Supporting Information

for

The Surface Trans Effect: Influence of Axial Ligands on the Surface Chemical Bonds of Adsorbed Metalloporphyrins

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Supporting Figures

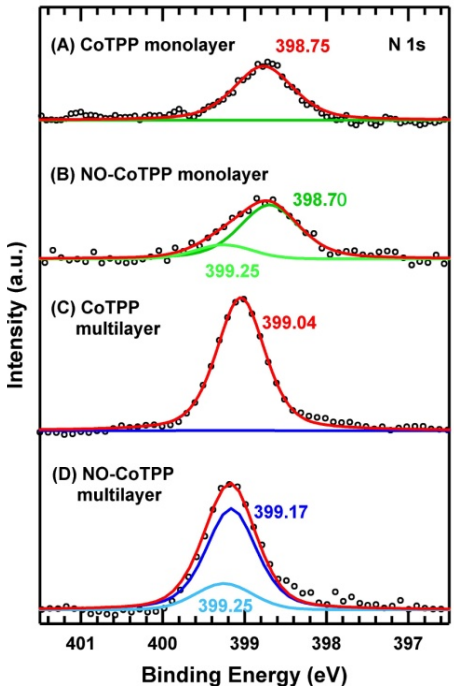

Figure S1. N 1s XP spectra of CoTPP and NO-CoTPP on Ag(111). (A) CoTPP monolayer, (B) NO-CoTPP monolayer, (C) CoTPP multilayer (ca. 4 monolayers), (D) NO-CoTPP multilayer (ca. 4 monolayers). The NO induced N 1s signal at 399.25 eV strongly overlaps with the signal of the nitrogen atoms in the porphyrin.

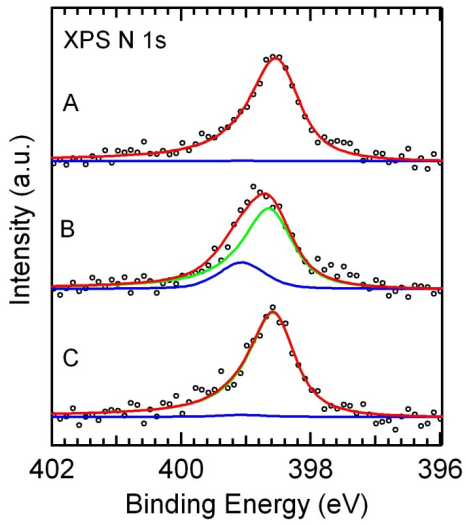

Figure S2. N 1s XP spectra of FeTPP and NO-FeTPP on Ag(111): (A) FeTPP monolayer, (B) NO-FeTPP monolayer, (C) after heating the NO-FeTPP monolayer to 550 K for removal of the NO ligand.

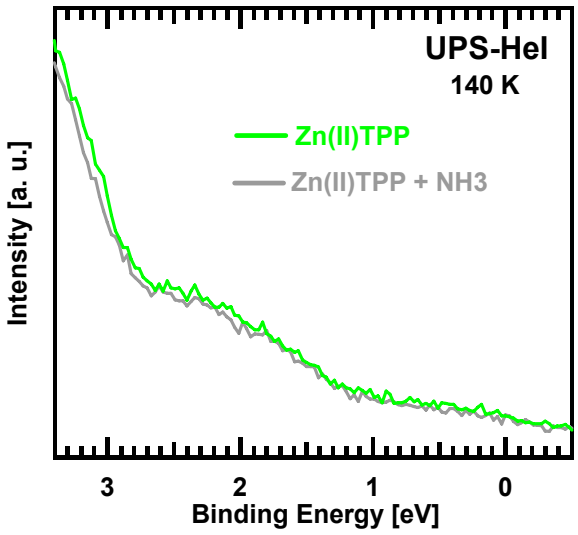

Figure S3. He-I UP spectra of monolayers of ZnTPP (green line) and NH_3-ZnTPP (grey line) on Ag(111).

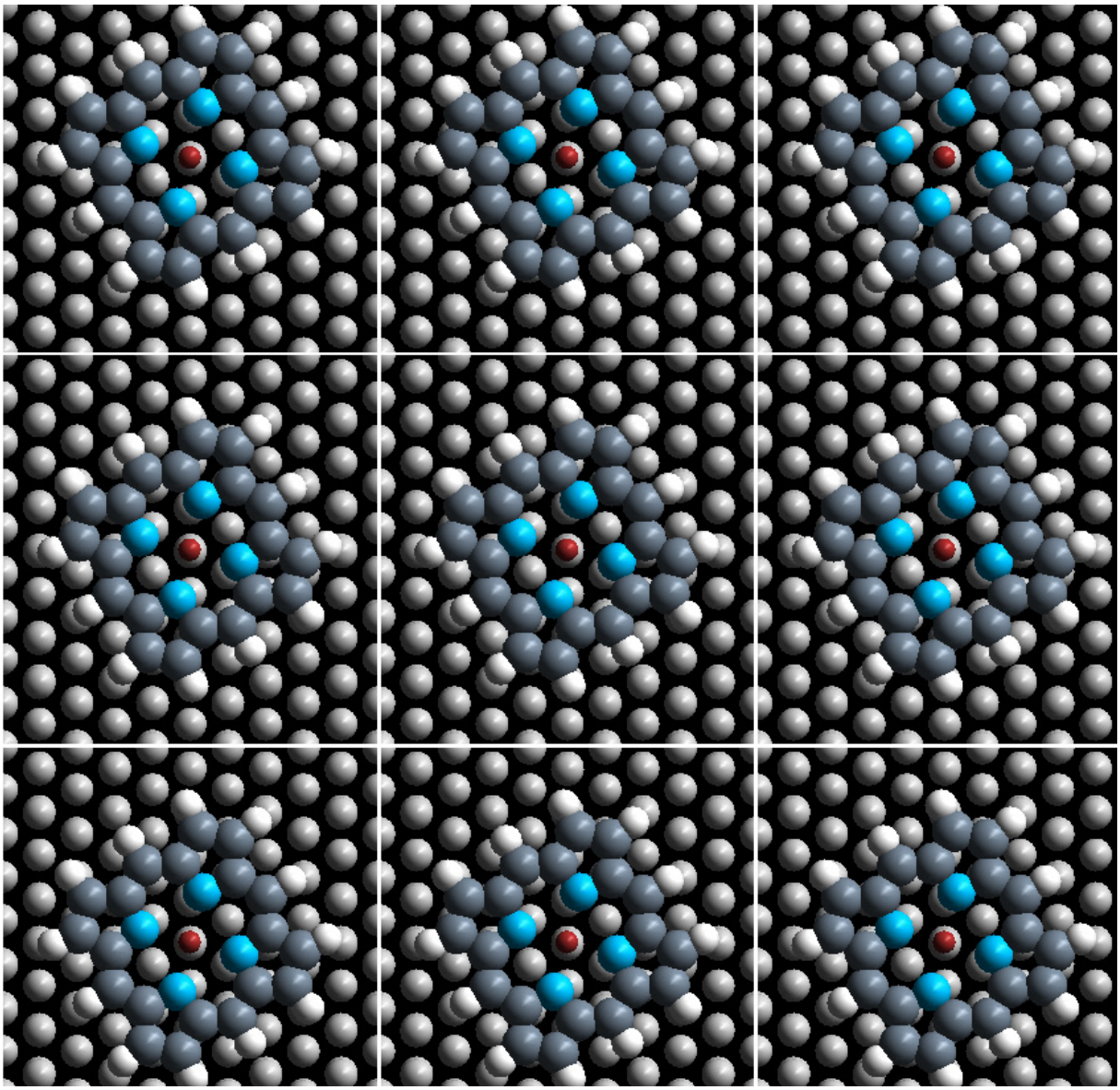

Figure S4. Metalloporphin superstructure used in the periodic calculations (CoP/Ag(111) shown, FeP/Ag(111) similar); while lines indicate unit cell boundaries.

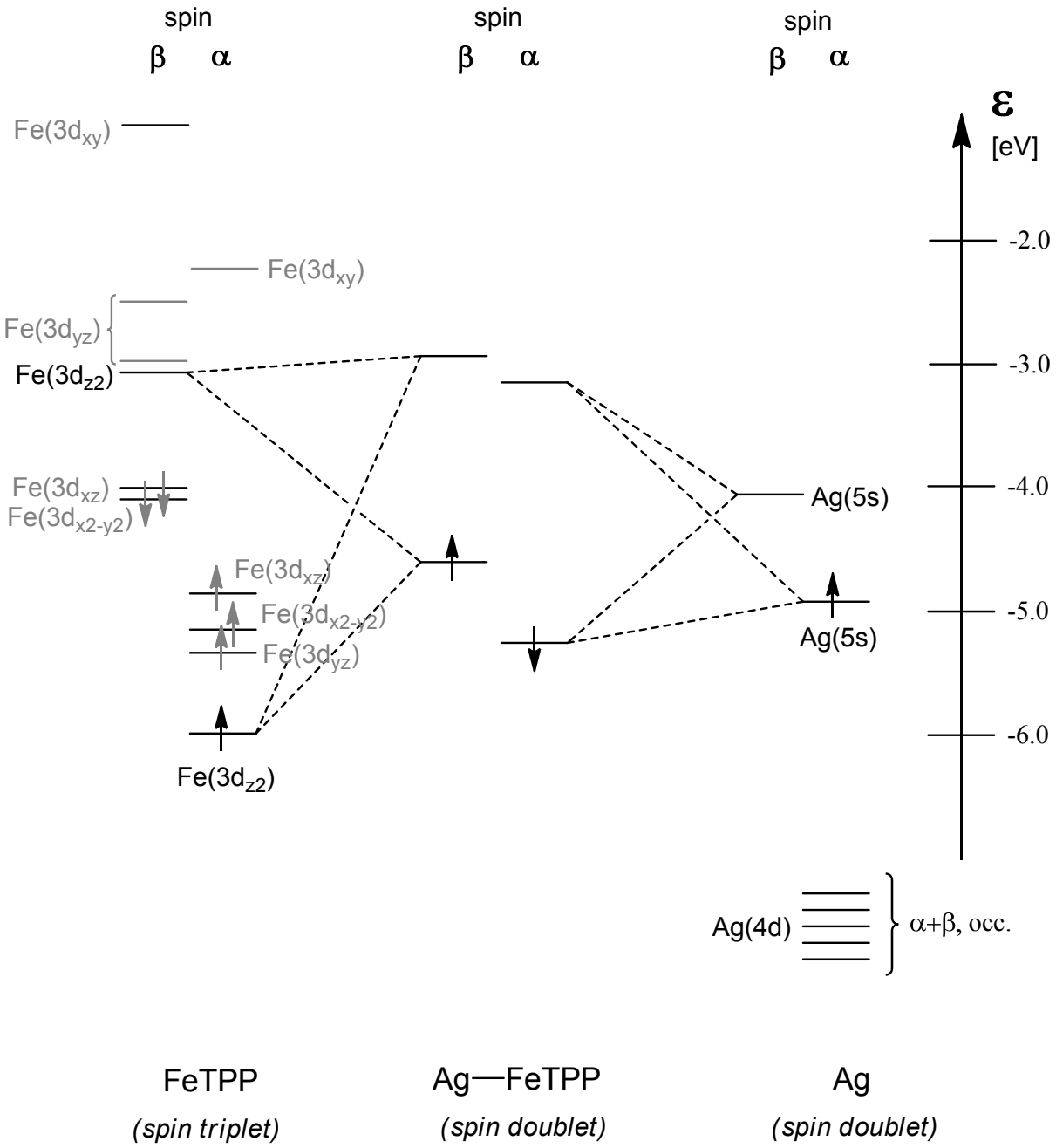

Figure S5. Qualitative orbital energy interaction diagram for the interaction of Ag and FeTPP, cf. Figure 12 of the main paper; orbital energy energies scales of the FeTPP and Ag fragments have been shifted for illustration purposes; Co and Ag d levels which are not involved in the bonding are shaded.

Supporting Tables

Table S1. Experimental UP signal positions of ZnTPP and CoTPP monolayer and multilayers and for the FeTPP monolayer.

	Porphyrin	Binding energy (eV) relative to E_F						
Multilayer	2H-TPP	12.0	9.9	9.5	7.4	4.7	2.5	
	CoTPP	11.8	9.8	9.2	7.2	4.4	2.3	
	ZnTPP	11.9	9.9	9.3	7.4	4.5	2.4	
Monolayer	2H-TPP	11.4	9.3	8.9	6.9	4.4	2.4	
	CoTPP	11.0	9.5	8.7	6.5	4.2	1.8	0.62
	FeTPP	11.3	9.4	8.7	6.9	4.2	1.7	0.23
	ZnTPP	11.4	9.5	8.8	6.9	4.4	2.3	

Table S2. Calculated Co(2p) and Fe(2p) core ionization energies and corresponding shifts; experimental XPS data for monolayers on Ag(111); calculated data for molecular complexes (Ag)**M**TPP and (NO)(Ag)**M**TPP (M = Co, Fe) using the Slater transition state method at the PBE/TZVP level.

Compound	**XPS (eV)**	**$\Delta E_{calc.}$ (eV)**	**XPS shift (eV)**	**calc. shift (eV)**
CoTPP [a]	780.1	779.1	0.0	0.0
(NO)**Co**TPP [a]	780.6	779.8	+0.5[c]	+0.7[c]
(Ag)**Co**TPP [a]	778.3	778.5	-1.8[c]	-0.6[c]
(NO)(Ag)**Co**TPP [a]	780.2	779.6	+0.1[c] /+2.0[d]	+0.5[c] / +1.1[d]
(Ag)**Fe**TPP [b]	706.8	707.5	0.0	0.0
(NO)(Ag)**Fe**TPP [b]	709.5	708.1	+2.7[d]	+0.6[d]

a: Co(2p) core level ionization energies / shifts; b: Fe(2p) core level ionization energies / shifts; c: shift with respect to MTPP (multilayer or gas-phase); d: shift with respect to (Ag)MTPP.

Table S3: Atomic partial charges of the metal center M in metalloporphin (MP) complexes in various binding situations according to the Bader partitioning scheme (PBE density functional; see Section 2.3 of the main paper for details on the underlying VASP calculations and references).

Structure	**M = Co**	**M = Fe**
MP	+1.14	+1.35
MP–Ag(111)	+0.96	+1.21
(NO)MP···Ag(111)	+1.15	+1.42
(NO)MP	+1.18	+1.46
MP–Ag_1	+0.98	+1.24
(NO)MP–Ag_1	+1.16	+1.37

According the Bader partial charge analysis, the entire MP moiety gains 0.37 (M = Co) or 0.22 (M = Fe) electron charges upon interaction with Ag(111). The charge-transfer from the surface to the complex is mitigated for the NO-coordinated complexes; e.g., NOCoP has a negative charge of only -0.03 e in the presence of the surface. In the isolated complexes (NO)MP (M = Co, Fe), i.e., in the absence of the surface, the coordinated NO ligand adopts a negative partial charge of 0.20e for M = Co and 0.35e for M = Fe.

Table S4. XYZ coordinates of the geometries of complexes (Ag)MTPP and (NO)(Ag)MTPP (M = Co, Fe) optimized at the RI-BP86/TZVP level of theory as illustrative examples. Further coordinate files on other optimized geometries quoted in the text can be obtained from the authors (contact W.H.).

CoTPP:

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77
Energy = -3296.388689982 <S2>=0.76
N     1.9589618   -0.1752732    0.0319008
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C     4.2112555    0.2617182    0.4122574
C     2.8892891    0.8236719    0.2946251
C     2.1931795   -2.6183483   -0.3235567
C     3.1567505   -3.7378162   -0.5552058
C     3.9211972   -3.7816792   -1.7340400
C     4.8276810   -4.8215695   -1.9586003
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C     2.6183772    2.1931790    0.3231989
C     1.3405156    2.7041006    0.0794168
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C    -0.2617689    4.2112398   -0.4123540
C     1.0714935    4.1002519   -0.1542797
Co    0.0000011   -0.0000081   -0.0000076
N    -0.1752635   -1.9589719   -0.0320524
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C    -1.2220695    2.7874344    0.1141922
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(Ag)FeTPP:

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C     7.6843949   -0.3500987    0.9788426
C     6.8617537   -1.3888646    1.4255606
C     5.4776899   -1.3164378    1.2447367
C     0.4206555    0.1052025   -3.4273366
C     0.6077784    0.1989754   -4.9083543
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C	1.2288264	1.3228274	-5.4800250
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C	0.9676890	0.3804647	-7.6977078
C	0.3512363	-0.7439931	-7.1399378
C	0.1712321	-0.8331323	-5.7567313
C	-3.4122437	-0.1298490	-0.4183515
C	-4.8939221	-0.2020848	-0.6092475
C	-5.7301092	0.8363570	-0.1636345
C	-7.1136727	0.7676614	-0.3492160
C	-7.6846271	-0.3428457	-0.9788313
C	-6.8629322	-1.3824774	-1.4252762
C	-5.4787869	-1.3111825	-1.2446257
Ag	-0.0013311	-2.6310573	0.0001038
N	1.5564434	-0.0599881	-1.2267861
C	1.5486537	-0.0679574	-2.6211489
C	2.8764221	-0.2656834	-3.1346501
C	3.7088360	-0.3591591	-2.0567409
C	2.8980293	-0.2041030	-0.8795813
N	-1.5564148	-0.0582821	1.2267991
C	-1.5486376	-0.0661173	2.6211635
C	-2.8766034	-0.2624693	3.1346822
C	-3.7091207	-0.3551233	2.0567813
C	-2.8981480	-0.2010535	0.8796073
H	2.0496171	0.5434096	4.7781583
H	4.1747802	0.3536465	3.1146944
H	4.7822863	-0.5183918	-2.0521890
H	3.1300397	-0.3315137	-4.1875078
H	-2.0489699	0.5451074	-4.7781974
H	-4.1743205	0.3577682	-3.1147021
H	-4.7827596	-0.5130830	2.0522470
H	-3.1302671	-0.3280958	4.1875420
H	-5.2848896	1.7066545	0.3218143
H	-4.8381585	-2.1243199	-1.5907259
H	-7.7470520	1.5870338	-0.0040876
H	-7.3006553	-2.2549341	-1.9140253
H	-8.7652399	-0.3972010	-1.1220303
H	1.5665720	2.1320262	-4.8299780
H	-0.3050725	-1.7137575	-5.3219583
H	1.8836311	2.2971819	-7.2910600
H	0.0113949	-1.5576711	-7.7834609
H	1.1067962	0.4508884	-8.7779348
H	5.2864720	1.7014979	-0.3218414
H	4.8363642	-2.1291036	1.5906545
H	7.7485659	1.5795222	0.0037004
H	7.2986567	-2.2614591	1.9147975
H	8.7649740	-0.4054786	1.1219031
H	-1.5647603	2.1339049	4.8296311
H	0.3042163	-1.7130916	5.3223021
H	-1.8800632	2.3005368	7.2908409
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H	-1.1065765	0.4529453	8.7778515

(NO)(Ag)CoTPP:

80
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C	-2.0566553	-3.8197421	-3.7249440
C	-0.7301681	-3.4378003	-3.4604254
C	0.3042587	-4.0337634	-4.2023395
C	0.0191226	-4.9893416	-5.1816346
C	-0.4389867	-2.4072788	-2.4166230
C	0.2185945	-2.7918257	-1.2441978
C	0.7184304	-4.1215422	-0.9963226
C	1.4273518	-4.0707796	0.1664790
C	1.3219232	-2.7218164	0.6650264
N	0.5671781	-1.9492461	-0.1994493
C	1.8244010	-2.3145607	1.9058008
C	2.7158104	-3.2556998	2.6511394
C	2.2656819	-3.9286563	3.8000958
C	3.1058070	-4.8137933	4.4814371
C	4.4091265	-5.0375356	4.0265445
C	4.8660715	-4.3746076	2.8833934
C	4.0252141	-3.4925156	2.1989179
Co	0.1191871	-0.0402358	0.0261682
N	-0.5822166	1.7950426	0.3265793
C	-0.7218865	2.4653682	1.5319122
C	-1.3211252	3.7592539	1.3149071
C	-1.4841485	3.9003110	-0.0307474
C	-1.0345484	2.6725895	-0.6407970
C	-0.2684364	2.0071270	2.7720699
C	-0.4750900	2.8584483	3.9838005
C	-1.3577945	2.4439575	4.9960356
C	-1.5561516	3.2300989	6.1344988
C	-0.8711584	4.4402031	6.2813402
C	0.0137474	4.8595573	5.2830215
C	0.2094256	4.0758158	4.1424554
C	-1.1597867	2.3990895	-2.0076103
C	-1.5553278	3.5171802	-2.9182966
C	-2.8380392	3.5732563	-3.4904761
C	-3.1969731	4.6300867	-4.3317599
C	-2.2788551	5.6458777	-4.6161921
C	-1.0010892	5.6013827	-4.0501954
C	-0.6429759	4.5470188	-3.2053957
Ag	-2.2790875	-0.9103599	0.8520444
N	1.7852953	0.5537012	-0.5330166
O	2.8044735	0.0728634	-0.1955680
N	-0.6568502	-0.0148527	-1.8058709
C	-0.7781985	-1.0770286	-2.6852334
C	-1.2133669	-0.6076680	-3.9772912
C	-1.3295379	0.7475560	-3.8899250
C	-1.0161338	1.1097797	-2.5291998
N	0.6394731	-0.1433531	1.9297900
C	1.4588712	-1.1037186	2.5011134
C	1.7987109	-0.7292001	3.8513029
C	1.1400749	0.4339139	4.1181290
C	0.4343040	0.8057343	2.9172567
H	0.5489722	-4.9762251	-1.6427203
H	1.9479134	-4.8768917	0.6730479
H	2.4492140	-1.2983095	4.5069268
H	1.1498563	1.0171234	5.0331228
H	-1.5747450	4.4641200	2.0997078
H	-1.9074906	4.7397789	-0.5726361

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H    -1.6143793    1.4481626   -4.6677437
H    -1.3738088   -1.2418408   -4.8430656
H    -3.5594388    2.7870810   -3.2605766
H     0.3553835    4.5105985   -2.7657938
H    -4.1995753    4.6619475   -4.7623110
H    -0.2776806    6.3891265   -4.2685145
H    -2.5592132    6.4702645   -5.2741477
H    -1.8956857    1.5013892    4.8793153
H     0.9076801    4.3997544    3.3686262
H    -2.2509198    2.8967532    6.9076034
H     0.5585475    5.7989911    5.3936023
H    -1.0247374    5.0532130    7.1711457
H     1.2451981   -3.7629140    4.1500633
H     4.3824926   -2.9716863    1.3088987
H     2.7384518   -5.3337853    5.3681407
H     5.8827566   -4.5418519    2.5229991
H     5.0651835   -5.7278361    4.5596532
H    -2.8657437   -3.3637317   -3.1515261
H     1.3366804   -3.7336426   -4.0142742
H    -3.3763112   -5.0683954   -4.8895309
H     0.8338991   -5.4374897   -5.7533665
H    -1.5261338   -6.1129853   -6.1968260
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(NO)(Ag)FeTPP:

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C    -0.7337583   -5.4353889   -5.4997430
C    -1.8478458   -4.9540326   -4.8052493
C    -1.6922119   -3.9771172   -3.8177274
C    -0.4196707   -3.4683168   -3.5063062
C     0.6930416   -3.9595790   -4.2106802
C     0.5369251   -4.9341626   -5.2003478
C    -0.2576224   -2.4220893   -2.4484523
C     0.3778506   -2.7775711   -1.2511761
C     0.8994773   -4.0935985   -0.9674028
C     1.5055114   -4.0265695    0.2516603
C     1.3344955   -2.6761833    0.7333986
N     0.6228991   -1.9311322   -0.1882427
C     1.7746787   -2.2366560    1.9896988
C     2.6072225   -3.1739973    2.8072020
C     2.0845290   -3.7919218    3.9561747
C     2.8663709   -4.6715491    4.7102914
C     4.1838442   -4.9445366    4.3291736
C     4.7137751   -4.3351380    3.1876510
C     3.9311110   -3.4584172    2.4310257
Fe    0.1579536    0.0337403   -0.0395522
N    -0.6437981    1.8511812    0.2355740
C    -0.6997932    2.5800471    1.4153529
C    -1.3873046    3.8289609    1.1938515
C    -1.7175259    3.8733008   -0.1276151
C    -1.2581867    2.6402762   -0.7191456
C    -0.1448213    2.2057420    2.6445631
C    -0.2536570    3.1523017    3.7980622
C    -1.0573843    2.8360714    4.9070251
C    -1.1595962    3.7156896    5.9884027
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C	-0.4558619	4.9240055	5.9807074
C	0.3501446	5.2473969	4.8846722
C	0.4493067	4.3696165	3.8015719
C	-1.4817195	2.2935199	-2.0577080
C	-2.0759344	3.3237837	-2.9647376
C	-3.3941766	3.2012744	-3.4375200
C	-3.9432499	4.1720051	-4.2799723
C	-3.1826927	5.2804340	-4.6654373
C	-1.8707808	5.4137379	-4.2003094
C	-1.3227529	4.4446081	-3.3552698
Ag	-2.0342548	-0.9351428	0.8932256
N	1.7945931	0.3987482	-0.4159622
O	2.9353934	0.1634353	-0.2517733
N	-0.6977139	-0.0477354	-1.8525245
C	-0.7145852	-1.1275143	-2.7227666
C	-1.2284567	-0.7202415	-4.0076136
C	-1.5255404	0.6068301	-3.9160791
C	-1.2215448	1.0150454	-2.5661293
N	0.6685301	-0.0190841	1.9221918
C	1.4441742	-0.9885787	2.5332889
C	1.8265749	-0.5549545	3.8562144
C	1.2557263	0.6669278	4.0539742
C	0.5414375	0.9995778	2.8442847
H	0.8064139	-4.9523278	-1.6239941
H	2.0049138	-4.8200994	0.7977447
H	2.4529809	-1.1207775	4.5377017
H	1.3247674	1.3061407	4.9280494
H	-1.5923244	4.5682269	1.9610309
H	-2.2512416	4.6537442	-0.6601365
H	-1.9173127	1.2606609	-4.6882004
H	-1.3243778	-1.3710273	-4.8704976
H	-3.9922595	2.3415851	-3.1298748
H	-0.2970145	4.5469812	-2.9963965
H	-4.9708392	4.0639518	-4.6322170
H	-1.2687512	6.2739973	-4.4988483
H	-3.6112500	6.0378934	-5.3240297
H	-1.6105992	1.8951262	4.9116763
H	1.0850471	4.6196751	2.9503322
H	-1.7941447	3.4570313	6.8381443
H	0.9085823	6.1852858	4.8735392
H	-0.5342905	5.6102394	6.8257306
H	1.0538886	-3.5853611	4.2503310
H	4.3460910	-2.9782715	1.5431128
H	2.4427256	-5.1481273	5.5963137
H	5.7425058	-4.5396888	2.8852756
H	4.7947178	-5.6301973	4.9189718
H	-2.5617017	-3.6048394	-3.2728881
H	1.6844962	-3.5637147	-3.9833389
H	-2.8429381	-5.3425535	-5.0298960
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CoTPP(Ag_{72}):

149
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C	-1.6348792	2.5991480	-1.9889701
C	-2.9445687	3.0738509	-1.6061485
C	-3.7764182	1.9771037	-1.6002285
Co	-0.0806809	0.0321442	-2.2177498
N	1.4811665	-1.1540623	-2.1775079
C	1.4798757	-2.5389159	-2.0702523
C	2.7980465	-3.0195906	-1.7281067
C	3.6286691	-1.9244762	-1.7183373
C	2.8137711	-0.7811964	-2.0606164
C	0.3925324	-3.3710928	-2.3964596
C	0.6175385	-4.8391347	-2.5452234
C	-0.1381340	-5.7761555	-1.8038573
C	0.0711066	-7.1555099	-1.9577994
C	1.0374694	-7.6283732	-2.8608038
C	1.7936145	-6.7094166	-3.6079174
C	1.5864411	-5.3305915	-3.4513668
C	3.3261163	0.4906126	-2.3810112
C	4.8018936	0.6699794	-2.5118883
C	5.4866878	1.6589392	-1.7688659
C	6.8740049	1.8284747	-1.8978938
C	7.6075987	1.0148972	-2.7769216
C	6.9411078	0.0302746	-3.5263120
C	5.5545839	-0.1398791	-3.3957873
C	-0.5581673	3.4367261	-2.3410533
C	-0.7968967	4.9026395	-2.4894059
C	-0.0230012	5.8515269	-1.7823087
C	-0.2411472	7.2284039	-1.9466474
C	-1.2366500	7.6875774	-2.8240081
C	-2.0133656	6.7575373	-3.5353250
C	-1.7961992	5.3812793	-3.3695422
C	-3.4887902	-0.4226431	-2.3273056
C	-4.9647040	-0.5920561	-2.4626186
C	-5.6551152	-1.6158433	-1.7725029
C	-7.0409424	-1.7804586	-1.9241087
C	-7.7667983	-0.9266194	-2.7708842
C	-7.0951923	0.0933200	-3.4660931
C	-5.7101917	0.2577643	-3.3142081
N	-1.2681072	-1.5272200	-2.4093721
C	-2.6409172	-1.5051494	-2.6217570
C	-3.0971160	-2.7866375	-3.1114503
C	-2.0075036	-3.6167828	-3.1240991
C	-0.8851104	-2.8408584	-2.6483650
N	1.1037420	1.5952553	-2.4074819
C	0.7148430	2.9117145	-2.6241827
C	1.8301442	3.6956963	-3.1041752
C	2.9221535	2.8686732	-3.1109000
C	2.4733808	1.5788707	-2.6375665
Ag	-5.7689334	-1.6974361	1.7344782
Ag	-4.3156546	0.8132986	1.6602927
Ag	-1.4014609	0.8160752	1.4909252
Ag	0.0512161	3.3736796	1.6041733
Ag	2.9472516	3.3395190	1.6811560
Ag	4.3765326	5.8219732	1.9019879
Ag	5.7288055	6.4975189	4.2897306
Ag	7.1270346	4.0687196	4.3603648
Ag	5.8209466	3.3201862	1.9019869

Ag	4.3997355	0.8135324	1.6853134
Ag	2.9969391	-1.7214287	1.5349154
Ag	0.0434748	-1.7091408	1.4689778
Ag	0.0495214	-3.3083150	4.1388360
Ag	-1.3816360	-0.8496490	4.0004165
Ag	-2.8929790	-1.7142072	1.6236636
Ag	-1.4145876	-4.2036178	1.7002397
Ag	0.0434466	-6.6867268	1.9019829
Ag	1.4858670	-5.7477508	4.3069496
Ag	2.8448871	-8.1911454	4.2967949
Ag	4.3789838	-5.8010682	4.2215254
Ag	5.7932759	-3.3379510	4.2274562
Ag	4.3491306	-0.8693489	4.1681926
Ag	1.4940234	-0.8513868	3.9293882
Ag	1.5115534	0.8285012	1.4517345
Ag	2.8998322	1.6270038	4.1321199
Ag	4.2917335	4.0951038	4.3146073
Ag	5.7260969	1.5987437	4.3114582
Ag	7.2653506	0.8183922	1.9019859
Ag	8.7096826	-1.6832618	1.9019669
Ag	7.2653476	-4.1850178	1.9019089
Ag	5.8209296	-6.6867258	1.9019659
Ag	4.4130198	-4.2153463	1.7499788
Ag	5.8642563	-1.7030183	1.7388264
Ag	7.2170295	-0.8834358	4.2145326
Ag	8.5207950	1.6391808	4.2963236
Ag	-8.6227824	-1.6832558	1.9019649
Ag	-7.1784464	0.8183982	1.9019839
Ag	-5.7340434	3.3201912	1.9019849
Ag	-4.1827261	4.0934274	4.2872697
Ag	-2.7967719	1.6319441	4.0777527
Ag	0.0577221	1.6376746	3.9867909
Ag	1.4685116	4.1269953	4.2073571
Ag	0.0515255	6.6117815	4.2144120
Ag	-1.4061570	5.8610991	1.7140132
Ag	-2.8453054	8.3236322	1.9019499
Ag	0.0434456	8.3236812	1.9018909
Ag	2.9321946	8.3236342	1.9019839
Ag	1.5003308	5.8554405	1.7573604
Ag	2.8891305	6.6244893	4.2217731
Ag	-7.1784484	-4.1850118	1.9019089
Ag	-5.6915145	-3.3288131	4.2148699
Ag	-2.8354863	-3.3171462	4.2146087
Ag	-4.2468939	-0.8577251	4.1982196
Ag	-5.6228757	1.6043984	4.3030425
Ag	-7.0180193	4.0777016	4.3706919
Ag	-5.6097311	6.4994354	4.3132529
Ag	-2.7786306	6.6228610	4.2061701
Ag	-1.3660547	4.1272335	4.1591213
Ag	-2.8548917	3.3448482	1.6123070
Ag	-4.2896264	5.8219752	1.9019849
Ag	-4.3164269	-4.2097175	1.7345046
Ag	-2.8453684	-6.6867178	1.9019859
Ag	-1.3921658	-5.7475925	4.3126590
Ag	0.0441186	-8.1950133	4.3548904
Ag	-2.7586246	-8.1862267	4.3037320
Ag	-4.2865645	-5.7915936	4.2124313
Ag	-5.7340314	-6.6867208	1.9019669

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Ag   -8.4148988    1.6491367    4.3045999
Ag    1.4998263   -4.2058299    1.6824243
Ag    2.9317094   -3.3210376    4.1785666
Ag    2.9322656   -6.6867208    1.9019829
H     1.7764642    4.7473439   -3.4071940
H     3.9466376    3.1024699   -3.4216722
H     4.7070389   -1.8938347   -1.5237482
H     3.0562794   -4.0676389   -1.5357088
H    -1.9590185   -4.6648375   -3.4400027
H    -4.1240560   -3.0143735   -3.4181429
H    -4.8511225    1.9454600   -1.3859544
H    -3.2021035    4.1214677   -1.4090114
H    -5.0933156   -2.2853680   -1.0990428
H    -5.1852126    1.0445100   -3.8794831
H    -7.5554240   -2.5798089   -1.3647199
H    -7.6528748    0.7628169   -4.1417171
H    -8.8549927   -1.0570574   -2.8910404
H    -0.8917362   -5.4147552   -1.0829778
H     2.1712306   -4.6156182   -4.0526059
H    -0.5258996   -7.8649222   -1.3596525
H     2.5481250   -7.0688334   -4.3271908
H     1.1999278   -8.7118465   -2.9841969
H     4.9211229    2.2952502   -1.0668525
H     5.0355858   -0.9015102   -3.9996878
H     7.3840708    2.6019179   -1.2985733
H     7.5052862   -0.6078014   -4.2264156
H     8.6971061    1.1486152   -2.8801768
H     0.7549056    5.5007350   -1.0830693
H    -2.3952390    4.6576190   -3.9458402
H     0.3719903    7.9452279   -1.3737465
H    -2.7913546    7.1060536   -4.2346565
H    -1.4061214    8.7690263   -2.9552795
```

(NO)CoTPP(Ag_{72}):

```
151
Energy = -14006.21198884 <S^2>=0
C     3.7150584   -1.9527217   -2.9786653
C     2.9097270   -0.8183015   -2.5878826
N     1.5919942   -1.2018448   -2.3937602
C     1.5770270   -2.5749610   -2.5832138
C     2.8876215   -3.0446494   -2.9721487
C     3.4182473    0.4733694   -2.3664789
C     4.8857854    0.7135565   -2.4966713
C     5.8205645    0.0037946   -1.7093694
C     7.1987817    0.2308454   -1.8475404
C     7.6718515    1.1687073   -2.7796493
C     6.7545279    1.8803833   -3.5711418
C     5.3766397    1.6565451   -3.4299502
Co    0.0209317    0.0118985   -2.4656675
N     0.0263157    0.0514019   -4.2761192
O     0.9974289    0.2589351   -4.9033350
C     0.4676034   -3.4147154   -2.3753584
C     0.6380522   -4.8931426   -2.4834158
C     1.5722531   -5.5838343   -1.6782131
```

C	1.7306545	-6.9738160	-1.7870260
C	0.9614894	-7.7038374	-2.7082606
C	0.0313363	-7.0310194	-3.5190116
C	-0.1292048	-5.6416524	-3.4072989
N	-1.1818162	-1.5639434	-2.2507658
C	-2.5628791	-1.5535038	-2.1367613
C	-3.0506568	-2.8690077	-1.7860727
C	-1.9603751	-3.7026733	-1.7674937
C	-0.8132563	-2.8926118	-2.1105163
C	-3.4016540	-0.4590297	-2.4220228
C	-2.8909188	0.8387656	-2.6056539
N	-1.5790428	1.2213767	-2.3872409
C	-1.5614117	2.5964248	-2.5608656
C	-2.8661017	3.0710708	-2.9642274
C	-3.6925822	1.9785304	-2.9911439
C	-0.4521706	3.4286912	-2.3266350
C	-0.6068864	4.9077326	-2.4502363
C	-1.5679389	5.6164555	-1.6920523
C	-1.7147362	7.0055732	-1.8314051
C	-0.9054790	7.7165335	-2.7329895
C	0.0520728	7.0265244	-3.4952452
C	0.1991557	5.6382032	-3.3556409
N	1.1952892	1.5700667	-2.1814503
C	0.8220328	2.8987255	-2.0366812
C	1.9661547	3.7044055	-1.6758396
C	3.0595179	2.8728556	-1.6932701
C	2.5770615	1.5612366	-2.0616534
C	-4.8679874	-0.6966176	-2.5662675
C	-5.8075630	-0.0024051	-1.7706054
C	-7.1847395	-0.2262780	-1.9212262
C	-7.6527031	-1.1465936	-2.8733316
C	-6.7308106	-1.8442092	-3.6718260
C	-5.3537327	-1.6227407	-3.5189188
Ag	-1.4503922	5.8481511	1.8419201
Ag	0.0105478	6.5939877	4.3068111
Ag	2.8326770	6.6288269	4.3121467
Ag	5.6543990	6.5452768	4.4166957
Ag	4.3315077	5.8175504	2.0112167
Ag	2.8871807	8.3192074	2.0112357
Ag	-0.0015693	8.3192604	2.0110697
Ag	-2.8903203	8.3192124	2.0111277
Ag	-2.8188793	6.6226205	4.3113935
Ag	-5.6328534	6.4905703	4.4435471
Ag	-4.2242226	4.0815626	4.4265050
Ag	-2.8401054	1.6152270	4.2217714
Ag	-1.4344614	-0.8656292	4.1413128
Ag	-0.0046507	-3.3358718	4.3101008
Ag	0.0017407	-1.6996953	1.7066036
Ag	-1.4705316	0.8248684	1.5776524
Ag	-4.3377546	0.8170652	1.7891329
Ag	-2.9375058	-1.7173351	1.7145146
Ag	-1.4677944	-4.2251869	1.8049950
Ag	-0.0015703	-6.6911386	2.0112157
Ag	1.4305190	-5.7787966	4.4255393
Ag	2.7669567	-8.2360334	4.3663047
Ag	4.3150199	-5.8188793	4.3371413
Ag	5.7583758	-3.3583588	4.3578098
Ag	4.2932294	-0.8764620	4.3765751

Ag	2.9353242	-1.7164556	1.8147745
Ag	1.4460412	-0.8684265	4.2297903
Ag	0.0032433	1.6185160	4.0898195
Ag	1.4331865	4.1305051	4.2552979
Ag	4.2368118	4.1114557	4.4078234
Ag	5.7759227	3.3157614	2.0112157
Ag	7.0547307	4.1121870	4.4675266
Ag	8.4462353	1.6877069	4.3823631
Ag	7.2203237	0.8139684	2.0112167
Ag	8.6646567	-1.6876866	2.0111967
Ag	7.1654013	-0.8733705	4.3444134
Ag	5.6656492	1.6130869	4.4185051
Ag	2.8535096	1.6274336	4.2315079
Ag	4.3499526	0.8072651	1.8004738
Ag	5.8027457	-1.7176566	1.8915102
Ag	4.3640261	-4.2110192	1.8662025
Ag	5.7759007	-6.6911476	2.0111277
Ag	7.2203197	-4.1894416	2.0111047
Ag	-4.3346503	5.8175554	2.0111477
Ag	-5.7790643	3.3157694	2.0111477
Ag	-5.6504514	1.5965781	4.4255066
Ag	-4.2921747	-0.8816535	4.3123761
Ag	-2.8867481	-3.3467903	4.2986066
Ag	-5.7390461	-3.3542165	4.3239812
Ag	-5.8060230	-1.7076678	1.8357967
Ag	-7.2234683	0.8139774	2.0111487
Ag	-8.6678043	-1.6876766	2.0111297
Ag	-7.2234723	-4.1894316	2.0110717
Ag	-4.3646727	-4.2222164	1.8413344
Ag	-2.8903943	-6.6911406	2.0111487
Ag	-1.4594499	-5.7834536	4.4170326
Ag	-0.0348002	-8.2265713	4.4545033
Ag	-2.8440936	-8.2385636	4.3848601
Ag	-4.3332898	-5.8157222	4.3217886
Ag	-5.7790563	-6.6911406	2.0111287
Ag	-1.4136202	4.1206784	4.2974802
Ag	0.0010871	3.3643414	1.6886566
Ag	1.4595916	0.8129356	1.6527513
Ag	2.9100981	3.3424674	1.7348285
Ag	1.4625800	5.8554685	1.8263957
Ag	-2.9003708	3.3227290	1.7843120
Ag	-7.0535906	4.0726759	4.4692291
Ag	-8.4244852	1.6346267	4.4344074
Ag	-7.1614385	-0.9001509	4.3178131
Ag	1.4634754	-4.2109225	1.8470420
Ag	2.8868667	-3.3336497	4.3687979
Ag	2.8872437	-6.6911446	2.0111487
H	1.9336128	4.7768370	-1.4494370
H	4.1066988	3.1223161	-1.4858742
H	4.7804592	-1.9131451	-3.2309110
H	3.1355967	-4.0823097	-3.2219111
H	-1.9302497	-4.7757790	-1.5442798
H	-4.0987784	-3.1161944	-1.5790413
H	-4.7547400	1.9412056	-3.2576635
H	-3.1120310	4.1104052	-3.2089672
H	-5.4496982	0.7131609	-1.0103582
H	-4.6352149	-2.1617667	-4.1576102
H	-7.8955970	0.3216871	-1.2790699

H	-7.0863791	-2.5639396	-4.4276468
H	-8.7347180	-1.3202054	-2.9935065
H	2.1715494	-5.0221106	-0.9410968
H	-0.8486658	-5.1166337	-4.0560850
H	2.4602965	-7.4881211	-1.1374654
H	-0.5710522	-7.5925151	-4.2521201
H	1.0873313	-8.7955207	-2.7961068
H	5.4588067	-0.7273038	-0.9659268
H	4.6615730	2.2058467	-4.0636555
H	7.9056873	-0.3307725	-1.2123891
H	7.1144755	2.6126968	-4.3126582
H	8.7544578	1.3443394	-2.8906338
H	-2.2010115	5.0684119	-0.9733700
H	0.9375233	5.0991366	-3.9706738
H	-2.4644668	7.5349871	-1.2192504
H	0.6857125	7.5725761	-4.2134257
H	-1.0221519	8.8073704	-2.8429351

Table S5. Coordinates and unit cell dimensions (VASP POSCAR format) for CoP/Ag(111) optimized at the PBE-D level (cf. Figure S4), as a representative example of the periodic calculations.

```
CoP on Ag111 top-site
   1.00000000000000
    14.4437211355000006    0.0000000000000000    0.0000000000000000
     0.0000000000000000   15.0103522455000000    0.0000000000000000
     0.0000000000000000    0.0000000000000000   35.3797356661999984
   1   4  20  12 150
Selective dynamics
Direct
  0.4989501555392183  0.4993519954343691  0.3546323596905409   T   T   T
  0.4664806325912250  0.3726634302370121  0.3568910402327063   T   T   T
  0.6306923755873529  0.4682333728485501  0.3572347644322381   T   T   T
  0.5314125347844804  0.6261455940195692  0.3567214562578183   T   T   T
  0.3671961704332877  0.5305768697368670  0.3569612144626607   T   T   T
  0.6141384875585082  0.7598328741519672  0.3580532562612805   T   T   T
  0.4755055682809909  0.2173367421874555  0.3589332365139088   T   T   T
  0.6190438840122294  0.6641652444280272  0.3569834709042117   T   T   T
  0.5257619346121128  0.2999835833478946  0.3580887958620810   T   T   T
  0.7014522040626239  0.6172563985640214  0.3572226725072926   T   T   T
  0.6213103183312475  0.3047965535542285  0.3584668520091094   T   T   T
  0.7063759066889047  0.5253447109771238  0.3577679705949718   T   T   T
  0.6700515241640563  0.3840684911096137  0.3586867166384345   T   T   T
  0.7921197602696102  0.4767584825301962  0.3594797908198669   T   T   T
  0.7694188612472785  0.3885068944624752  0.3601371566306856   T   T   T
  0.3837155228516467  0.2389750994957203  0.3583038839023951   T   T   T
  0.5223126265788967  0.7814865726887082  0.3585861862141518   T   T   T
  0.3788410274352079  0.3346530565807327  0.3571095437745305   T   T   T
  0.4721101136952971  0.6988266036759595  0.3578059852958471   T   T   T
  0.2964453125776480  0.3815382072310312  0.3570593725154767   T   T   T
  0.3765770231267404  0.6940069544457992  0.3580813639105173   T   T   T
  0.2914810314569981  0.4734851385338111  0.3573662663434891   T   T   T
  0.3278303143601428  0.6147539335779433  0.3582315869527531   T   T   T
  0.2057191785678663  0.5221028034916257  0.3588228200002493   T   T   T
  0.2284342593383027  0.6103769995955332  0.3594105675994859   T   T   T
  0.6743195019722117  0.8032435801473881  0.3589409700951685   T   T   T
  0.5079503700674225  0.1521284063663900  0.3604982981338339   T   T   T
  0.7660251036631485  0.6549317543288917  0.3576987705913838   T   T   T
  0.8599509879158773  0.5079984140341013  0.3605720558520796   T   T   T
  0.8142937209802422  0.3305373432520119  0.3618754038258861   T   T   T
  0.3375052663624299  0.7561364151587673  0.3589774280795155   T   T   T
  0.2318445047447288  0.3438833626582466  0.3574373096615756   T   T   T
  0.6603802630398585  0.2426798412217324  0.3594979042019837   T   T   T
  0.3234983483120369  0.1956067239652266  0.3591086753650626   T   T   T
  0.4898428409130551  0.8466848942045692  0.3601520502954165   T   T   T
  0.1378538604830503  0.4909068906291944  0.3597955710222292   T   T   T
  0.1835482121294295  0.6683426597007791  0.3610880498023933   T   T   T
  0.0000000000000000  0.1111110001099433  0.0000000000000000   F   F   F
  0.0999999997542176  0.2777776664934706  0.0000000000000000   F   F   F
  0.0000000000000000  0.0000000000000000  0.0666666589104352   F   F   F
  0.0999999997542176  0.1666666663835272  0.0666666589104352   F   F   F
  0.0999999997542176  0.0555556669397959  0.1333333178208775   F   F   F
  0.0000000000000000  0.2222223333233231  0.1333333178208775   F   F   F
 -0.0000630999517393  0.1068813824965626  0.2019824701367797   T   T   T
  0.0997909225465030  0.2733243950046895  0.2017922101576325   T   T   T
```

-0.0000072661377088	0.9946397476717529	0.2705066676238780	T	T	T
0.0997288859996977	0.1607221031468900	0.2702731246537032	T	T	T
0.0000000000000000	0.4444443335432027	0.0000000000000000	F	F	F
0.0999999997542176	0.6111109999267370	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333334332664	0.0666666589104352	F	F	F
0.0999999997542176	0.4999999998167937	0.0666666589104352	F	F	F
0.0999999997542176	0.3888889997068503	0.1333333178208775	F	F	F
0.0000000000000000	0.5555556667565895	0.1333333178208775	F	F	F
-0.0000326141341055	0.4401268067258905	0.2019953816351538	T	T	T
0.1000368854351289	0.6072169769817116	0.2020464200180048	T	T	T
0.0001835889629165	0.3273885829419038	0.2701215023518596	T	T	T
0.0993093968455091	0.4945528926673130	0.2697872461481895	T	T	T
0.0000000000000000	0.7777776669764691	0.0000000000000000	F	F	F
0.0999999997542176	0.9444443333599963	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666668665258	0.0666666589104352	F	F	F
0.0999999997542176	0.8333333332500601	0.0666666589104352	F	F	F
0.0999999997542176	0.7222223331401167	0.1333333178208775	F	F	F
0.0000000000000000	0.8888890001898488	0.1333333178208775	F	F	F
0.0000344744896773	0.7740784870096050	0.2021486632506101	T	T	T
0.0998241372945803	0.9406354728790555	0.2021344889364482	T	T	T
0.9997401995408087	0.6618189365020685	0.2702019927259574	T	T	T
0.0996676466387681	0.8284131429665543	0.2704336396316554	T	T	T
0.2000000002007809	0.1111110001099433	0.0000000000000000	F	F	F
0.2999999999549985	0.2777776664934706	0.0000000000000000	F	F	F
0.2000000002007809	0.0000000000000000	0.0666666589104352	F	F	F
0.2999999999549985	0.1666666663835272	0.0666666589104352	F	F	F
0.2999999999549985	0.0555556669397959	0.1333333178208775	F	F	F
0.2000000002007809	0.2222223333233231	0.1333333178208775	F	F	F
0.1999406405523643	0.1070234742759013	0.2019676685517811	T	T	T
0.3001555699444258	0.2740505153095417	0.2017538413671024	T	T	T
0.1998187252806103	0.9945352252235703	0.2703995372115316	T	T	T
0.2993773497448333	0.1604973855385383	0.2695837461155590	T	T	T
0.2000000002007809	0.4444443335432027	0.0000000000000000	F	F	F
0.2999999999549985	0.6111109999267370	0.0000000000000000	F	F	F
0.2000000002007809	0.3333333334332664	0.0666666589104352	F	F	F
0.2999999999549985	0.4999999998167937	0.0666666589104352	F	F	F
0.2999999999549985	0.3888889997068503	0.1333333178208775	F	F	F
0.2000000002007809	0.5555556667565895	0.1333333178208775	F	F	F
0.2001624018913318	0.4405606988293091	0.2017180927499119	T	T	T
0.3000042207034586	0.6074745890087153	0.2021239593002970	T	T	T
0.1991458530940954	0.3272948036071787	0.2691685335174325	T	T	T
0.2993326750149016	0.4941986811581017	0.2685329005964733	T	T	T
0.2000000002007809	0.7777776669764691	0.0000000000000000	F	F	F
0.2999999999549985	0.9444443333599963	0.0000000000000000	F	F	F
0.2000000002007809	0.6666666668665258	0.0666666589104352	F	F	F
0.2999999999549985	0.8333333332500601	0.0666666589104352	F	F	F
0.2999999999549985	0.7222223331401167	0.1333333178208775	F	F	F
0.2000000002007809	0.8888890001898488	0.1333333178208775	F	F	F
0.1999497450248253	0.7739951500756083	0.2021629924941886	T	T	T
0.2998789798854433	0.9409366492358399	0.2019425967448420	T	T	T
0.1989298429863623	0.6615455761000476	0.2700787054677544	T	T	T
0.2992597978306666	0.8287612075714248	0.2697319616686750	T	T	T
0.3999999997092161	0.1111110001099433	0.0000000000000000	F	F	F
0.5000000001557794	0.2777776664934706	0.0000000000000000	F	F	F
0.3999999997092161	0.0000000000000000	0.0666666589104352	F	F	F
0.5000000001557794	0.1666666663835272	0.0666666589104352	F	F	F
0.5000000001557794	0.0555556669397959	0.1333333178208775	F	F	F
0.3999999997092161	0.2222223333233231	0.1333333178208775	F	F	F

0.4001583617290986	0.1073292349375100	0.2020022048336971	T	T	T
0.5002514316217970	0.2739328575809123	0.2021575594569818	T	T	T
0.3999043548314116	0.9942797837879963	0.2702290020562241	T	T	T
0.4998412090615841	0.1604673542997872	0.2699670931342332	T	T	T
0.3999999997092161	0.4444443335432027	0.0000000000000000	F	F	F
0.5000000001557794	0.6111109999267370	0.0000000000000000	F	F	F
0.3999999997092161	0.3333333334332664	0.0666666589104352	F	F	F
0.5000000001557794	0.4999999998167937	0.0666666589104352	F	F	F
0.5000000001557794	0.3888889997068503	0.1333333178208775	F	F	F
0.3999999997092161	0.5555556667565895	0.1333333178208775	F	F	F
0.4014072066288219	0.4412694201294500	0.2026600857810310	T	T	T
0.4998196640990697	0.6060317873749578	0.2030411985145439	T	T	T
0.3994928409092654	0.3276672163404064	0.2686360829679664	T	T	T
0.4999789289476549	0.4948709059530271	0.2748000165269273	T	T	T
0.3999999997092161	0.7777776669764691	0.0000000000000000	F	F	F
0.5000000001557794	0.9444443333599963	0.0000000000000000	F	F	F
0.3999999997092161	0.6666666668665258	0.0666666589104352	F	F	F
0.5000000001557794	0.8333333332500601	0.0666666589104352	F	F	F
0.5000000001557794	0.7222223331401167	0.1333333178208775	F	F	F
0.3999999997092161	0.8888890001898488	0.1333333178208775	F	F	F
0.4003459041798123	0.7736828048896905	0.2022166485079880	T	T	T
0.5000263656773806	0.9404814365542916	0.2021598705639179	T	T	T
0.3992842147611055	0.6618010931720245	0.2696630737963434	T	T	T
0.5002828199406590	0.8283961501079294	0.2700830448676348	T	T	T
0.5999999999099970	0.1111110001099433	0.0000000000000000	F	F	F
0.6999999996642146	0.2777776664934706	0.0000000000000000	F	F	F
0.5999999999099970	0.0000000000000000	0.0666666589104352	F	F	F
0.6999999996642146	0.1666666663835272	0.0666666589104352	F	F	F
0.6999999996642146	0.0555556669397959	0.1333333178208775	F	F	F
0.5999999999099970	0.2222223333233231	0.1333333178208775	F	F	F
0.5998594406523369	0.1074471990496041	0.2019901739471236	T	T	T
0.6999219077939398	0.2742659439018427	0.2021495740951227	T	T	T
0.6000416776554821	0.9947611032375644	0.2701899229008131	T	T	T
0.7007239180523760	0.1605302715158324	0.2696997817524830	T	T	T
0.5999999999099970	0.4444443335432027	0.0000000000000000	F	F	F
0.6999999996642146	0.6111109999267370	0.0000000000000000	F	F	F
0.5999999999099970	0.3333333334332664	0.0666666589104352	F	F	F
0.6999999996642146	0.4999999998167937	0.0666666589104352	F	F	F
0.6999999996642146	0.3888889997068503	0.1333333178208775	F	F	F
0.5999999999099970	0.5555556667565895	0.1333333178208775	F	F	F
0.5985265485437715	0.4410465226835512	0.2030077814560040	T	T	T
0.7000487983157476	0.6071796670982489	0.2016272888814040	T	T	T
0.6004682815300210	0.3272862382429522	0.2696758254829965	T	T	T
0.7007485611009876	0.4948984456866651	0.2685034128062782	T	T	T
0.5999999999099970	0.7777776669764691	0.0000000000000000	F	F	F
0.6999999996642146	0.9444443333599963	0.0000000000000000	F	F	F
0.5999999999099970	0.6666666668665258	0.0666666589104352	F	F	F
0.6999999996642146	0.8333333332500601	0.0666666589104352	F	F	F
0.6999999996642146	0.7222223331401167	0.1333333178208775	F	F	F
0.5999999999099970	0.8888890001898488	0.1333333178208775	F	F	F
0.5998721905711702	0.7739314434858122	0.2020206306624605	T	T	T
0.7001218157793186	0.9409702395184528	0.2020268892469307	T	T	T
0.6009227662722331	0.6612576125011876	0.2687302132167244	T	T	T
0.7007292717418883	0.8287781983488653	0.2696479518748078	T	T	T
0.8000000001107779	0.1111110001099433	0.0000000000000000	F	F	F
0.8999999998649955	0.2777776664934706	0.0000000000000000	F	F	F
0.8000000001107779	0.0000000000000000	0.0666666589104352	F	F	F
0.8999999998649955	0.1666666663835272	0.0666666589104352	F	F	F

```
0.8999999998649955  0.0555556669397959  0.1333333178208775   F   F   F
0.8000000001107779  0.2222223333233231  0.1333333178208775   F   F   F
0.8000498731443445  0.1070365544881949  0.2019205621447148   T   T   T
0.8999240363165839  0.2734622801280441  0.2020455001953559   T   T   T
0.8002090697918102  0.9946332556038604  0.2703887728459656   T   T   T
0.9002840970693572  0.1607908645174461  0.2702978457573233   T   T   T
0.8000000001107779  0.4444443335432027  0.0000000000000000   F   F   F
0.8999999998649955  0.6111109999267370  0.0000000000000000   F   F   F
0.8000000001107779  0.3333333334332664  0.0666666589104352   F   F   F
0.8999999998649955  0.4999999998167937  0.0666666589104352   F   F   F
0.8999999998649955  0.3888889997068503  0.1333333178208775   F   F   F
0.8000000001107779  0.5555556667565895  0.1333333178208775   F   F   F
0.7998739008325435  0.4402290731458465  0.2018320484039046   T   T   T
0.9001840440387772  0.6070004012765484  0.2018652116319652   T   T   T
0.8009347778628069  0.3276859328965209  0.2698544196952009   T   T   T
0.9006952349419477  0.4946670586149147  0.2698501666744966   T   T   T
0.8000000001107779  0.7777776669764691  0.0000000000000000   F   F   F
0.8999999998649955  0.9444443333599963  0.0000000000000000   F   F   F
0.8000000001107779  0.6666666668665258  0.0666666589104352   F   F   F
0.8999999998649955  0.8333333332500601  0.0666666589104352   F   F   F
0.8999999998649955  0.7222223331401167  0.1333333178208775   F   F   F
0.8000000001107779  0.8888890001898488  0.1333333178208775   F   F   F
0.8001521101198346  0.7741456864455928  0.2019761156071919   T   T   T
0.9001881117097116  0.9406760034175585  0.2021442912033192   T   T   T
0.8008833043501824  0.6618292424043775  0.2692297445747717   T   T   T
0.9003200128131286  0.8285271731621168  0.2704512484670111   T   T   T
```

Further coordinate files on other optimized geometries quoted in the text can be obtained from the authors (contact W.H.).

Table S6. Fragment orbital analysis for MTPP, (Ag)MTPP, (NO)(Ag)MTPP (M = Co, Fe): transcript adopted from ADF program output corresponding to Figures 12, 13 of the main paper, showing the composition of each molecular orbital (1st column) in terms of fragment orbitals located on the metal center, the tpp ligand, or the NO ligand, respectively. 1st column ("`E(eV)`"): molecular orbital energy; 2nd column ("`Occ`"): occupancy of that molecular orbital; 3rd column ("`MO`"): label of that molecular orbital (Schoenflies symbol of irreducible representation preceded by numer within that representation); 4th column ("`%`"): composition of the molecular orbital in terms of the symmetrized fragment orbital (`SFO`) specified in the 5th column ("`SFO`"); 6th column ("`E(eV)`"): orbital energy of the SFO in the *isolated fragment calculation*; 7th column ("`Occ`"): occupancy of the SFO in the *isolated fragment calculation*; 8th column ("`Fragment`"): fragment nicknames, `tpp` = TPP fragment, `silv` = Ag atom fragment, `cobalt` = Co atom fragment, `no` = NO fragment. Note that for spin-polarized systems, a separate table is given for each spin channel ("`SPIN 1`" or "`SPIN 2`"). Molecular orbitals (columns 1-3) are ordered according to increasing energy; columns 4-8 in general contain several entries corresponding to each entry in columns 1-3, i.e., they give the composition of each molecular orbitals in terms of fragment orbitals.

Example: The HOMO in spin channel 1 (line entry "`-4.934  1.00 35 A1`" in columns 1-3) of CoTPP is composed of three SFOs given in the three lines to the right (columns 4-8), i.e., it is composed to 77.76% of an SFO labeled 32 A_1 (column 5) of the isolated TPP fragment (column 8). In the isolated fragment calculation, this SFO is unoccupied (column 7) and has an energy of -4.674 eV (column 6). The HOMO furthermore is composed from SFO 29 A_1 by 11.62%, which is a doubly occupied SFO of energy -5.919 eV in the isolated TPP fragment calculation. Finally, the smallest contribution (7.34%) given for the HOMO in spin channel 1 comes from SFO 31 A_1, which is a doubly occupied fragment orbital on TPP with an energy of -4.714.

In the sections for (Ag)CoTPP and (NO)(Ag)CoTPP (see below), the molecular orbitals included in Figures 12 and 13 of the main paper are highlighted (bold or grey, cf. Figures 12 and 13).

CoTPP:

```
                          *** SPIN 1 *** (α)


  E(eV)  Occ    MO     %     SFO           E(eV)  Occ  Fragment
-------------------------------------------------------------

-23.838  1.00  2 B1  98.27%     1 B1      -23.338  2.00 1 tpp
   (...)
 -9.569  1.00 24 A1  30.02%    23 A1       -8.871  2.00 1 tpp
                     25.81%    21 A1       -9.340  2.00 1 tpp
                     17.42%    31 A1       -4.714  2.00 1 tpp
                     15.09%     1 D:x2-y2  -8.344  1.40 2 cobalt
                      5.29%    14 A1      -12.039  2.00 1 tpp
```

```
  (...)
-8.539  1.00 28 A1  45.62%    23 A1       -8.871  2.00 1 tpp
                    25.38%    31 A1       -4.714  2.00 1 tpp
                    16.41%     1 D:x2-y2  -8.344  1.40 2 cobalt
  (...)
-6.630  1.00 27 B1  35.82%    28 B1       -5.439  2.00 1 tpp
                    26.16%     1 D:xz     -8.344  1.40 2 cobalt
                    18.68%    25 B1       -6.619  2.00 1 tpp
                    13.90%    27 B1       -5.682  2.00 1 tpp
-6.625  1.00 27 B2  38.97%    28 B2       -5.411  2.00 1 tpp
                    25.27%     1 D:yz     -8.344  1.40 2 cobalt
                    19.03%    25 B2       -6.619  2.00 1 tpp
                    11.44%    27 B2       -5.686  2.00 1 tpp
-6.575  1.00 30 A1  92.10%    26 A1       -6.712  2.00 1 tpp
-6.504  1.00 31 A1  90.97%    28 A1       -6.617  2.00 1 tpp
                     6.00%    27 A1       -6.698  2.00 1 tpp
-6.503  1.00 23 A2  99.95%    23 A2       -6.638  2.00 1 tpp
-6.449  1.00 28 B1  80.48%    25 B1       -6.619  2.00 1 tpp
                     6.89%    28 B1       -5.439  2.00 1 tpp
                     5.44%    27 B1       -5.682  2.00 1 tpp
                     5.13%     1 D:xz     -8.344  1.40 2 cobalt
-6.449  1.00 28 B2  80.16%    25 B2       -6.619  2.00 1 tpp
                     7.66%    28 B2       -5.411  2.00 1 tpp
                     5.36%     1 D:yz     -8.344  1.40 2 cobalt
                     5.09%    27 B2       -5.686  2.00 1 tpp
-6.405  1.00 32 A1  75.00%    29 A1       -5.919  2.00 1 tpp
                     6.78%    32 A1       -4.674  0.00 1 tpp
                     5.35%     1 D:z2     -8.344  1.40 2 cobalt
-6.320  1.00 24 A2  99.92%    24 A2       -6.456  2.00 1 tpp
-6.295  1.00 29 B2  97.08%    26 B2       -6.412  2.00 1 tpp
-6.295  1.00 29 B1  96.36%    26 B1       -6.412  2.00 1 tpp
-6.214  1.00 33 A1  74.29%     1 D:z2     -8.344  1.40 2 cobalt
                     6.25%    29 A1       -5.919  2.00 1 tpp
                     6.00%     2 S        -5.621  2.00 2 cobalt
                     5.48%    30 A1       -5.423  2.00 1 tpp
-5.961  1.00 34 A1  89.91%    30 A1       -5.423  2.00 1 tpp
                     6.43%     1 D:z2     -8.344  1.40 2 cobalt
-5.600  1.00 25 A2  92.95%     1 D:xy     -8.344  1.40 2 cobalt
-5.041  1.00 26 A2  99.67%    25 A2       -4.922  2.00 1 tpp
-4.995  1.00 30 B1  62.07%     1 D:xz     -8.344  1.40 2 cobalt
                    25.51%    28 B1       -5.439  2.00 1 tpp
                    10.17%    27 B1       -5.682  2.00 1 tpp
-4.995  1.00 30 B2  61.87%     1 D:yz     -8.344  1.40 2 cobalt
                    20.54%    28 B2       -5.411  2.00 1 tpp
                    15.15%    27 B2       -5.686  2.00 1 tpp
-4.934  1.00 35 A1  77.76%    32 A1       -4.674  0.00 1 tpp
                    11.62%    29 A1       -5.919  2.00 1 tpp
                     7.34%    31 A1       -4.714  2.00 1 tpp
-2.896  0.00 31 B2  96.44%    29 B2       -2.900  0.00 1 tpp
-2.896  0.00 31 B1  96.58%    29 B1       -2.895  0.00 1 tpp
-2.643  0.00 36 A1  57.83%     1 D:x2-y2  -8.344  1.40 2 cobalt
                    35.43%    31 A1       -4.714  2.00 1 tpp
                     5.15%    32 A1       -4.674  0.00 1 tpp
-1.735  0.00 27 A2  98.23%    26 A2       -1.807  0.00 1 tpp
-1.464  0.00 37 A1  99.34%    33 A1       -1.584  0.00 1 tpp
-1.426  0.00 32 B2  99.64%    30 B2       -1.558  0.00 1 tpp
-1.425  0.00 32 B1  99.59%    30 B1       -1.557  0.00 1 tpp
-1.372  0.00 28 A2  99.97%    27 A2       -1.500  0.00 1 tpp
```

-1.363	0.00	38	A1	99.87%	34	A1	-1.496	0.00	1	tpp
-1.330	0.00	33	B2	99.45%	31	B2	-1.452	0.00	1	tpp
-1.329	0.00	33	B1	99.39%	31	B1	-1.452	0.00	1	tpp
-1.280	0.00	29	A2	98.24%	28	A2	-1.370	0.00	1	tpp
-0.133	0.00	39	A1	97.70%	36	A1	0.404	0.00	1	tpp
0.030	0.00	40	A1	71.20%	35	A1	0.117	0.00	1	tpp
				18.11%	3	S	1.392	0.00	2	cobalt
				9.46%	2	S	-5.621	2.00	2	cobalt
0.242	0.00	34	B1	99.59%	32	B1	0.206	0.00	1	tpp
0.244	0.00	34	B2	99.56%	32	B2	0.208	0.00	1	tpp
0.357	0.00	30	A2	99.96%	29	A2	0.300	0.00	1	tpp
0.513	0.00	35	B1	96.56%	33	B1	0.722	0.00	1	tpp
0.514	0.00	35	B2	96.20%	33	B2	0.720	0.00	1	tpp
0.590	0.00	41	A1	30.61%	38	A1	0.938	0.00	1	tpp
				23.64%	3	S	1.392	0.00	2	cobalt
				22.39%	35	A1	0.117	0.00	1	tpp
				19.37%	2	S	-5.621	2.00	2	cobalt
0.774	0.00	42	A1	62.13%	37	A1	0.837	0.00	1	tpp
				15.57%	2	P:z	-0.679	0.00	2	cobalt
				5.94%	41	A1	1.775	0.00	1	tpp
0.929	0.00	36	B1	97.24%	34	B1	0.937	0.00	1	tpp
0.936	0.00	36	B2	96.55%	34	B2	0.936	0.00	1	tpp
0.959	0.00	31	A2	99.84%	30	A2	1.097	0.00	1	tpp
0.982	0.00	43	A1	34.99%	37	A1	0.837	0.00	1	tpp
				22.70%	2	P:z	-0.679	0.00	2	cobalt
				13.01%	39	A1	1.332	0.00	1	tpp
				10.67%	41	A1	1.775	0.00	1	tpp
				7.75%	44	A1	2.706	0.00	1	tpp
1.217	0.00	32	A2	99.94%	31	A2	1.168	0.00	1	tpp
1.223	0.00	44	A1	74.17%	40	A1	1.335	0.00	1	tpp
				14.27%	38	A1	0.938	0.00	1	tpp
				6.71%	39	A1	1.332	0.00	1	tpp
1.230	0.00	37	B2	97.25%	35	B2	1.227	0.00	1	tpp
1.236	0.00	37	B1	97.00%	35	B1	1.226	0.00	1	tpp
1.369	0.00	45	A1	74.34%	39	A1	1.332	0.00	1	tpp
				7.96%	40	A1	1.335	0.00	1	tpp
				6.78%	41	A1	1.775	0.00	1	tpp
1.432	0.00	38	B1	97.49%	36	B1	1.449	0.00	1	tpp
1.438	0.00	38	B2	97.76%	36	B2	1.454	0.00	1	tpp
1.548	0.00	33	A2	99.71%	32	A2	1.514	0.00	1	tpp
1.560	0.00	46	A1	30.23%	38	A1	0.938	0.00	1	tpp
				27.26%	42	A1	1.965	0.00	1	tpp
				20.08%	2	S	-5.621	2.00	2	cobalt
				9.97%	40	A1	1.335	0.00	1	tpp
				6.03%	3	S	1.392	0.00	2	cobalt
1.640	0.00	34	A2	99.27%	33	A2	1.655	0.00	1	tpp
1.859	0.00	39	B1	88.86%	37	B1	1.874	0.00	1	tpp
				8.69%	38	B1	1.949	0.00	1	tpp
1.860	0.00	39	B2	84.19%	37	B2	1.876	0.00	1	tpp
				13.45%	38	B2	1.945	0.00	1	tpp
1.904	0.00	40	B2	83.59%	38	B2	1.945	0.00	1	tpp
				14.06%	37	B2	1.876	0.00	1	tpp
1.907	0.00	40	B1	88.02%	38	B1	1.949	0.00	1	tpp
				9.37%	37	B1	1.874	0.00	1	tpp
1.934	0.00	35	A2	99.60%	34	A2	1.910	0.00	1	tpp
1.941	0.00	47	A1	58.44%	41	A1	1.775	0.00	1	tpp
				29.24%	43	A1	2.062	0.00	1	tpp
				7.97%	44	A1	2.706	0.00	1	tpp

2.102	0.00	36	A2	98.32%	35	A2	2.070	0.00	1	tpp
2.135	0.00	41	B2	95.70%	39	B2	2.104	0.00	1	tpp
2.139	0.00	41	B1	95.24%	39	B1	2.097	0.00	1	tpp
2.238	0.00	48	A1	62.00%	43	A1	2.062	0.00	1	tpp
				11.23%	41	A1	1.775	0.00	1	tpp
				10.59%	44	A1	2.706	0.00	1	tpp
				8.04%	2	P:z	-0.679	0.00	2	cobalt
2.333	0.00	42	B1	96.84%	40	B1	2.334	0.00	1	tpp
2.338	0.00	42	B2	97.06%	40	B2	2.325	0.00	1	tpp
2.464	0.00	49	A1	51.17%	42	A1	1.965	0.00	1	tpp
				20.58%	45	A1	3.008	0.00	1	tpp
				18.30%	2	S	-5.621	2.00	2	cobalt
				5.09%	38	A1	0.938	0.00	1	tpp
2.528	0.00	37	A2	95.50%	36	A2	2.482	0.00	1	tpp

*** SPIN 2 *** (β)

E(eV)	Occ	MO		%	SFO		E(eV)	Occ	Fragment	
-23.846	1.00	2	B1	98.29%	1	B1	-23.338	2.00	1	tpp
(...)										
-8.392	1.00	29	A1	28.64%	31	A1	-4.714	2.00	1	tpp
				24.41%	25	A1	-8.583	2.00	1	tpp
				24.23%	23	A1	-8.871	2.00	1	tpp
				14.30%	1	D:x2-y2	-8.344	1.40	2	cobalt
-8.340	1.00	21	A2	95.07%	21	A2	-8.359	2.00	1	tpp
-7.880	1.00	25	B2	52.29%	27	B2	-5.686	2.00	1	tpp
				24.73%	28	B2	-5.411	2.00	1	tpp
				9.26%	21	B2	-8.762	2.00	1	tpp
-7.865	1.00	25	B1	54.23%	27	B1	-5.682	2.00	1	tpp
				23.94%	28	B1	-5.439	2.00	1	tpp
				8.48%	21	B1	-8.761	2.00	1	tpp
-7.833	1.00	22	A2	99.78%	22	A2	-7.925	2.00	1	tpp
-7.028	1.00	26	B2	98.35%	24	B2	-7.077	2.00	1	tpp
-7.025	1.00	26	B1	98.21%	24	B1	-7.075	2.00	1	tpp
-6.575	1.00	30	A1	92.49%	26	A1	-6.712	2.00	1	tpp
-6.543	1.00	27	B1	55.38%	25	B1	-6.619	2.00	1	tpp
				24.46%	28	B1	-5.439	2.00	1	tpp
				9.69%	1	D:xz	-8.344	1.40	2	cobalt
				7.54%	27	B1	-5.682	2.00	1	tpp
-6.541	1.00	27	B2	56.72%	25	B2	-6.619	2.00	1	tpp
				24.77%	28	B2	-5.411	2.00	1	tpp
				9.10%	1	D:yz	-8.344	1.40	2	cobalt
				6.69%	27	B2	-5.686	2.00	1	tpp
-6.504	1.00	23	A2	99.96%	23	A2	-6.638	2.00	1	tpp
-6.504	1.00	31	A1	92.48%	28	A1	-6.617	2.00	1	tpp
				5.15%	27	A1	-6.698	2.00	1	tpp
-6.410	1.00	28	B1	43.36%	25	B1	-6.619	2.00	1	tpp
				26.10%	28	B1	-5.439	2.00	1	tpp
				13.75%	27	B1	-5.682	2.00	1	tpp
				9.94%	1	D:xz	-8.344	1.40	2	cobalt
-6.407	1.00	28	B2	42.18%	25	B2	-6.619	2.00	1	tpp
				28.09%	28	B2	-5.411	2.00	1	tpp
				13.84%	27	B2	-5.686	2.00	1	tpp
				10.30%	1	D:yz	-8.344	1.40	2	cobalt

```
-6.384  1.00 32 A1  82.60%    29 A1       -5.919  2.00 1 tpp
                     6.76%    32 A1       -4.674  0.00 1 tpp
-6.320  1.00 24 A2  99.92%    24 A2       -6.456  2.00 1 tpp
-6.296  1.00 29 B2  94.78%    26 B2       -6.412  2.00 1 tpp
-6.295  1.00 29 B1  93.12%    26 B1       -6.412  2.00 1 tpp
-5.988  1.00 33 A1  95.39%    30 A1       -5.423  2.00 1 tpp
-5.068  1.00 25 A2  87.30%    25 A2       -4.922  2.00 1 tpp
                    11.83%     1 D:xy     -8.344  1.40 2 cobalt
-4.972  1.00 26 A2  81.84%     1 D:xy     -8.344  1.40 2 cobalt
                    12.65%    25 A2       -4.922  2.00 1 tpp
-4.930  1.00 34 A1  79.15%    32 A1       -4.674  0.00 1 tpp
                    11.00%    29 A1       -5.919  2.00 1 tpp
                     7.01%    31 A1       -4.714  2.00 1 tpp
-4.613  1.00 30 B2  70.90%     1 D:yz     -8.344  1.40 2 cobalt
                    13.32%    28 B2       -5.411  2.00 1 tpp
                    10.39%    27 B2       -5.686  2.00 1 tpp
-4.612  1.00 30 B1  71.35%     1 D:xz     -8.344  1.40 2 cobalt
                    16.90%    28 B1       -5.439  2.00 1 tpp
                     6.70%    27 B1       -5.682  2.00 1 tpp
-3.697  0.00 35 A1  87.11%     1 D:z2     -8.344  1.40 2 cobalt
                    11.38%     2 S        -5.621  2.00 2 cobalt
-2.879  0.00 31 B1  94.70%    29 B1       -2.895  0.00 1 tpp
                     5.06%     1 D:xz     -8.344  1.40 2 cobalt
-2.878  0.00 31 B2  94.47%    29 B2       -2.900  0.00 1 tpp
                     5.32%     1 D:yz     -8.344  1.40 2 cobalt
-1.987  0.00 36 A1  64.37%     1 D:x2-y2  -8.344  1.40 2 cobalt
                    30.29%    31 A1       -4.714  2.00 1 tpp
-1.740  0.00 27 A2  98.05%    26 A2       -1.807  0.00 1 tpp
-1.463  0.00 37 A1  99.49%    33 A1       -1.584  0.00 1 tpp
-1.426  0.00 32 B2  99.67%    30 B2       -1.558  0.00 1 tpp
-1.425  0.00 32 B1  99.62%    30 B1       -1.557  0.00 1 tpp
-1.372  0.00 28 A2  99.96%    27 A2       -1.500  0.00 1 tpp
-1.363  0.00 38 A1  99.89%    34 A1       -1.496  0.00 1 tpp
-1.329  0.00 33 B1  99.40%    31 B1       -1.452  0.00 1 tpp
-1.329  0.00 33 B2  99.45%    31 B2       -1.452  0.00 1 tpp
-1.283  0.00 29 A2  98.06%    28 A2       -1.370  0.00 1 tpp
-0.142  0.00 39 A1  98.39%    36 A1        0.404  0.00 1 tpp
 0.068  0.00 40 A1  80.82%    35 A1        0.117  0.00 1 tpp
                    13.26%     3 S         1.392  0.00 2 cobalt
 0.243  0.00 34 B1  99.62%    32 B1        0.206  0.00 1 tpp
 0.244  0.00 34 B2  99.56%    32 B2        0.208  0.00 1 tpp
 0.357  0.00 30 A2  99.96%    29 A2        0.300  0.00 1 tpp
 0.511  0.00 35 B1  96.41%    33 B1        0.722  0.00 1 tpp
 0.513  0.00 35 B2  96.08%    33 B2        0.720  0.00 1 tpp
 0.676  0.00 41 A1  44.66%    38 A1        0.938  0.00 1 tpp
                    26.87%     3 S         1.392  0.00 2 cobalt
                    13.66%    35 A1        0.117  0.00 1 tpp
                    13.62%     2 S        -5.621  2.00 2 cobalt
 0.827  0.00 42 A1  92.84%    37 A1        0.837  0.00 1 tpp
 0.933  0.00 36 B1  97.25%    34 B1        0.937  0.00 1 tpp
 0.936  0.00 36 B2  96.58%    34 B2        0.936  0.00 1 tpp
 0.950  0.00 31 A2  99.82%    30 A2        1.097  0.00 1 tpp
 1.161  0.00 43 A1  38.85%    39 A1        1.332  0.00 1 tpp
                    17.53%     2 P:z      -0.679  0.00 2 cobalt
                    15.55%    41 A1        1.775  0.00 1 tpp
                     7.64%    44 A1        2.706  0.00 1 tpp
                     5.69%    40 A1        1.335  0.00 1 tpp
 1.218  0.00 32 A2  99.94%    31 A2        1.168  0.00 1 tpp
```

```
  1.228  0.00 44 A1  72.21%    40 A1        1.335  0.00 1 tpp
                     12.04%    38 A1        0.938  0.00 1 tpp
                     10.39%    39 A1        1.332  0.00 1 tpp
  1.231  0.00 37 B2  97.15%    35 B2        1.227  0.00 1 tpp
  1.236  0.00 37 B1  97.13%    35 B1        1.226  0.00 1 tpp
  1.417  0.00 45 A1  47.39%    39 A1        1.332  0.00 1 tpp
                     21.87%    41 A1        1.775  0.00 1 tpp
                      8.05%     2 P:z      -0.679  0.00 2 cobalt
                      7.62%    44 A1        2.706  0.00 1 tpp
                      6.01%    40 A1        1.335  0.00 1 tpp
  1.435  0.00 38 B1  97.62%    36 B1        1.449  0.00 1 tpp
  1.438  0.00 38 B2  97.59%    36 B2        1.454  0.00 1 tpp
  1.549  0.00 33 A2  99.69%    32 A2        1.514  0.00 1 tpp
  1.633  0.00 34 A2  99.25%    33 A2        1.655  0.00 1 tpp
  1.638  0.00 46 A1  36.94%    42 A1        1.965  0.00 1 tpp
                     22.05%    38 A1        0.938  0.00 1 tpp
                     15.41%     2 S        -5.621  2.00 2 cobalt
                     10.23%     3 S         1.392  0.00 2 cobalt
                      8.70%    40 A1        1.335  0.00 1 tpp
  1.856  0.00 39 B1  86.93%    37 B1        1.874  0.00 1 tpp
                     10.40%    38 B1        1.949  0.00 1 tpp
  1.858  0.00 39 B2  82.75%    37 B2        1.876  0.00 1 tpp
                     14.73%    38 B2        1.945  0.00 1 tpp
  1.904  0.00 40 B2  82.09%    38 B2        1.945  0.00 1 tpp
                     15.48%    37 B2        1.876  0.00 1 tpp
  1.906  0.00 40 B1  86.17%    38 B1        1.949  0.00 1 tpp
                     11.25%    37 B1        1.874  0.00 1 tpp
  1.934  0.00 35 A2  99.58%    34 A2        1.910  0.00 1 tpp
  1.966  0.00 47 A1  44.02%    43 A1        2.062  0.00 1 tpp
                     42.79%    41 A1        1.775  0.00 1 tpp
                      9.60%    44 A1        2.706  0.00 1 tpp
  2.102  0.00 36 A2  98.29%    35 A2        2.070  0.00 1 tpp
  2.134  0.00 41 B2  95.45%    39 B2        2.104  0.00 1 tpp
  2.140  0.00 41 B1  95.08%    39 B1        2.097  0.00 1 tpp
  2.308  0.00 48 A1  45.66%    43 A1        2.062  0.00 1 tpp
                     25.91%    44 A1        2.706  0.00 1 tpp
                     11.22%    41 A1        1.775  0.00 1 tpp
                      9.19%     2 P:z      -0.679  0.00 2 cobalt
  2.333  0.00 42 B1  96.78%    40 B1        2.334  0.00 1 tpp
  2.340  0.00 42 B2  96.98%    40 B2        2.325  0.00 1 tpp
  2.529  0.00 37 A2  92.83%    36 A2        2.482  0.00 1 tpp
                      5.42%    37 A2        2.507  0.00 1 tpp
```

(Ag)CoTPP:

```
  E(eV)  Occ       MO    %     SFO           E(eV)  Occ   Fragment
-------------------------------------------------------------------

-21.633  2.00     1 A2 99.87%     1 A2      -21.878  2.00  1 tpp
                      0.03%     2 A2      -20.678  2.00  1 tpp
(...)
 -9.393  2.00    26 A1 40.63%    21 A1       -9.340  2.00  1 tpp
                     27.92%    23 A1       -8.871  2.00  1 tpp
                     12.38%    31 A1       -4.714  2.00  1 tpp
```

```
                      9.04%     1 D:x2-y2  -8.344  1.40  2 cobalt
                      3.42%    14 A1      -12.039  2.00  1 tpp
                      1.72%    27 A1       -6.698  2.00  1 tpp
                      1.43%    32 A1       -4.674  0.00  1 tpp
(...)
-8.286  2.00    31 A1 34.04%    31 A1       -4.714  2.00  1 tpp
                     30.11%    23 A1       -8.871  2.00  1 tpp
                     17.82%     1 D:x2-y2  -8.344  1.40  2 cobalt
                      7.77%    25 A1       -8.583  2.00  1 tpp
                      2.98%    32 A1       -4.674  0.00  1 tpp
                      2.87%    14 A1      -12.039  2.00  1 tpp
                      2.18%    21 A1       -9.340  2.00  1 tpp
-8.277  2.00    21 A2 95.53%    21 A2       -8.359  2.00  1 tpp
                      2.60%    17 A2       -9.436  2.00  1 tpp
                      1.04%     1 D:xy     -8.344  1.40  2 cobalt
-7.829  2.00    26 B2 35.48%    27 B2       -5.686  2.00  1 tpp
                     24.48%    28 B2       -5.411  2.00  1 tpp
                     18.87%     1 D:yz     -7.552  2.00  3 silv
                      7.58%    21 B2       -8.762  2.00  1 tpp
                      4.54%     2 P:y      -0.679  0.00  2 cobalt
                      2.17%    23 B2       -8.551  2.00  1 tpp
                      1.66%    12 B2      -12.165  2.00  1 tpp
                      1.51%    22 B2       -8.580  2.00  1 tpp
-7.822  2.00    26 B1 46.27%    27 B1       -5.682  2.00  1 tpp
                     19.73%     1 D:xz     -7.552  2.00  3 silv
                     12.63%    28 B1       -5.439  2.00  1 tpp
                      8.34%    21 B1       -8.761  2.00  1 tpp
                      4.27%     2 P:x      -0.679  0.00  2 cobalt
                      2.49%    19 B1       -9.591  2.00  1 tpp
                      1.55%    12 B1      -12.171  2.00  1 tpp
-7.753  2.00    22 A2 97.59%    22 A2       -7.925  2.00  1 tpp
                      2.16%     1 D:xy     -7.552  2.00  3 silv
-7.738  2.00    32 A1 86.64%     1 D:z2     -7.552  2.00  3 silv
                      8.04%     1 D:z2     -8.344  1.40  2 cobalt
                      1.81%     2 P:z      -0.679  0.00  2 cobalt
                      1.41%     2 S        -5.621  2.00  2 cobalt
-7.370  2.00    27 B2 69.73%     1 D:yz     -7.552  2.00  3 silv
                     20.35%    27 B2       -5.686  2.00  1 tpp
                      4.63%     1 D:yz     -8.344  1.40  2 cobalt
-7.342  2.00    27 B1 67.55%     1 D:xz     -7.552  2.00  3 silv
                     17.94%    28 B1       -5.439  2.00  1 tpp
                      6.84%    27 B1       -5.682  2.00  1 tpp
                      3.64%     1 D:xz     -8.344  1.40  2 cobalt
                      1.25%    18 B1       -9.751  2.00  1 tpp
-7.202  2.00    33 A1 97.90%     1 D:x2-y2  -7.552  2.00  3 silv
                      0.86%    30 A1       -5.423  2.00  1 tpp
-7.201  2.00    23 A2 97.43%     1 D:xy     -7.552  2.00  3 silv
                      2.19%    22 A2       -7.925  2.00  1 tpp
-6.938  2.00    28 B2 98.65%    24 B2       -7.077  2.00  1 tpp
                      0.48%    26 B2       -6.412  2.00  1 tpp
-6.932  2.00    28 B1 98.58%    24 B1       -7.075  2.00  1 tpp
                      0.48%    26 B1       -6.412  2.00  1 tpp
-6.516  2.00    34 A1 93.04%    26 A1       -6.712  2.00  1 tpp
                      3.69%    29 A1       -5.919  2.00  1 tpp
                      2.17%    27 A1       -6.698  2.00  1 tpp
-6.456  2.00    24 A2 99.97%    23 A2       -6.638  2.00  1 tpp
                      0.02%    25 A2       -4.922  2.00  1 tpp
-6.453  2.00    35 A1 93.25%    28 A1       -6.617  2.00  1 tpp
```

				4.96%	27	A1	-6.698	2.00	1	tpp
				1.39%	30	A1	-5.423	2.00	1	tpp
-6.449	2.00	29	B1	93.44%	25	B1	-6.619	2.00	1	tpp
				3.53%	28	B1	-5.439	2.00	1	tpp
				1.22%	1	D:xz	-7.552	2.00	3	silv
-6.448	2.00	29	B2	92.45%	25	B2	-6.619	2.00	1	tpp
				4.62%	28	B2	-5.411	2.00	1	tpp
				1.22%	1	D:yz	-7.552	2.00	3	silv
-6.361	2.00	36	A1	76.31%	29	A1	-5.919	2.00	1	tpp
				7.45%	32	A1	-4.674	0.00	1	tpp
				4.19%	26	A1	-6.712	2.00	1	tpp
				2.66%	31	A1	-4.714	2.00	1	tpp
				2.62%	2	P:z	-0.679	0.00	2	cobalt
				2.54%	2	S	-4.552	1.00	3	silv
				1.66%	1	D:z2	-7.552	2.00	3	silv
				1.09%	20	A1	-10.055	2.00	1	tpp
-6.263	2.00	25	A2	99.90%	24	A2	-6.456	2.00	1	tpp
				0.04%	1	D:xy	-7.552	2.00	3	silv
-6.254	2.00	30	B1	69.80%	26	B1	-6.412	2.00	1	tpp
				15.79%	28	B1	-5.439	2.00	1	tpp
				4.56%	27	B1	-5.682	2.00	1	tpp
				3.69%	1	D:xz	-8.344	1.40	2	cobalt
				2.81%	1	D:xz	-7.552	2.00	3	silv
				1.98%	25	B1	-6.619	2.00	1	tpp
-6.248	2.00	30	B2	68.99%	26	B2	-6.412	2.00	1	tpp
				17.94%	28	B2	-5.411	2.00	1	tpp
				3.54%	1	D:yz	-8.344	1.40	2	cobalt
				3.44%	27	B2	-5.686	2.00	1	tpp
				2.85%	1	D:yz	-7.552	2.00	3	silv
				1.72%	25	B2	-6.619	2.00	1	tpp
-6.215	2.00	31	B2	32.26%	28	B2	-5.411	2.00	1	tpp
				29.52%	26	B2	-6.412	2.00	1	tpp
				18.42%	27	B2	-5.686	2.00	1	tpp
				7.85%	1	D:yz	-8.344	1.40	2	cobalt
				5.09%	25	B2	-6.619	2.00	1	tpp
				4.18%	1	D:yz	-7.552	2.00	3	silv
-6.199	2.00	31	B1	29.75%	28	B1	-5.439	2.00	1	tpp
				28.98%	26	B1	-6.412	2.00	1	tpp
				21.60%	27	B1	-5.682	2.00	1	tpp
				7.72%	1	D:xz	-8.344	1.40	2	cobalt
				5.45%	1	D:xz	-7.552	2.00	3	silv
				4.07%	25	B1	-6.619	2.00	1	tpp
-5.883	2.00	37	A1	94.79%	30	A1	-5.423	2.00	1	tpp
				2.11%	28	A1	-6.617	2.00	1	tpp
-5.017	**2.00**	**38**	**A1**	**27.30%**	**32**	**A1**	**-4.674**	**0.00**	**1**	**tpp**
				22.99%	**1**	**D:z2**	**-8.344**	**1.40**	**2**	**cobalt**
				22.88%	**2**	**S**	**-4.552**	**1.00**	**3**	**silv**
				13.26%	29	A1	-5.919	2.00	1	tpp
				4.95%	1	D:z2	-7.552	2.00	3	silv
				3.74%	2	S	-5.621	2.00	2	cobalt
				1.84%	31	A1	-4.714	2.00	1	tpp
				1.36%	2	P:z	-0.679	0.00	2	cobalt
-4.957	2.00	26	A2	89.79%	25	A2	-4.922	2.00	1	tpp
				9.48%	1	D:xy	-8.344	1.40	2	cobalt
-4.856	2.00	27	A2	84.23%	1	D:xy	-8.344	1.40	2	cobalt
				10.16%	25	A2	-4.922	2.00	1	tpp
				1.53%	21	A2	-8.359	2.00	1	tpp
-4.769	2.00	39	A1	46.96%	32	A1	-4.674	0.00	1	tpp

				29.60%	1	D:z2	-8.344	1.40	2	cobalt
				8.07%	2	S	-4.552	1.00	3	silv
				4.50%	31	A1	-4.714	2.00	1	tpp
				3.46%	29	A1	-5.919	2.00	1	tpp
				2.64%	2	S	-5.621	2.00	2	cobalt
				2.42%	1	D:z2	-7.552	2.00	3	silv
-4.332	2.00	32	B2	71.86%	1	D:yz	-8.344	1.40	2	cobalt
				10.82%	28	B2	-5.411	2.00	1	tpp
				8.61%	27	B2	-5.686	2.00	1	tpp
				5.00%	29	B2	-2.900	0.00	1	tpp
				1.40%	1	D:yz	-7.552	2.00	3	silv
-4.323	2.00	32	B1	73.21%	1	D:xz	-8.344	1.40	2	cobalt
				13.56%	28	B1	-5.439	2.00	1	tpp
				5.35%	27	B1	-5.682	2.00	1	tpp
				4.76%	29	B1	-2.895	0.00	1	tpp
				1.13%	1	D:xz	-7.552	2.00	3	silv
-3.261	**0.00**	**40**	**A1**	**56.64%**	**2**	**S**	**-4.552**	**1.00**	**3**	**silv**
				26.03%	**1**	**D:z2**	**-8.344**	**1.40**	**2**	**cobalt**
				8.92%	2	P:z	0.033	0.00	3	silv
				3.19%	32	A1	-4.674	0.00	1	tpp
				1.97%	27	A1	-6.698	2.00	1	tpp
				1.94%	2	P:z	-0.679	0.00	2	cobalt
				-1.07%	3	S	1.392	0.00	2	cobalt
-2.769	0.00	33	B2	93.21%	29	B2	-2.900	0.00	1	tpp
				6.64%	1	D:yz	-8.344	1.40	2	cobalt
-2.765	0.00	33	B1	93.52%	29	B1	-2.895	0.00	1	tpp
				6.33%	1	D:xz	-8.344	1.40	2	cobalt
-1.990	0.00	41	A1	63.05%	1	D:x2-y2	-8.344	1.40	2	cobalt
				31.04%	31	A1	-4.714	2.00	1	tpp
				4.37%	32	A1	-4.674	0.00	1	tpp
-1.656	0.00	28	A2	99.15%	26	A2	-1.807	0.00	1	tpp
				0.69%	28	A2	-1.370	0.00	1	tpp
-1.413	0.00	42	A1	99.06%	33	A1	-1.584	0.00	1	tpp
				0.18%	2	P:z	0.033	0.00	3	silv
-1.377	0.00	34	B1	99.73%	30	B1	-1.557	0.00	1	tpp
				0.13%	2	P:x	0.033	0.00	3	silv
-1.373	0.00	34	B2	99.84%	30	B2	-1.558	0.00	1	tpp
				0.07%	1	D:yz	-8.344	1.40	2	cobalt
-1.324	0.00	29	A2	99.97%	27	A2	-1.500	0.00	1	tpp
				0.02%	30	A2	1.097	0.00	1	tpp
-1.315	0.00	43	A1	99.78%	34	A1	-1.496	0.00	1	tpp
				0.09%	33	A1	-1.584	0.00	1	tpp
-1.279	0.00	35	B2	99.62%	31	B2	-1.452	0.00	1	tpp
				0.23%	1	D:yz	-8.344	1.40	2	cobalt
-1.279	0.00	35	B1	99.57%	31	B1	-1.452	0.00	1	tpp
				0.26%	1	D:xz	-8.344	1.40	2	cobalt
-1.215	0.00	30	A2	99.15%	28	A2	-1.370	0.00	1	tpp
				0.71%	26	A2	-1.807	0.00	1	tpp
-0.040	0.00	44	A1	97.18%	36	A1	0.404	0.00	1	tpp
				0.48%	2	P:z	0.033	0.00	3	silv
0.005	0.00	36	B2	40.17%	32	B2	0.208	0.00	1	tpp
				37.68%	2	P:y	0.033	0.00	3	silv
				12.02%	34	B2	0.936	0.00	1	tpp
				3.18%	36	B2	1.454	0.00	1	tpp
				1.82%	39	B2	2.104	0.00	1	tpp
0.120	0.00	36	B1	54.43%	32	B1	0.206	0.00	1	tpp
				30.85%	2	P:x	0.033	0.00	3	silv
				4.77%	35	B1	1.226	0.00	1	tpp

				2.26%	42	B1	3.430	0.00	1	tpp
				2.15%	40	B1	2.334	0.00	1	tpp
				1.66%	34	B1	0.937	0.00	1	tpp
0.170	0.00	45	A1	82.90%	35	A1	0.117	0.00	1	tpp
				7.70%	3	S	1.392	0.00	2	cobalt
				4.27%	3	S	1.341	0.00	3	silv
				1.89%	2	P:z	-0.679	0.00	2	cobalt
				1.49%	2	S	-5.621	2.00	2	cobalt
0.388	0.00	31	A2	99.85%	29	A2	0.300	0.00	1	tpp
				0.08%	31	A2	1.168	0.00	1	tpp
0.438	0.00	46	A1	32.73%	2	P:z	0.033	0.00	3	silv
				17.17%	3	S	1.341	0.00	3	silv
				16.02%	2	P:z	-0.679	0.00	2	cobalt
				8.41%	35	A1	0.117	0.00	1	tpp
				5.80%	44	A1	2.706	0.00	1	tpp
				2.86%	3	S	1.392	0.00	2	cobalt
				2.84%	41	A1	1.775	0.00	1	tpp
				2.78%	43	A1	2.062	0.00	1	tpp
				2.57%	32	A1	-4.674	0.00	1	tpp
				2.17%	1	D:z2	-8.344	1.40	2	cobalt
				1.25%	36	A1	0.404	0.00	1	tpp
				1.24%	40	A1	1.335	0.00	1	tpp
0.438	0.00	37	B2	54.77%	32	B2	0.208	0.00	1	tpp
				15.03%	2	P:y	0.033	0.00	3	silv
				12.69%	34	B2	0.936	0.00	1	tpp
				10.59%	33	B2	0.720	0.00	1	tpp
				2.83%	36	B2	1.454	0.00	1	tpp
				1.09%	39	B2	2.104	0.00	1	tpp
0.479	0.00	37	B1	43.85%	32	B1	0.206	0.00	1	tpp
				29.46%	2	P:x	0.033	0.00	3	silv
				7.02%	35	B1	1.226	0.00	1	tpp
				5.05%	33	B1	0.722	0.00	1	tpp
				3.59%	34	B1	0.937	0.00	1	tpp
				3.09%	40	B1	2.334	0.00	1	tpp
				2.74%	42	B1	3.430	0.00	1	tpp
0.625	0.00	38	B1	90.96%	33	B1	0.722	0.00	1	tpp
				3.49%	34	B1	0.937	0.00	1	tpp
				1.46%	2	P:x	0.033	0.00	3	silv
				1.16%	32	B1	0.206	0.00	1	tpp
0.646	0.00	38	B2	86.61%	33	B2	0.720	0.00	1	tpp
				3.78%	32	B2	0.208	0.00	1	tpp
				3.21%	34	B2	0.936	0.00	1	tpp
				2.89%	2	P:y	0.033	0.00	3	silv
				1.15%	36	B2	1.454	0.00	1	tpp
0.773	0.00	47	A1	41.14%	37	A1	0.837	0.00	1	tpp
				21.58%	3	S	1.392	0.00	2	cobalt
				18.79%	38	A1	0.938	0.00	1	tpp
				17.79%	2	S	-5.621	2.00	2	cobalt
				2.23%	35	A1	0.117	0.00	1	tpp
				1.56%	39	A1	1.332	0.00	1	tpp
				-1.55%	45	A1	3.008	0.00	1	tpp
				-1.45%	2	S	-4.552	1.00	3	silv
				-1.38%	55	A1	5.665	0.00	1	tpp
				1.35%	3	S	1.341	0.00	3	silv
				1.28%	1	D:z2	-8.344	1.40	2	cobalt
				1.05%	27	A1	-6.698	2.00	1	tpp
				-1.04%	42	A1	1.965	0.00	1	tpp
0.930	0.00	48	A1	50.70%	37	A1	0.837	0.00	1	tpp

				30.30%	38	A1	0.938	0.00	1	tpp
				7.33%	3	S	1.392	0.00	2	cobalt
				5.25%	2	S	-5.621	2.00	2	cobalt
				3.69%	2	P:z	0.033	0.00	3	silv
				1.61%	39	A1	1.332	0.00	1	tpp
1.019	0.00	39	B1	89.27%	34	B1	0.937	0.00	1	tpp
				4.78%	35	B1	1.226	0.00	1	tpp
				2.18%	2	P:x	0.033	0.00	3	silv
				1.89%	33	B1	0.722	0.00	1	tpp
1.050	0.00	32	A2	99.87%	30	A2	1.097	0.00	1	tpp
				0.04%	1	D:xy	-8.344	1.40	2	cobalt
1.203	0.00	39	B2	63.05%	34	B2	0.936	0.00	1	tpp
				18.72%	36	B2	1.454	0.00	1	tpp
				8.54%	2	P:y	0.033	0.00	3	silv
				3.58%	35	B2	1.227	0.00	1	tpp
				2.59%	39	B2	2.104	0.00	1	tpp
1.241	0.00	33	A2	99.48%	31	A2	1.168	0.00	1	tpp
				0.26%	32	A2	1.514	0.00	1	tpp
1.252	0.00	49	A1	54.37%	39	A1	1.332	0.00	1	tpp
				20.42%	38	A1	0.938	0.00	1	tpp
				7.63%	40	A1	1.335	0.00	1	tpp
				7.56%	3	S	1.341	0.00	3	silv
				4.19%	3	S	1.392	0.00	2	cobalt
				3.81%	2	S	-5.621	2.00	2	cobalt
				1.88%	37	A1	0.837	0.00	1	tpp
				1.36%	41	A1	1.775	0.00	1	tpp
1.282	0.00	40	B2	93.32%	35	B2	1.227	0.00	1	tpp
				5.06%	36	B2	1.454	0.00	1	tpp
1.329	0.00	50	A1	81.79%	40	A1	1.335	0.00	1	tpp
				4.76%	39	A1	1.332	0.00	1	tpp
				3.46%	3	S	1.341	0.00	3	silv
				2.08%	2	P:z	0.033	0.00	3	silv
				2.07%	41	A1	1.775	0.00	1	tpp
				1.22%	2	P:z	-0.679	0.00	2	cobalt
				1.03%	3	S	1.392	0.00	2	cobalt
1.379	0.00	40	B1	62.81%	35	B1	1.226	0.00	1	tpp
				25.66%	36	B1	1.449	0.00	1	tpp
				4.09%	2	P:x	0.033	0.00	3	silv
				2.16%	40	B1	2.334	0.00	1	tpp
				1.88%	37	B1	1.874	0.00	1	tpp
				1.31%	42	B1	3.430	0.00	1	tpp
1.527	0.00	41	B1	72.42%	36	B1	1.449	0.00	1	tpp
				17.49%	35	B1	1.226	0.00	1	tpp
				3.25%	2	P:x	0.033	0.00	3	silv
				1.42%	40	B1	2.334	0.00	1	tpp
				1.35%	38	B1	1.949	0.00	1	tpp
				1.23%	37	B1	1.874	0.00	1	tpp
1.573	0.00	51	A1	30.15%	39	A1	1.332	0.00	1	tpp
				29.24%	41	A1	1.775	0.00	1	tpp
				14.53%	2	S	-5.621	2.00	2	cobalt
				8.51%	38	A1	0.938	0.00	1	tpp
				5.75%	42	A1	1.965	0.00	1	tpp
				5.63%	3	S	1.392	0.00	2	cobalt
				3.06%	37	A1	0.837	0.00	1	tpp
				2.67%	3	S	1.341	0.00	3	silv
				-1.32%	2	S	-4.552	1.00	3	silv
				-1.28%	55	A1	5.665	0.00	1	tpp
				1.13%	44	A1	2.706	0.00	1	tpp

				1.06%	27	A1	-6.698	2.00	1 tpp
1.579	0.00	34	A2	98.93%	32	A2	1.514	0.00	1 tpp
				0.28%	33	A2	1.655	0.00	1 tpp
1.676	0.00	41	B2	63.99%	36	B2	1.454	0.00	1 tpp
				8.62%	39	B2	2.104	0.00	1 tpp
				8.36%	2	P:y	0.033	0.00	3 silv
				6.34%	37	B2	1.876	0.00	1 tpp
				5.62%	34	B2	0.936	0.00	1 tpp
				2.14%	35	B2	1.227	0.00	1 tpp
				1.01%	2	P:y	-0.679	0.00	2 cobalt
1.710	0.00	35	A2	98.95%	33	A2	1.655	0.00	1 tpp
				0.30%	35	A2	2.070	0.00	1 tpp
1.905	0.00	52	A1	38.44%	41	A1	1.775	0.00	1 tpp
				34.09%	42	A1	1.965	0.00	1 tpp
				6.98%	3	S	1.341	0.00	3 silv
				5.96%	3	S	1.392	0.00	2 cobalt
				4.64%	2	S	-5.621	2.00	2 cobalt
				4.00%	38	A1	0.938	0.00	1 tpp
				2.02%	40	A1	1.335	0.00	1 tpp
1.923	0.00	42	B1	63.12%	37	B1	1.874	0.00	1 tpp
				33.76%	38	B1	1.949	0.00	1 tpp
				1.41%	40	B1	2.334	0.00	1 tpp
1.954	0.00	42	B2	53.24%	38	B2	1.945	0.00	1 tpp
				39.82%	37	B2	1.876	0.00	1 tpp
				3.42%	39	B2	2.104	0.00	1 tpp
				1.20%	41	B2	2.805	0.00	1 tpp
1.968	0.00	43	B2	47.88%	37	B2	1.876	0.00	1 tpp
				45.30%	38	B2	1.945	0.00	1 tpp
				3.34%	39	B2	2.104	0.00	1 tpp
				1.50%	36	B2	1.454	0.00	1 tpp
1.976	0.00	36	A2	99.51%	34	A2	1.910	0.00	1 tpp
				0.10%	37	A2	2.507	0.00	1 tpp
2.035	0.00	43	B1	60.81%	38	B1	1.949	0.00	1 tpp
				28.18%	37	B1	1.874	0.00	1 tpp
				6.88%	40	B1	2.334	0.00	1 tpp
				1.51%	2	P:x	0.033	0.00	3 silv
2.143	0.00	37	A2	97.83%	35	A2	2.070	0.00	1 tpp
				0.88%	36	A2	2.482	0.00	1 tpp
2.180	0.00	53	A1	87.73%	43	A1	2.062	0.00	1 tpp
				3.19%	2	P:z	0.033	0.00	3 silv
				1.76%	42	A1	1.965	0.00	1 tpp
				1.31%	44	A1	2.706	0.00	1 tpp

(NO)(Ag)CoTPP:

*** SPIN 1 *** (α)

E(eV)	Occ	MO	%	SFO	E(eV)	Occ	Fragment
-21.724	1.00	14 A	99.40%	5 A	-21.866	2.00	1 tpp
	(...)						
-9.567	1.00	90 A	28.70%	77 A	-9.336	2.00	1 tpp

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                      26.69%    81 A       -8.910  2.00 1 tpp
                      11.73%    97 A       -6.649  2.00 1 tpp
                      11.11%   113 A       -4.707  0.00 1 tpp
                       8.30%     1 D:x2-y2 -8.344  1.40 2 cobalt
  (...)
-8.515  1.00   103 A 25.59%    81 A       -8.910  2.00 1 tpp
                      24.31%   113 A       -4.707  0.00 1 tpp
                      17.66%    88 A       -8.576  2.00 1 tpp
                      14.16%     1 D:x2-y2 -8.344  1.40 2 cobalt
      (...)
-7.238  1.00   111 A 73.92%     1 D:z2    -7.552  2.00 3 silv
                       8.68%     1 D:z2    -8.344  1.40 2 cobalt
                       6.63%   105 A       -5.935  2.00 1 tpp
-7.060  1.00   112 A 86.79%    94 A       -7.047  2.00 1 tpp
                       5.80%    95 A       -7.038  2.00 1 tpp
-7.048  1.00   113 A 85.34%    95 A       -7.038  2.00 1 tpp
                       6.74%    94 A       -7.047  2.00 1 tpp
-7.007  1.00   114 A 27.06%     1 D:yz    -7.552  2.00 3 silv
                      26.85%     1 D:xz    -7.552  2.00 3 silv
                      14.71%   107 A       -5.662  2.00 1 tpp
                       5.27%     1 D:yz    -8.344  1.40 2 cobalt
                       5.18%     1 D:xz    -8.344  1.40 2 cobalt
-6.934  1.00   115 A 32.49%     1 D:yz    -7.552  2.00 3 silv
                      31.70%     1 D:xz    -7.552  2.00 3 silv
                      15.35%   110 A       -5.446  2.00 1 tpp
                       4.63%    95 A       -7.038  2.00 1 tpp
-6.797  1.00   116 A 94.78%     1 D:x2-y2 -7.552  2.00 3 silv
-6.782  1.00   117 A 98.51%     1 D:xy    -7.552  2.00 3 silv
-6.557  1.00   118 A 88.15%    96 A       -6.665  2.00 1 tpp
                       6.60%   105 A       -5.935  2.00 1 tpp
-6.530  1.00   119 A 46.50%   100 A       -6.607  2.00 1 tpp
                      10.90%   101 A       -6.606  2.00 1 tpp
                      10.21%    98 A       -6.626  2.00 1 tpp
                       6.91%     1 D:xz    -7.552  2.00 3 silv
                       6.38%     1 D:yz    -7.552  2.00 3 silv
                       5.57%    99 A       -6.610  2.00 1 tpp
-6.521  1.00   120 A 64.53%    98 A       -6.626  2.00 1 tpp
                      17.73%    99 A       -6.610  2.00 1 tpp
                       9.65%   100 A       -6.607  2.00 1 tpp
                       3.85%   101 A       -6.606  2.00 1 tpp
-6.516  1.00   121 A 61.01%    99 A       -6.610  2.00 1 tpp
                      22.41%    98 A       -6.626  2.00 1 tpp
                       8.40%   101 A       -6.606  2.00 1 tpp
-6.515  1.00   122 A 59.54%   101 A       -6.606  2.00 1 tpp
                      16.64%   100 A       -6.607  2.00 1 tpp
                       5.34%    99 A       -6.610  2.00 1 tpp
-6.501  1.00   123 A 55.86%   105 A       -5.935  2.00 1 tpp
                      13.61%     1 D:z2    -7.552  2.00 3 silv
                       7.99%    96 A       -6.665  2.00 1 tpp
                       6.17%   112 A       -4.712  2.00 1 tpp
                       4.70%   101 A       -6.606  2.00 1 tpp
-6.426  1.00   124 A 21.81%   100 A       -6.607  2.00 1 tpp
                      10.46%     1 D:yz    -7.552  2.00 3 silv
                      10.01%   108 A       -5.472  2.00 1 tpp
                       8.95%     1 D:xz    -7.552  2.00 3 silv
                       8.33%   107 A       -5.662  2.00 1 tpp
                       6.74%   109 A       -5.458  2.00 1 tpp
                       6.02%    99 A       -6.610  2.00 1 tpp
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				5.99%	1	D:yz	-8.344	1.40	2	cobalt
				5.98%	104	A	-6.423	2.00	1	tpp
				5.14%	1	D:xz	-8.344	1.40	2	cobalt
-6.370	1.00	125	A	48.74%	103	A	-6.428	2.00	1	tpp
				10.92%	110	A	-5.446	2.00	1	tpp
				9.91%	106	A	-5.678	2.00	1	tpp
				5.86%	1	D:xz	-7.552	2.00	3	silv
				5.80%	1	D:yz	-7.552	2.00	3	silv
				5.22%	101	A	-6.606	2.00	1	tpp
-6.346	1.00	126	A	91.59%	102	A	-6.446	2.00	1	tpp
-6.333	1.00	127	A	89.13%	104	A	-6.423	2.00	1	tpp
-6.316	1.00	128	A	45.96%	103	A	-6.428	2.00	1	tpp
				12.98%	110	A	-5.446	2.00	1	tpp
				8.16%	106	A	-5.678	2.00	1	tpp
				5.88%	102	A	-6.446	2.00	1	tpp
-6.039	1.00	129	A	46.11%	109	A	-5.458	2.00	1	tpp
				39.60%	108	A	-5.472	2.00	1	tpp
				7.36%	110	A	-5.446	2.00	1	tpp
-5.458	1.00	130	A	81.55%	1	D:xy	-8.344	1.40	2	cobalt
				7.05%	105	A	-5.935	2.00	1	tpp
-5.300	**1.00**	**131**	**A**	**21.95%**	**1**	**D:z2**	**-8.344**	**1.40**	**2**	**cobalt**
				11.62%	**105**	**A**	**-5.935**	**2.00**	**1**	**tpp**
				10.35%	**2**	**PI:x**	**-4.149**	**0.50**	**4**	**no**
				9.30%	**2**	**PI:y**	**-4.149**	**0.50**	**4**	**no**
				6.96%	**112**	**A**	**-4.712**	**2.00**	**1**	**tpp**
				6.78%	2	S	-4.552	1.00	3	silv
				5.16%	1	D:z2	-7.552	2.00	3	silv
				4.67%	1	D:xz	-8.344	1.40	2	cobalt
				4.04%	1	D:yz	-8.344	1.40	2	cobalt
-5.210	1.00	132	A	23.34%	1	D:yz	-8.344	1.40	2	cobalt
				22.43%	1	D:xz	-8.344	1.40	2	cobalt
				13.28%	108	A	-5.472	2.00	1	tpp
				10.66%	107	A	-5.662	2.00	1	tpp
				6.35%	109	A	-5.458	2.00	1	tpp
				5.72%	111	A	-4.953	2.00	1	tpp
				5.44%	2	PI:y	-4.149	0.50	4	no
-5.117	1.00	133	A	89.87%	111	A	-4.953	2.00	1	tpp
-5.028	1.00	134	A	42.73%	112	A	-4.712	2.00	1	tpp
				10.85%	1	D:yz	-8.344	1.40	2	cobalt
				10.65%	1	D:xz	-8.344	1.40	2	cobalt
				5.40%	105	A	-5.935	2.00	1	tpp
				4.96%	1	D:xy	-8.344	1.40	2	cobalt
-4.664	**1.00**	**135**	**A**	19.60%	1	D:xz	-8.344	1.40	2	cobalt
				19.53%	112	A	-4.712	2.00	1	tpp
				18.35%	1	D:yz	-8.344	1.40	2	cobalt
				11.65%	1	D:z2	-8.344	1.40	2	cobalt
				5.99%	2	PI:x	-4.149	0.50	4	no
-3.778	**1.00**	**136**	**A**	**65.27%**	**2**	**S**	**-4.552**	**1.00**	**3**	**silv**
				9.04%	**2**	**PI:x**	**-4.149**	**0.50**	**4**	**no**
				8.37%	112	A	-4.712	2.00	1	tpp
				7.74%	**2**	**PI:y**	**-4.149**	**0.50**	**4**	**no**
-3.094	0.00	137	A	42.87%	2	PI:y	-4.149	0.50	4	no
				38.47%	2	PI:x	-4.149	0.50	4	no
				8.47%	1	D:yz	-8.344	1.40	2	cobalt
				6.83%	1	D:xz	-8.344	1.40	2	cobalt
-2.978	0.00	138	A	67.12%	114	A	-2.913	0.00	1	tpp
				29.51%	115	A	-2.905	0.00	1	tpp
-2.970	0.00	139	A	67.00%	115	A	-2.905	0.00	1	tpp

				28.99%	114	A	-2.913	0.00	1	tpp
-2.574	0.00	140	A	60.85%	1	D:x2-y2	-8.344	1.40	2	cobalt
				35.90%	113	A	-4.707	0.00	1	tpp
-2.362	**0.00**	**141**	**A**	**30.49%**	**1**	**D:z2**	**-8.344**	**1.40**	**2**	**cobalt**
				18.46%	**2**	**PI:x**	**-4.149**	**0.50**	**4**	**no**
				16.99%	**2**	**PI:y**	**-4.149**	**0.50**	**4**	**no**
				13.38%	**2**	**S**	**-4.552**	**1.00**	**3**	**silv**
				7.10%	2	P:z	0.033	0.00	3	silv
-1.759	0.00	142	A	97.23%	116	A	-1.771	0.00	1	tpp
				2.53%	124	A	-1.417	0.00	1	tpp
-1.463	0.00	143	A	92.77%	117	A	-1.565	0.00	1	tpp
-1.446	0.00	144	A	87.43%	118	A	-1.544	0.00	1	tpp
				9.17%	119	A	-1.542	0.00	1	tpp
-1.441	0.00	145	A	88.16%	119	A	-1.542	0.00	1	tpp
				7.42%	118	A	-1.544	0.00	1	tpp
-1.389	0.00	146	A	51.04%	121	A	-1.488	0.00	1	tpp
				48.66%	120	A	-1.493	0.00	1	tpp
-1.388	0.00	147	A	48.54%	120	A	-1.493	0.00	1	tpp
				47.07%	121	A	-1.488	0.00	1	tpp
-1.357	0.00	148	A	46.31%	122	A	-1.449	0.00	1	tpp
				35.35%	123	A	-1.447	0.00	1	tpp
				17.13%	124	A	-1.417	0.00	1	tpp
-1.354	0.00	149	A	47.95%	122	A	-1.449	0.00	1	tpp
				34.75%	124	A	-1.417	0.00	1	tpp
				13.83%	123	A	-1.447	0.00	1	tpp
-1.350	0.00	150	A	48.02%	123	A	-1.447	0.00	1	tpp
				44.92%	124	A	-1.417	0.00	1	tpp
-0.079	0.00	151	A	95.53%	129	A	0.507	0.00	1	tpp
-0.059	0.00	152	A	32.08%	2	P:y	0.033	0.00	3	silv
				32.06%	127	A	0.226	0.00	1	tpp
				7.37%	134	A	0.979	0.00	1	tpp
				7.18%	2	P:x	0.033	0.00	3	silv
0.087	0.00	153	A	44.62%	126	A	0.224	0.00	1	tpp
				27.59%	2	P:x	0.033	0.00	3	silv
				6.35%	2	P:y	0.033	0.00	3	silv
(...)										
2.283	0.00	185	A	88.06%	157	A	2.281	0.00	1	tpp
				4.98%	154	A	2.147	0.00	1	tpp
				2.42%	155	A	2.148	0.00	1	tpp
				1.21%	4	SIGMA	4.304	0.00	4	no

*** SPIN 2 *** (β)

E(eV)	Occ	MO		%	SFO		E(eV)	Occ	Fragment	
-21.723	1.00	14	A	99.44%	5	A	-21.866	2.00	1	tpp
				0.41%	6	A	-21.751	2.00	1	tpp
(...)										
-9.573	1.00	90	A	26.58%	77	A	-9.336	2.00	1	tpp
				25.26%	81	A	-8.910	2.00	1	tpp
				13.93%	97	A	-6.649	2.00	1	tpp
				10.80%	113	A	-4.707	0.00	1	tpp

```
                      8.37%     1 D:x2-y2 -8.344  1.40 2 cobalt
                      3.20%    51 A      -12.034  2.00 1 tpp
                      1.71%     1 D:z2    -8.344  1.40 2 cobalt
                      1.50%    45 A      -12.539  2.00 1 tpp
                      1.26%    80 A       -9.180  2.00 1 tpp
      (...)
-8.538  1.00   100 A 45.04%    89 A       -8.548  2.00 1 tpp
                     13.09%    81 A       -8.910  2.00 1 tpp
                     11.70%   113 A       -4.707  0.00 1 tpp
                      7.02%     1 D:x2-y2 -8.344  1.40 2 cobalt
                      6.34%    90 A       -8.547  2.00 1 tpp
                      4.11%    87 A       -8.579  2.00 1 tpp
                      2.49%    88 A       -8.576  2.00 1 tpp
                      1.32%   107 A       -5.662  2.00 1 tpp
                      1.19%    51 A      -12.034  2.00 1 tpp
                      1.16%    73 A       -9.611  2.00 1 tpp
                      1.05%    77 A       -9.336  2.00 1 tpp
      (...)
-8.525  1.00   103 A 22.53%    85 A       -8.678  2.00 1 tpp
                     16.32%    89 A       -8.548  2.00 1 tpp
                     13.49%    91 A       -8.501  2.00 1 tpp
                     11.36%    81 A       -8.910  2.00 1 tpp
                     10.36%   113 A       -4.707  0.00 1 tpp
                      7.46%    90 A       -8.547  2.00 1 tpp
                      6.32%     1 D:x2-y2 -8.344  1.40 2 cobalt
                      5.33%    88 A       -8.576  2.00 1 tpp
      (...)
-7.147  1.00   111 A 67.62%     1 D:z2    -7.552  2.00 3 silv
                     10.26%     1 D:z2    -8.344  1.40 2 cobalt
                      9.26%   105 A       -5.935  2.00 1 tpp
                      4.04%     2 P:z     -0.679  0.00 2 cobalt
-7.054  1.00   112 A 92.18%    94 A       -7.047  2.00 1 tpp
                      5.38%    95 A       -7.038  2.00 1 tpp
-7.039  1.00   113 A 90.64%    95 A       -7.038  2.00 1 tpp
                      5.33%    94 A       -7.047  2.00 1 tpp
-6.934  1.00   114 A 22.26%     1 D:xz    -7.552  2.00 3 silv
                     22.02%     1 D:yz    -7.552  2.00 3 silv
                     17.70%   107 A       -5.662  2.00 1 tpp
                      8.07%     1 D:yz    -8.344  1.40 2 cobalt
                      8.02%     1 D:xz    -8.344  1.40 2 cobalt
-6.835  1.00   115 A 28.55%     1 D:xz    -7.552  2.00 3 silv
                     27.58%     1 D:yz    -7.552  2.00 3 silv
                     19.83%   110 A       -5.446  2.00 1 tpp
-6.647  1.00   116 A 89.01%     1 D:x2-y2 -7.552  2.00 3 silv
-6.623  1.00   117 A 97.46%     1 D:xy    -7.552  2.00 3 silv
-6.554  1.00   118 A 93.12%    96 A       -6.665  2.00 1 tpp
-6.522  1.00   119 A 87.37%    98 A       -6.626  2.00 1 tpp
                      7.79%    99 A       -6.610  2.00 1 tpp
-6.513  1.00   120 A 37.77%    99 A       -6.610  2.00 1 tpp
                     34.09%   100 A       -6.607  2.00 1 tpp
                     19.43%   101 A       -6.606  2.00 1 tpp
                      5.01%     1 D:x2-y2 -7.552  2.00 3 silv
-6.506  1.00   121 A 43.45%    99 A       -6.610  2.00 1 tpp
                     26.05%   101 A       -6.606  2.00 1 tpp
                     10.15%    98 A       -6.626  2.00 1 tpp
                      8.91%   100 A       -6.607  2.00 1 tpp
                      6.68%     1 D:xz    -7.552  2.00 3 silv
-6.503  1.00   122 A 46.17%   101 A       -6.606  2.00 1 tpp
```

				40.81%	100	A	-6.607	2.00	1	tpp
				6.93%	1	D:yz	-7.552	2.00	3	silv
-6.451	1.00	123	A	63.08%	105	A	-5.935	2.00	1	tpp
				19.34%	1	D:z2	-7.552	2.00	3	silv
				6.00%	112	A	-4.712	2.00	1	tpp
-6.390	1.00	124	A	19.49%	1	D:yz	-7.552	2.00	3	silv
				17.79%	1	D:xz	-7.552	2.00	3	silv
				10.07%	108	A	-5.472	2.00	1	tpp
				9.54%	104	A	-6.423	2.00	1	tpp
				7.82%	100	A	-6.607	2.00	1	tpp
				6.71%	107	A	-5.662	2.00	1	tpp
				6.07%	109	A	-5.458	2.00	1	tpp
				6.02%	1	D:yz	-8.344	1.40	2	cobalt
				5.50%	1	D:xz	-8.344	1.40	2	cobalt
-6.354	1.00	125	A	75.67%	103	A	-6.428	2.00	1	tpp
				8.86%	102	A	-6.446	2.00	1	tpp
				4.34%	1	D:yz	-7.552	2.00	3	silv
-6.343	1.00	126	A	86.54%	102	A	-6.446	2.00	1	tpp
				5.41%	103	A	-6.428	2.00	1	tpp
-6.332	1.00	127	A	85.54%	104	A	-6.423	2.00	1	tpp
-6.288	1.00	128	A	19.57%	110	A	-5.446	2.00	1	tpp
				15.90%	103	A	-6.428	2.00	1	tpp
				14.70%	106	A	-5.678	2.00	1	tpp
				13.52%	1	D:xz	-7.552	2.00	3	silv
				9.87%	1	D:yz	-7.552	2.00	3	silv
				5.22%	1	D:xz	-8.344	1.40	2	cobalt
-6.019	1.00	129	A	45.75%	109	A	-5.458	2.00	1	tpp
				39.16%	108	A	-5.472	2.00	1	tpp
				7.31%	110	A	-5.446	2.00	1	tpp
				4.28%	1	D:x2-y2	-7.552	2.00	3	silv
-5.532	1.00	130	A	84.90%	1	D:xy	-8.344	1.40	2	cobalt
				6.01%	105	A	-5.935	2.00	1	tpp
-5.247	1.00	131	A	24.45%	1	D:xz	-8.344	1.40	2	cobalt
				22.92%	1	D:yz	-8.344	1.40	2	cobalt
				14.83%	108	A	-5.472	2.00	1	tpp
				11.08%	107	A	-5.662	2.00	1	tpp
				7.07%	109	A	-5.458	2.00	1	tpp
-5.235	**1.00**	**132**	**A**	**22.34%**	**1**	**D:z2**	**-8.344**	**1.40**	**2**	**cobalt**
				13.46%	112	A	-4.712	2.00	1	tpp
				12.51%	105	A	-5.935	2.00	1	tpp
				6.48%	1	D:z2	-7.552	2.00	3	silv
				6.31%	1	D:yz	-8.344	1.40	2	cobalt
				5.97%	**2**	**PI:y**	**-4.149**	**0.50**	**4**	**no**
				5.31%	**2**	**PI:x**	**-4.149**	**0.50**	**4**	**no**
-5.120	1.00	133	A	93.31%	111	A	-4.953	2.00	1	tpp
-4.998	1.00	134	A	36.30%	112	A	-4.712	2.00	1	tpp
				16.37%	1	D:xz	-8.344	1.40	2	cobalt
				15.91%	1	D:yz	-8.344	1.40	2	cobalt
				6.65%	106	A	-5.678	2.00	1	tpp
				5.52%	110	A	-5.446	2.00	1	tpp
-4.620	**1.00**	**135**	**A**	26.14%	112	A	-4.712	2.00	1	tpp
				18.75%	1	D:z2	-8.344	1.40	2	cobalt
				12.95%	1	D:xz	-8.344	1.40	2	cobalt
				12.14%	1	D:yz	-8.344	1.40	2	cobalt
				6.13%	2	PI:x	-4.149	0.50	4	no
				5.29%	2	PI:y	-4.149	0.50	4	no
-3.198	**0.00**	**136**	**A**	**61.32%**	**2**	**S**	**-4.552**	**1.00**	**3**	**silv**
				11.75%	**2**	**PI:x**	**-4.149**	**0.50**	**4**	**no**

				10.29%	**2**	**PI:y**	**-4.149**	**0.50**	**4**	**no**
				5.41%	112	A	-4.712	2.00	1	tpp
-2.984	0.00	137	A	28.66%	115	A	-2.905	0.00	1	tpp
				20.83%	2	PI:y	-4.149	0.50	4	no
				18.83%	2	PI:x	-4.149	0.50	4	no
				17.27%	114	A	-2.913	0.00	1	tpp
				8.38%	1	D:yz	-8.344	1.40	2	cobalt
-2.962	0.00	138	A	67.48%	115	A	-2.905	0.00	1	tpp
				13.42%	114	A	-2.913	0.00	1	tpp
				9.23%	2	PI:y	-4.149	0.50	4	no
				7.68%	2	PI:x	-4.149	0.50	4	no
-2.960	0.00	139	A	65.61%	114	A	-2.913	0.00	1	tpp
				14.32%	2	PI:y	-4.149	0.50	4	no
				13.28%	2	PI:x	-4.149	0.50	4	no
-2.658	0.00	140	A	59.83%	1	D:x2-y2	-8.344	1.40	2	cobalt
				36.80%	113	A	-4.707	0.00	1	tpp
-2.064	**0.00**	**141**	**A**	**22.71%**	**1**	**D:z2**	**-8.344**	**1.40**	**2**	**cobalt**
				21.71%	**2**	**S**	**-4.552**	**1.00**	**3**	**silv**
				21.52%	**2**	**PI:x**	**-4.149**	**0.50**	**4**	**no**
				19.27%	**2**	**PI:y**	**-4.149**	**0.50**	**4**	**no**
-1.754	0.00	142	A	97.38%	116	A	-1.771	0.00	1	tpp
-1.461	0.00	143	A	92.61%	117	A	-1.565	0.00	1	tpp
-1.445	0.00	144	A	85.48%	118	A	-1.544	0.00	1	tpp
				11.60%	119	A	-1.542	0.00	1	tpp
-1.440	0.00	145	A	85.80%	119	A	-1.542	0.00	1	tpp
				9.70%	118	A	-1.544	0.00	1	tpp
-1.388	0.00	146	A	60.58%	121	A	-1.488	0.00	1	tpp
				39.11%	120	A	-1.493	0.00	1	tpp
-1.387	0.00	147	A	58.17%	120	A	-1.493	0.00	1	tpp
				37.49%	121	A	-1.488	0.00	1	tpp
-1.356	0.00	148	A	43.28%	122	A	-1.449	0.00	1	tpp
				39.32%	123	A	-1.447	0.00	1	tpp
				16.32%	124	A	-1.417	0.00	1	tpp
-1.353	0.00	149	A	51.60%	122	A	-1.449	0.00	1	tpp
				29.51%	124	A	-1.417	0.00	1	tpp
				15.41%	123	A	-1.447	0.00	1	tpp
-1.349	0.00	150	A	51.14%	124	A	-1.417	0.00	1	tpp
				42.52%	123	A	-1.447	0.00	1	tpp
-0.065	0.00	151	A	98.35%	129	A	0.507	0.00	1	tpp
0.144	0.00	152	A	71.50%	127	A	0.226	0.00	1	tpp
				10.43%	2	P:y	0.033	0.00	3	silv
				5.37%	126	A	0.224	0.00	1	tpp
(...)										
2.286	0.00	185	A	88.36%	157	A	2.281	0.00	1	tpp

Similar data for the FeTPP system can be obtained from the authors upon request (contact W.H.).

Table S7. Structural *trans* effect exerted by NO on Co–L bond lengths (d(Co–L) in Å) in octahedral (NO)(L)CoTPP complexes.

	d(Co–L)		
L	**(L)CoTPP**	**(NO)(L)CoTPP**	**Δd(Co–L)**
NH_3	2.19	2.32	0.13 (+6%)
NCMe[a]	2.06	*dissociation*	---
Cl^-	2.46	2.53	0.07 (+3%)
NCS^-	2.06	2.18	0.12 (+6%)
Ag[b]	2.48	2.68	0.20 (+8%)

BP86/TZVP level; a: acetonitrile; b: single silver atom.