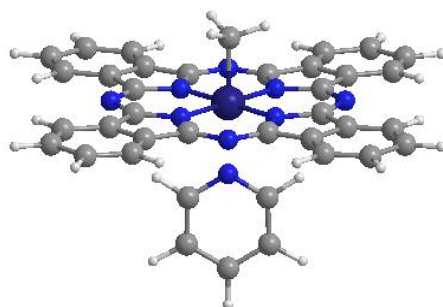
Table S15: B3LYP/6-31G(d) (5d) optimized xyz coordinates of [Co^{III}Pc]-Et



	X	Y	Z
C	2.404148	-1.762095	-0.126094
N	1.891129	-0.481969	-0.119269
C	2.962816	0.385349	-0.126746
C	4.210904	-0.361131	-0.162909
C	3.857601	-1.718645	-0.162241
C	4.828636	-2.721474	-0.193257
C	6.164122	-2.323689	-0.222472
C	6.519266	-0.959715	-0.222878
C	5.548028	0.039630	-0.194287
Co	0.031130	-0.000491	0.041331
N	0.510543	1.862307	-0.089687
C	-0.355798	2.935292	-0.101080
C	0.391033	4.183642	-0.110171
C	1.748198	3.830243	-0.106387
C	1.791437	2.376391	-0.094552
C	2.751416	4.801309	-0.121215
C	2.353968	6.137106	-0.135435
C	0.989999	6.492432	-0.139289
C	-0.009566	5.521086	-0.129037
N	-1.676000	2.903398	-0.125027
C	-2.345539	1.765389	-0.154081
N	-1.831345	0.485812	-0.127256
C	-2.903825	-0.381057	-0.168076
C	-4.150716	0.364980	-0.233771
C	-3.797686	1.722142	-0.224915
C	-4.767556	2.725080	-0.281830
C	-6.101802	2.327133	-0.343706
C	-6.456829	0.963033	-0.351664
C	-5.486605	-0.036178	-0.298646
N	-2.873171	-1.701292	-0.151382
C	-1.736010	-2.373130	-0.122678
N	-0.456652	-1.859095	-0.098808
C	0.411350	-2.931955	-0.101832
C	-0.335044	-4.180248	-0.122943
C	-1.692328	-3.826961	-0.137180
C	-2.695099	-4.798148	-0.166796
C	-2.297372	-6.133899	-0.176945
C	-0.933446	-6.489122	-0.162423
C	0.065781	-5.517733	-0.137681
N	1.731699	-2.898832	-0.107162
N	2.928983	1.705635	-0.105842

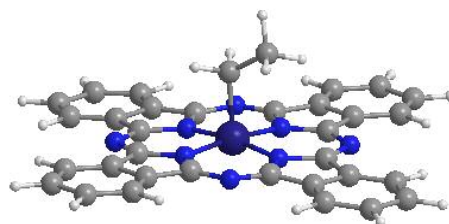
C	0.174889	-0.061232	1.987035
C	-1.121269	0.010192	2.776239
H	0.700543	-0.998095	2.195958
H	0.835535	0.770844	2.249414
H	-0.894405	-0.091583	3.848651
H	-1.816255	-0.795019	2.517125
H	-1.640296	0.964753	2.643853
H	1.118309	-5.782559	-0.129010
H	-0.659527	-7.540603	-0.171594
H	-3.049334	-6.917998	-0.196996
H	-3.742633	-4.514278	-0.180484
H	-5.750989	-1.088821	-0.306207
H	-7.507204	0.689129	-0.400756
H	-6.885019	3.079056	-0.386825
H	-4.483855	3.772732	-0.276649
H	-1.062102	5.785958	-0.134740
H	0.716313	7.543947	-0.151306
H	3.106183	6.921166	-0.144647
H	3.798983	4.517249	-0.120960
H	5.812833	1.092202	-0.195260
H	7.570530	-0.685795	-0.246067
H	6.948065	-3.075738	-0.245298
H	4.544915	-3.769140	-0.193469

Table S16: B3LYP/6-311G(d,p) (5d) optimized xyz coordinates of Py-[Co^{III}Pc]-Me



	X	Y	Z
C	4.116791	-5.114662	-0.398258
C	2.766623	-4.780189	-0.359888
C	2.436124	-3.426793	-0.373527
C	3.427533	-2.437425	-0.426059
C	4.779785	-2.770886	-0.465665
C	5.111120	-4.122294	-0.450836
C	2.729231	-1.158816	-0.424686
N	1.375482	-1.371917	-0.371416
C	1.158809	-2.726306	-0.350033
Co	-0.001734	0.000008	-0.389919
N	1.375471	1.371937	-0.371393
C	2.729220	1.158851	-0.424667
C	3.427509	2.437467	-0.426021
C	2.436089	3.426824	-0.373480
C	1.158782	2.726324	-0.350000
C	2.766576	4.780223	-0.359824
C	4.116740	5.114710	-0.398186
C	5.111079	4.122353	-0.450774

C	4.779758	2.770941	-0.465620
N	0.000855	-3.360367	-0.328858
C	-1.157698	-2.727035	-0.349789
N	-1.374491	-1.373457	-0.369855
C	-2.728294	-1.159441	-0.423122
C	-3.426576	-2.437951	-0.422644
C	-2.435023	-3.427432	-0.371247
C	-2.765638	-4.780759	-0.356074
C	-4.115905	-5.115189	-0.391403
C	-5.110285	-4.122811	-0.442602
C	-4.778916	-2.771438	-0.459196
N	3.364579	0.000020	-0.450963
N	-3.362858	-0.000015	-0.448633
C	-2.728307	1.159419	-0.423126
N	-1.374508	1.373449	-0.369847
C	-1.157727	2.727029	-0.349777
C	-2.435059	3.427412	-0.371244
C	-3.426602	2.437921	-0.422652
C	-4.778944	2.771394	-0.459213
C	-5.110327	4.122763	-0.442617
C	-4.115959	5.115152	-0.391407
C	-2.765688	4.780736	-0.356068
N	0.000820	3.360371	-0.328830
C	-0.041818	0.000114	-2.352654
N	0.005573	-0.000037	1.881526
C	-1.140524	-0.000037	2.576690
C	-1.186272	-0.000048	3.966201
C	0.009546	-0.000060	4.676085
C	1.203354	-0.000060	3.962788
C	1.153637	-0.000048	2.573446
H	-1.079652	-0.000710	-2.688215
H	0.463795	-0.890956	-2.727239
H	0.462331	0.892078	-2.727084
H	-2.056066	-0.000028	1.999400
H	-2.143430	-0.000048	4.472650
H	0.011105	-0.000070	5.760012
H	2.161992	-0.000069	4.466438
H	2.067497	-0.000048	1.993539
H	1.993587	-5.537819	-0.321809
H	4.411151	-6.158147	-0.389494
H	6.153439	-4.419234	-0.482356
H	5.538882	-1.999505	-0.508989
H	-5.538111	-2.000083	-0.501357
H	-6.152691	-4.419711	-0.471517
H	-4.410304	-6.158649	-0.381160
H	-1.992613	-5.538445	-0.318879
H	-1.992671	5.538429	-0.318865
H	-4.410368	6.158608	-0.381163
H	-6.152737	4.419653	-0.471539
H	-5.538131	2.000032	-0.501382
H	5.538863	1.999569	-0.508953
H	6.153395	4.419304	-0.482288
H	4.411089	6.158198	-0.389408
H	1.993532	5.537845	-0.321738

Table S17: B3LYP/6-311G(d,p) (5d) optimized xyz coordinates of [Co^{III}Pc]-Et

	X	Y	Z
C	2.479422	-1.658125	-0.120374
N	1.916650	-0.402378	-0.107483
C	2.944005	0.512480	-0.119086
C	4.222364	-0.179960	-0.160342
C	3.929004	-1.549591	-0.161271
C	4.941753	-2.506500	-0.197748
C	6.255624	-2.051686	-0.230541
C	6.550378	-0.676429	-0.229438
C	5.538596	0.277286	-0.195657
Co	0.030712	-0.001104	0.047891
N	0.430975	1.887173	-0.085664
C	-0.483143	2.915726	-0.102573
C	0.209640	4.194457	-0.116326
C	1.579035	3.901035	-0.110218
C	1.687531	2.451024	-0.092042
C	2.536305	4.914041	-0.128064
C	2.081796	6.228227	-0.147374
C	0.706511	6.523079	-0.153422
C	-0.247410	5.511074	-0.140430
N	-1.797979	2.821488	-0.128231
C	-2.419772	1.659253	-0.154753
N	-1.855994	0.404030	-0.122464
C	-2.884221	-0.510272	-0.164374
C	-4.161179	0.181760	-0.235107
C	-3.867927	1.551003	-0.228933
C	-4.879434	2.508157	-0.290020
C	-6.192071	2.053345	-0.353755
C	-6.486831	0.677974	-0.359526
C	-5.476237	-0.275710	-0.302029
N	-2.792319	-1.825257	-0.145604
C	-1.631211	-2.449702	-0.117101
N	-0.376291	-1.885635	-0.091930
C	0.539663	-2.913947	-0.098228
C	-0.152530	-4.192661	-0.123444
C	-1.522075	-3.899657	-0.135716
C	-2.478692	-4.912917	-0.167728
C	-2.023586	-6.226963	-0.182067
C	-0.648255	-6.521434	-0.169605
C	0.305092	-5.509205	-0.142637
N	1.854666	-2.819184	-0.103922
N	2.849020	1.827517	-0.100682
C	0.168136	-0.050390	2.009461
C	-1.130215	0.029128	2.788959
H	0.691042	-0.985817	2.213237
H	0.828086	0.783909	2.251246
H	-0.904731	-0.037890	3.862229

H	-1.812286	-0.790973	2.554865
H	-1.659409	0.970741	2.630252
H	1.366008	-5.726497	-0.135470
H	-0.329609	-7.557628	-0.182120
H	-2.738342	-7.041822	-0.203928
H	-3.535399	-4.676081	-0.179629
H	-5.693620	-1.336615	-0.307431
H	-7.521968	0.359677	-0.410210
H	-7.005714	2.768330	-0.400051
H	-4.642322	3.564859	-0.286157
H	-1.308266	5.728641	-0.147705
H	0.388346	7.559374	-0.169413
H	2.797000	7.042906	-0.158778
H	3.592996	4.676854	-0.125791
H	5.756186	1.338167	-0.195369
H	7.586394	-0.358034	-0.255577
H	7.070092	-2.766718	-0.257425
H	4.704788	-3.563248	-0.198919