A Series of Dimeric Cobalt Complexes Bridged by N-Heterocyclic Phosphido Ligands.

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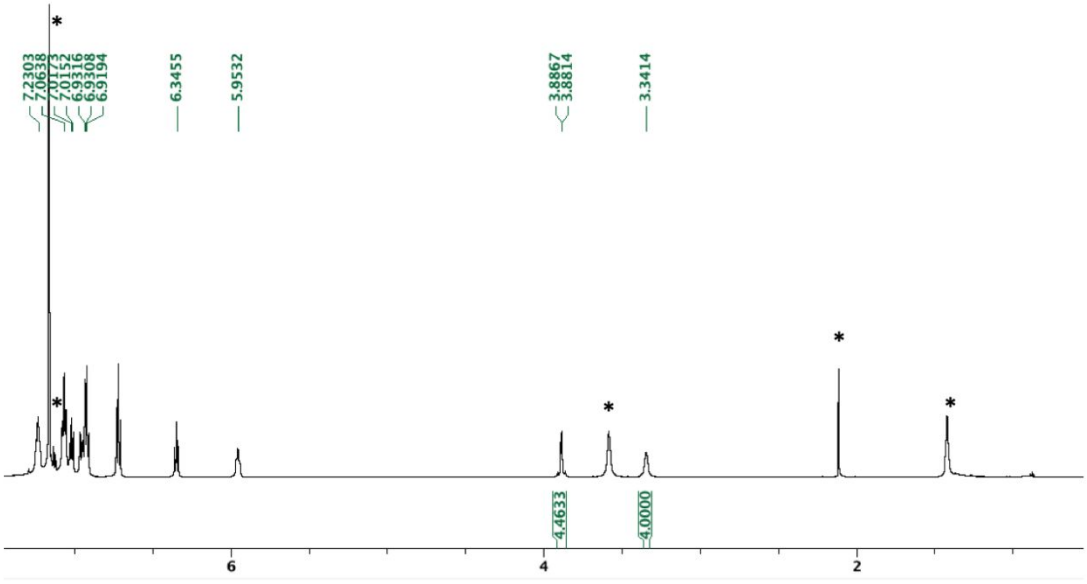


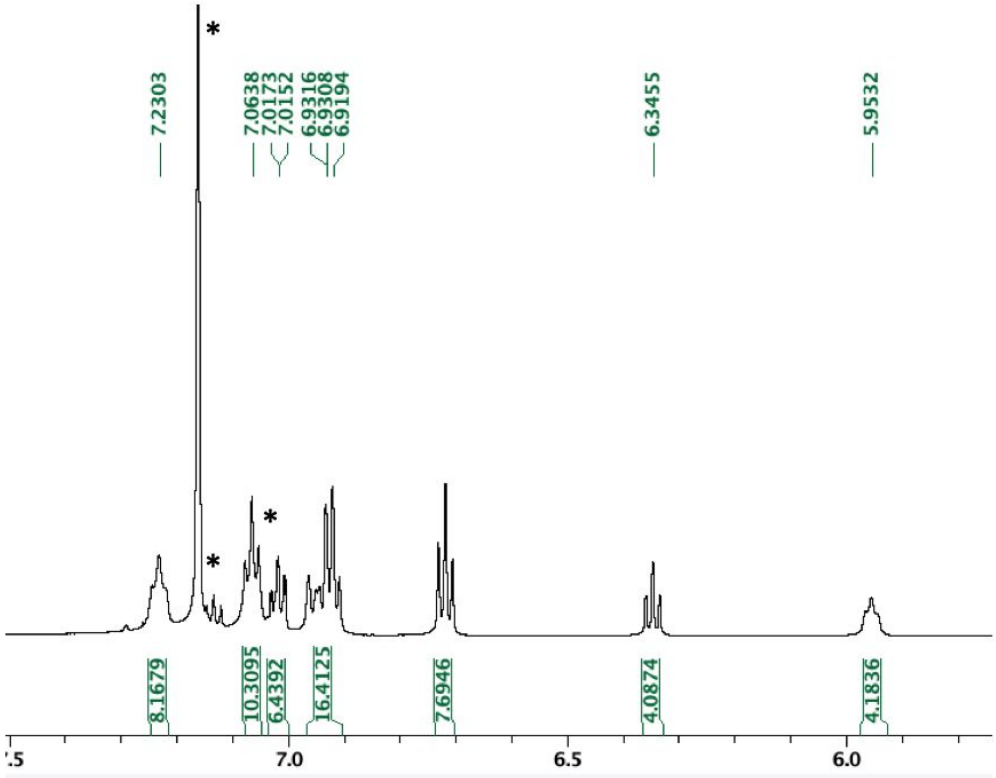


Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum of **2** (242.8 MHz, C_6D_6).

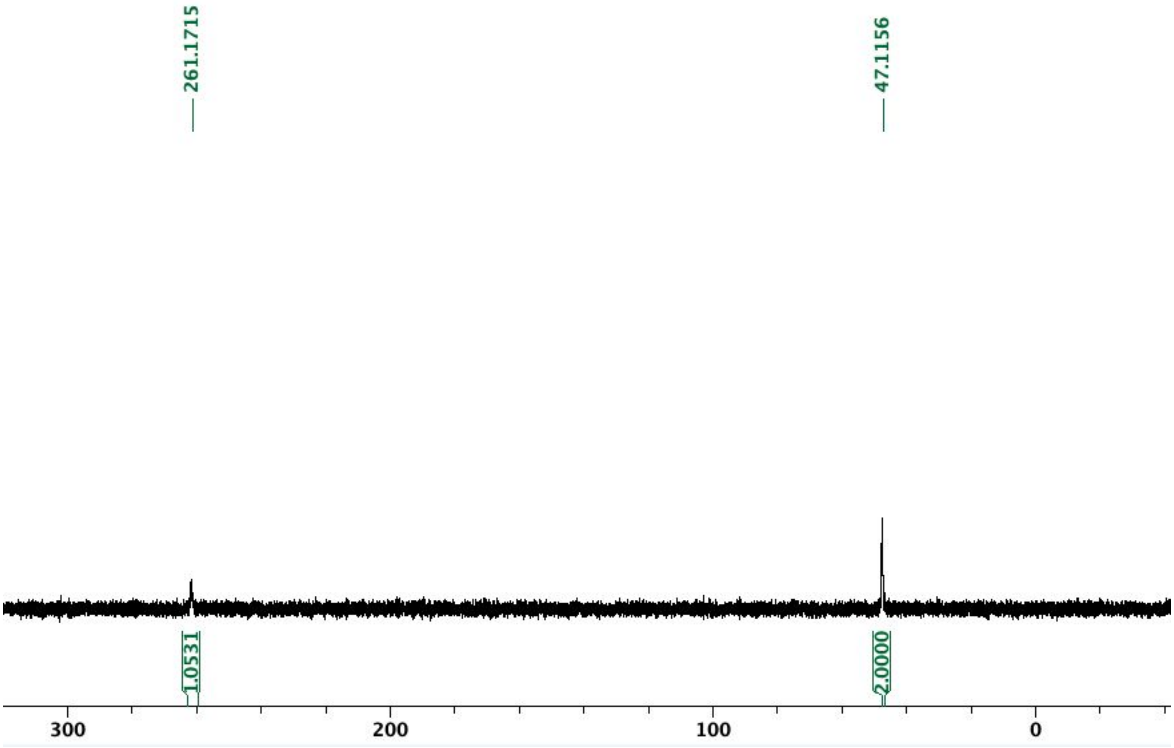


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of **2** (150.8 MHz, C_6D_6). Stars denote residual solvent, in this case C_6D_5H, THF and toluene.

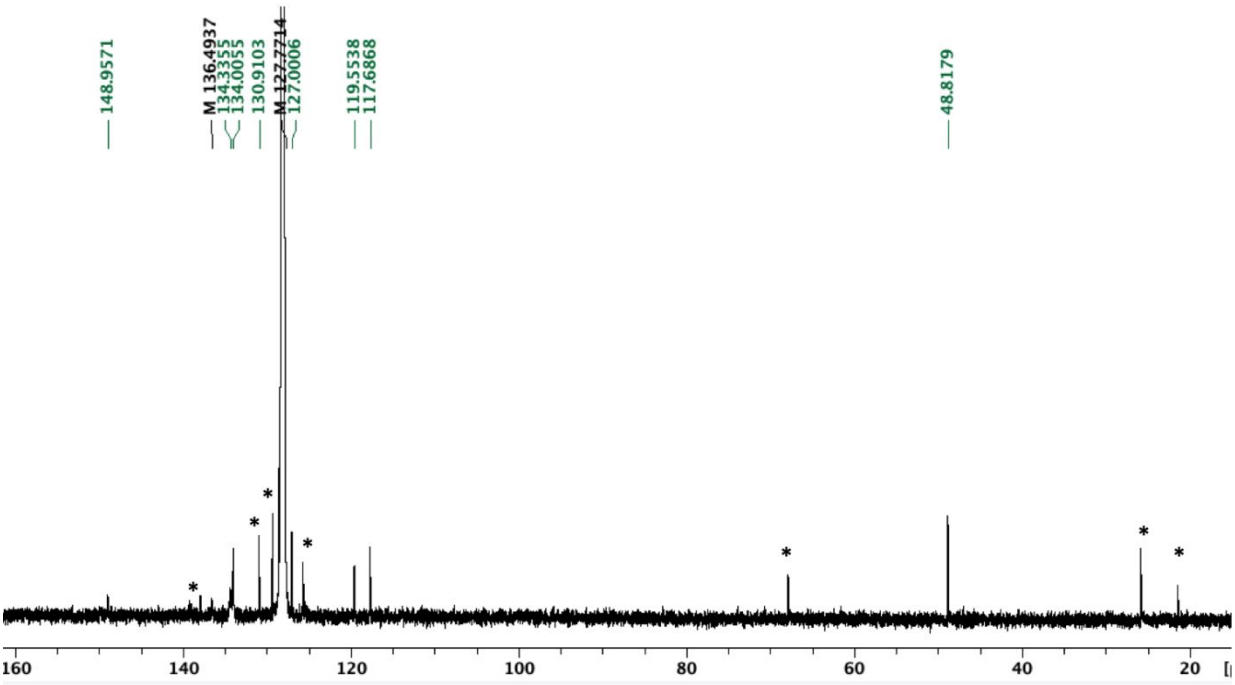


Figure S4. Variable temperature $^{31}P\{^{1}H\}$ NMR spectra of **2** (242.8 MHz, THF-d_8).

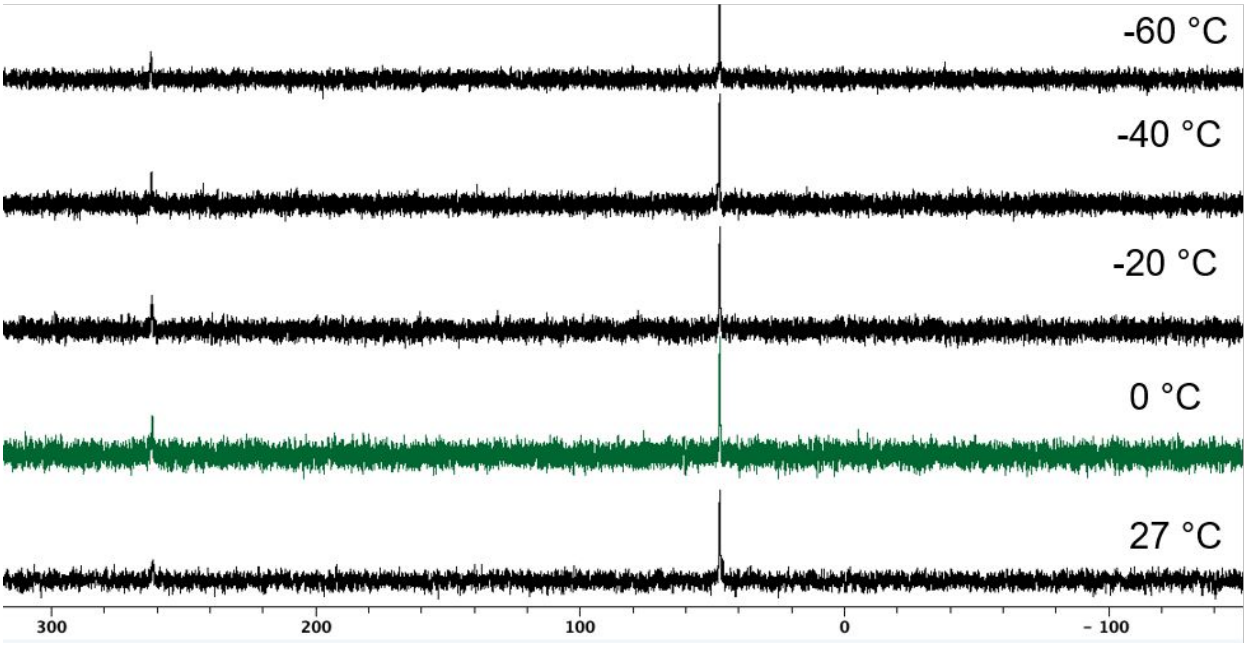


Figure S5. Variable temperature ^{1}H NMR spectra of **2** (600 MHz, THF-d_8), revealing the absence of any significant changes or new paramagnetic peaks appearing at low temperature. Resonances attributed to residual solvents are denoted with a *.

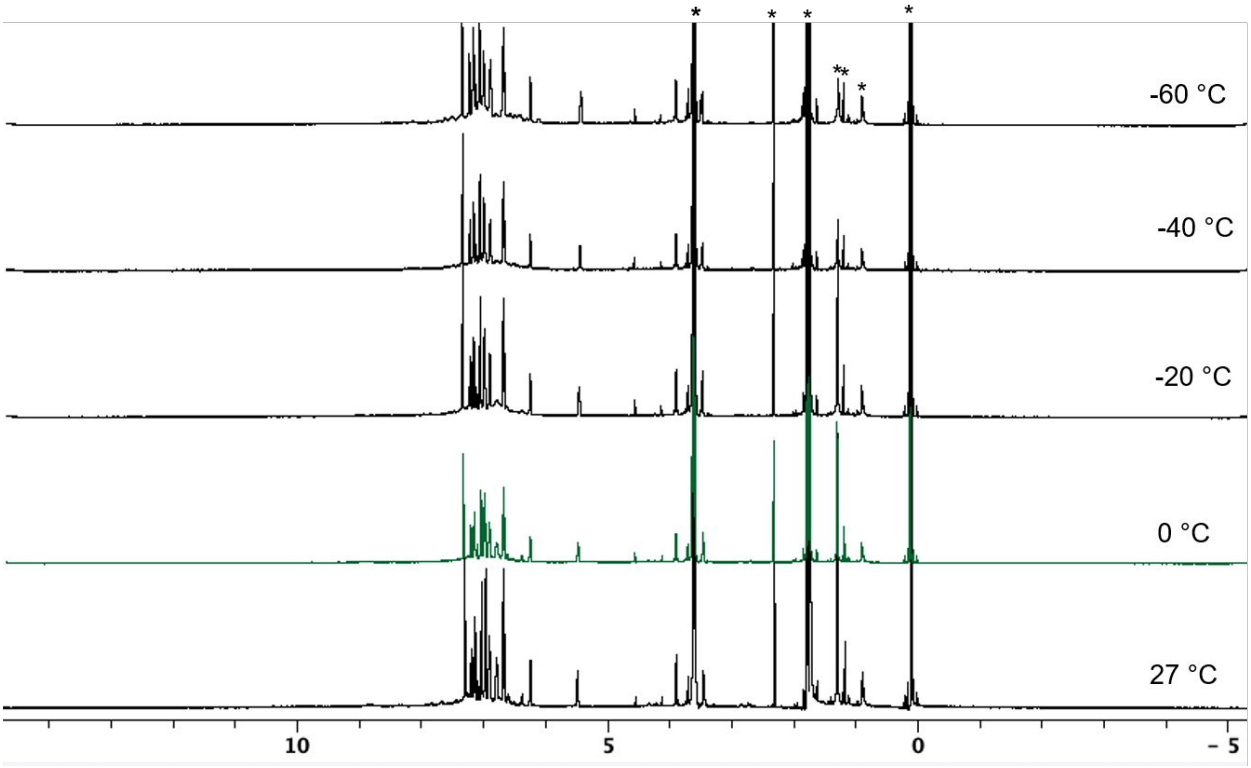


Figure S6. An expanded chemical shift window of the ^{1}H NMR spectrum of **2** (600 MHz, THF-d_8) at -60 °C revealing the absence of any resonances in the paramagnetic region.

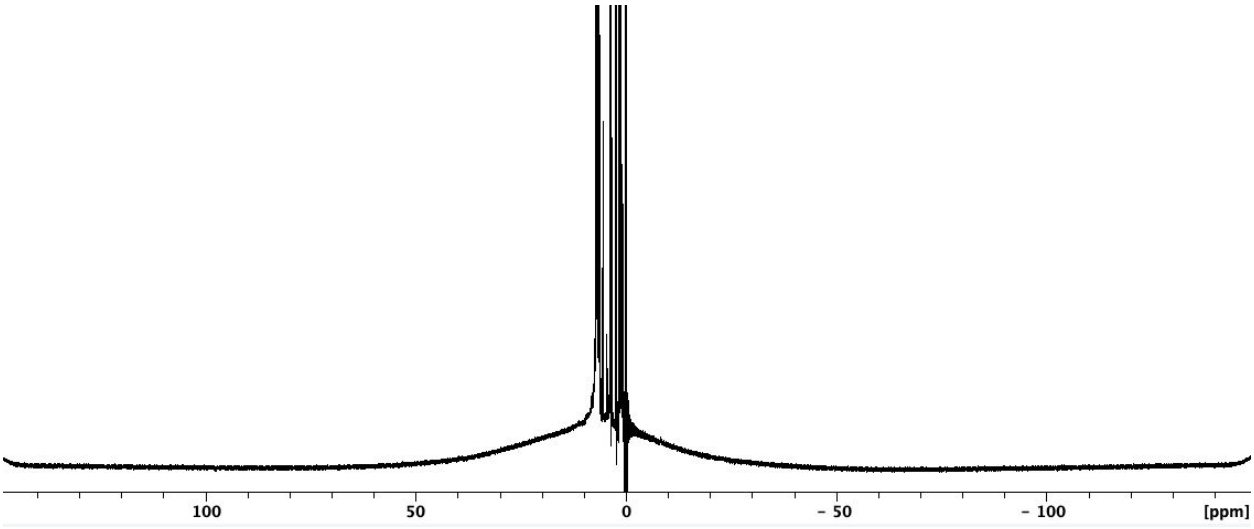


Figure S7. ^{1}H NMR spectrum of **3** (400 MHz, CD_2Cl_2). Stars denote residual solvent, in this case $CDHCl_2$ and THF, Et_2O, and paratone.

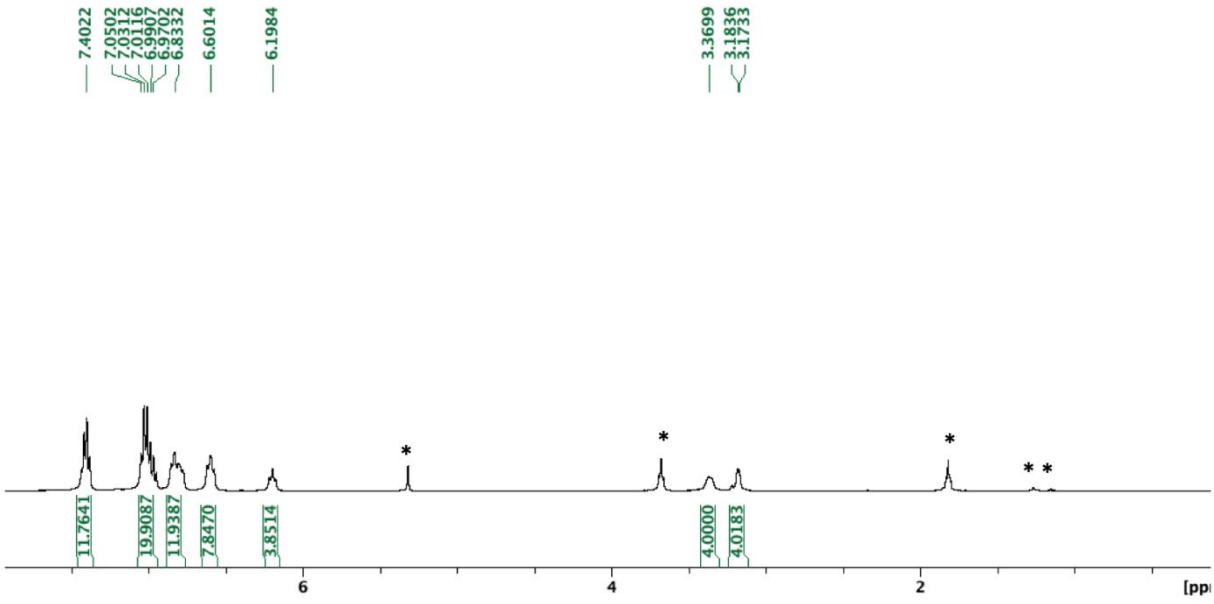


Figure S8. $^{31}P\{^{1}H\}$ NMR spectrum of **3** (242.8 MHz, CD_2Cl_2).

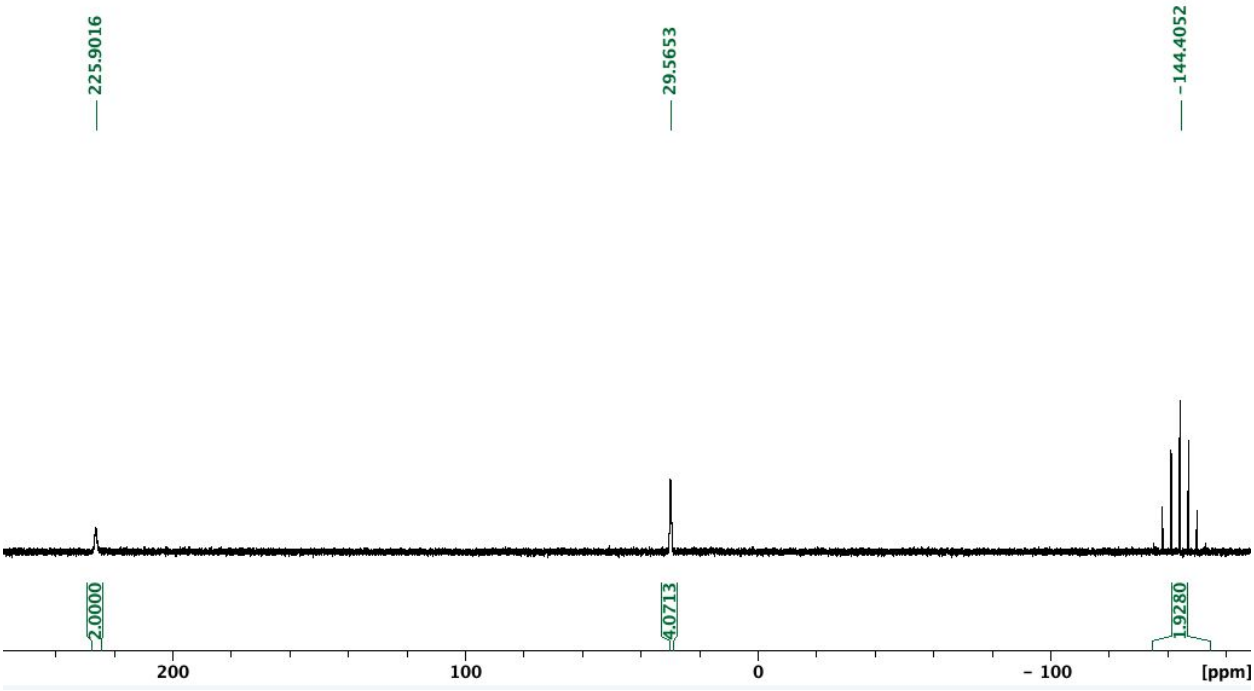
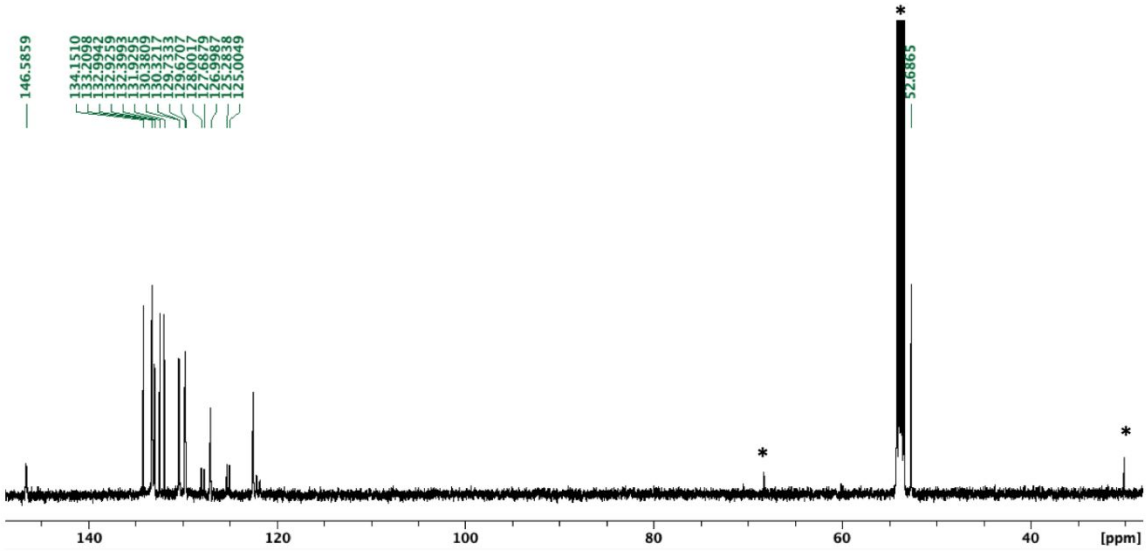


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of **3** (150.8 MHz, CD_2Cl_2). Stars denote residual solvent, in this case $CDHCl_2$ and THF.



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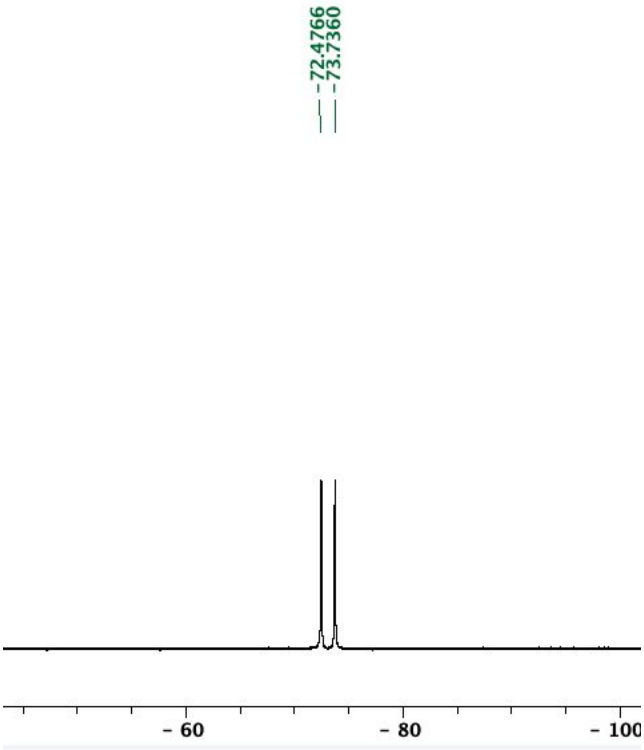


Figure S11. (top) ^{1}H NMR spectrum of **4** (400 MHz, CD_2Cl_2). (bottom) Expansion of the aromatic region of the ^{1}H NMR spectrum of **4**. Stars denote residual solvent, in this case $CDHCl_2$.

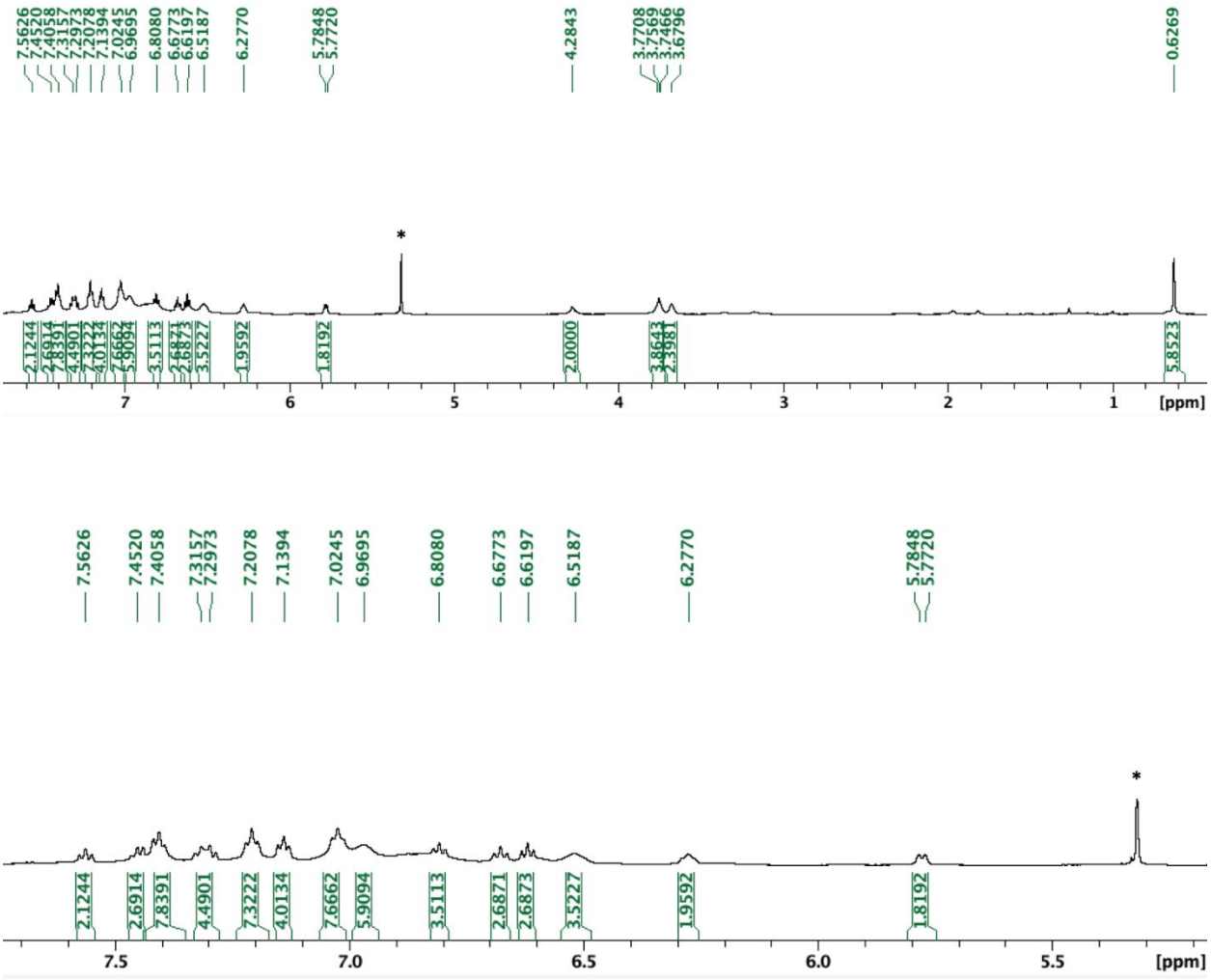


Figure S12. $^{31}P\{^{1}H\}$ NMR spectrum of **4** (161.8 MHz, CD_2Cl_2).

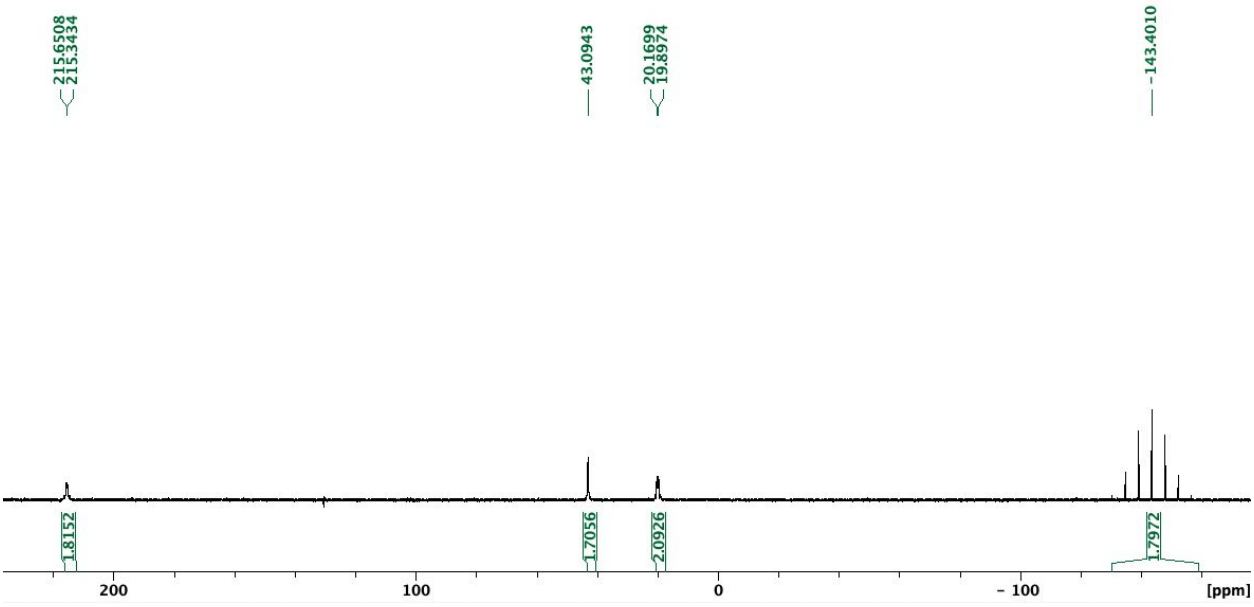


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of **4** (150.8 MHz, C_6D_6). Stars denote residual solvent, in this case $CDHCl_2$.

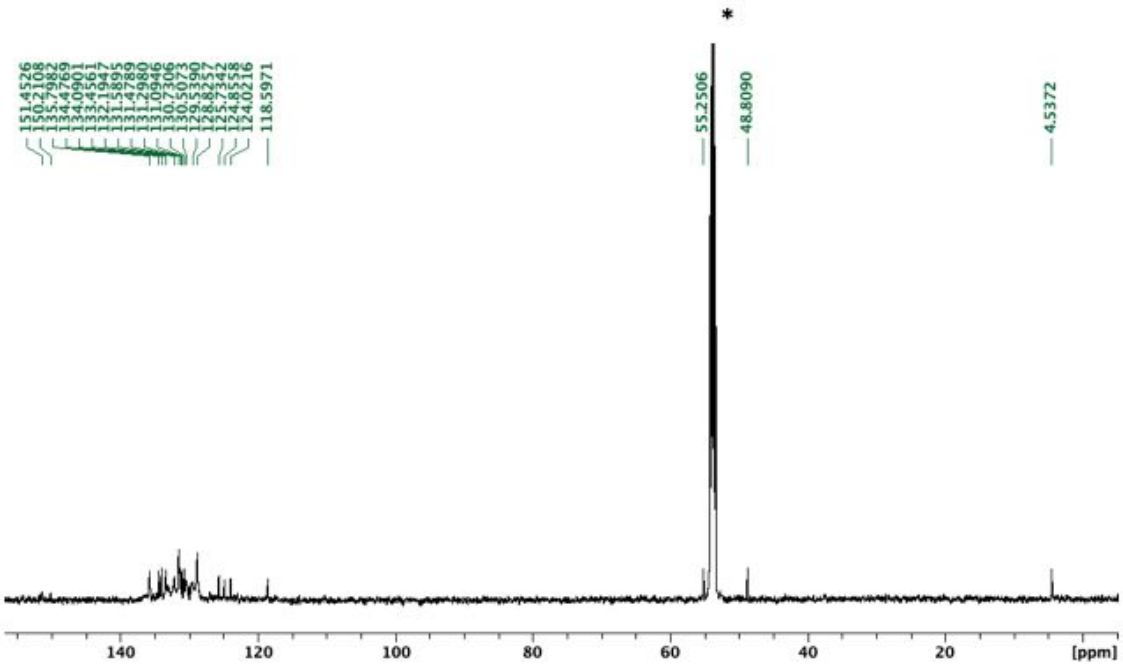


Figure S14. ^{19}F NMR spectrum of **4** (376 MHz, CD_2Cl_2).

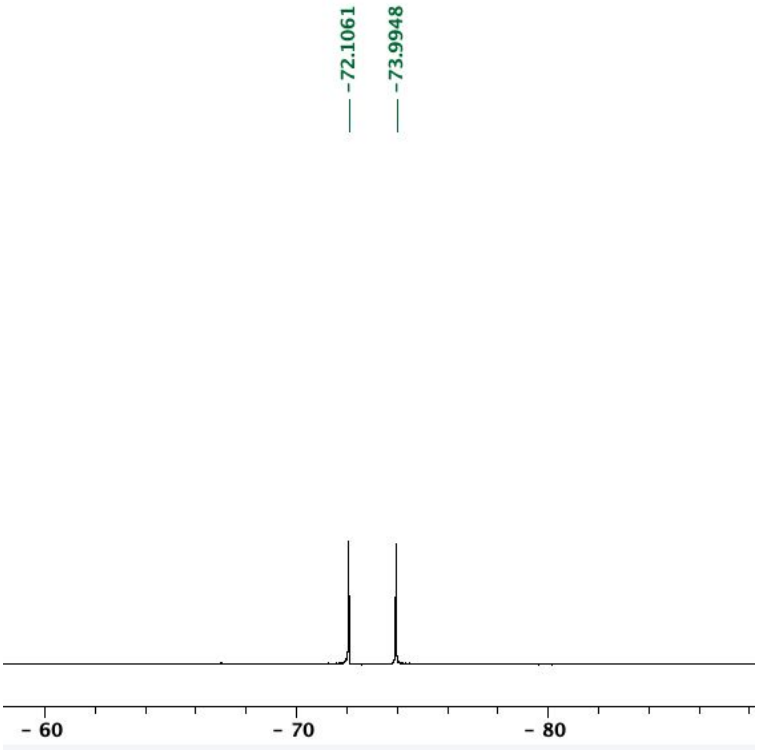


Figure S15. ^{1}H NMR spectrum of $\mathbf{5^{PF6}}$ (400 MHz, CD_2Cl_2). Stars denote residual solvent in this case $CDHCl_2$, THF.

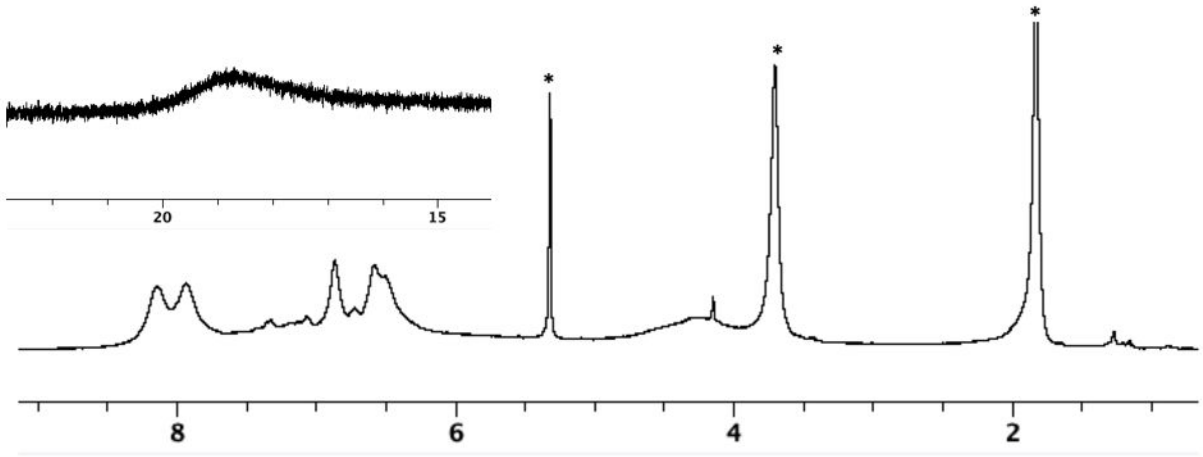


Figure S16. $^{31}P\{^{1}H\}$ NMR spectrum of **5^{PF6}** (161.8 MHz, CD_2Cl_2).

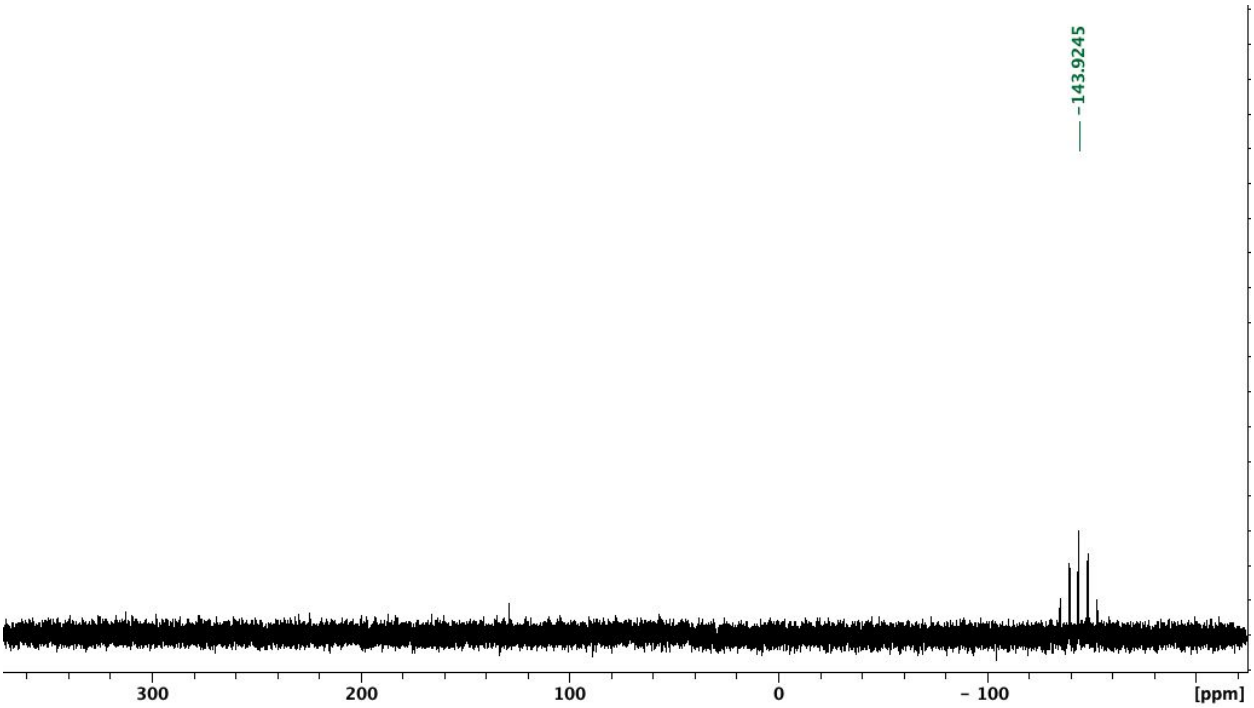


Figure S17. ^{19}F NMR spectrum of **5^{PF6}** (376 MHz, CD_2Cl_2).

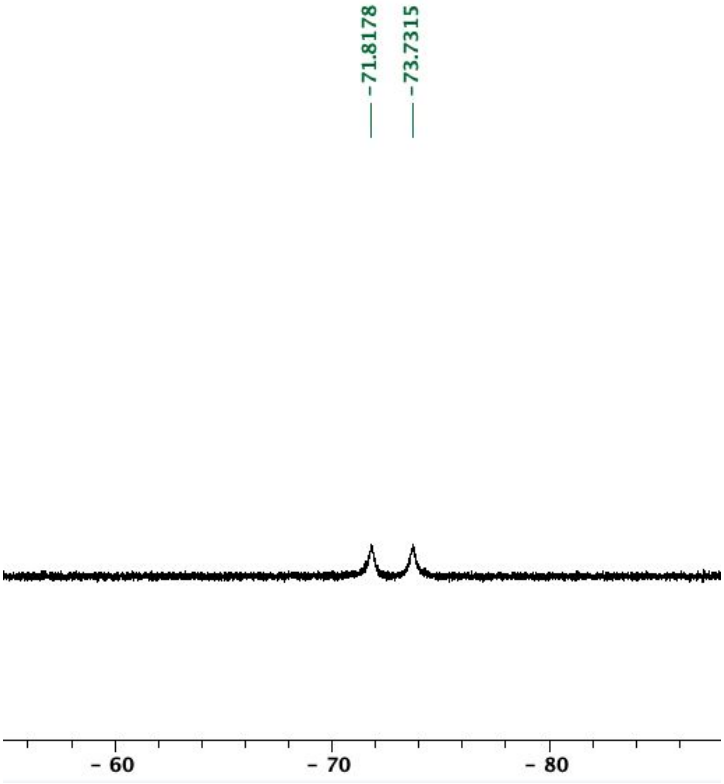


Figure S18. ^{1}H NMR spectrum of **5^{BPh4}** (400 MHz, CD_2Cl_2). Peak at 18.9 shown below. Stars denote residual solvent in this case $CDHCl_2$.

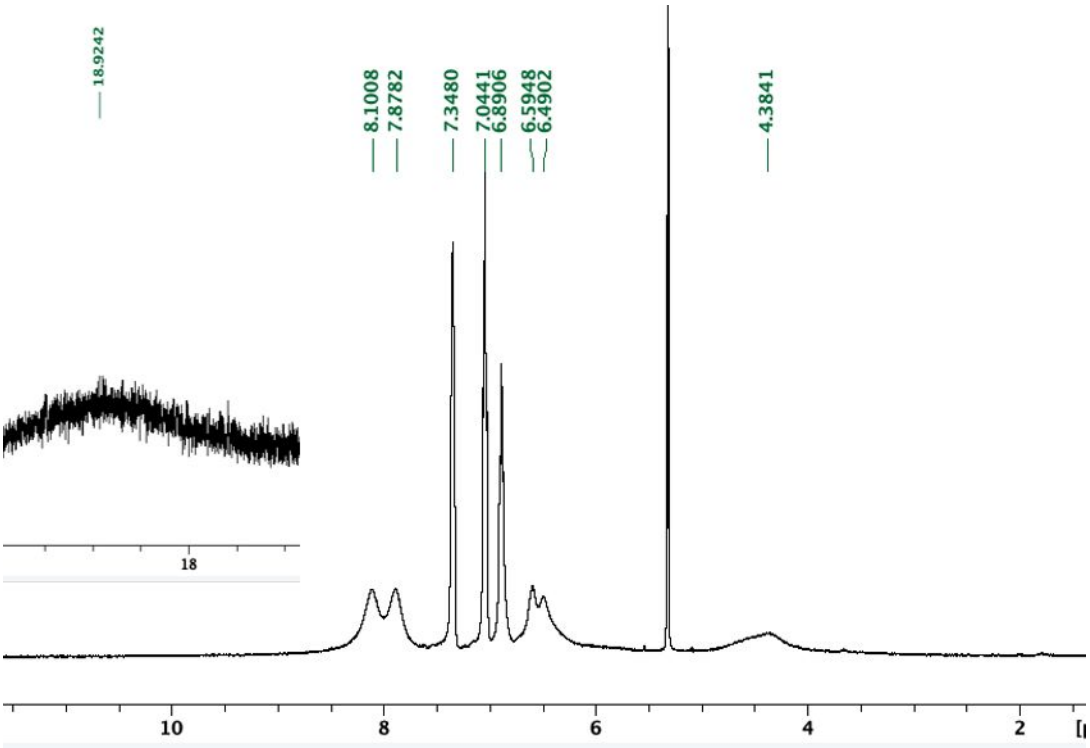


Figure S19. ^{11}B NMR spectrum of **5^{BPh4}** (64.47 MHz, CD_2Cl_2).

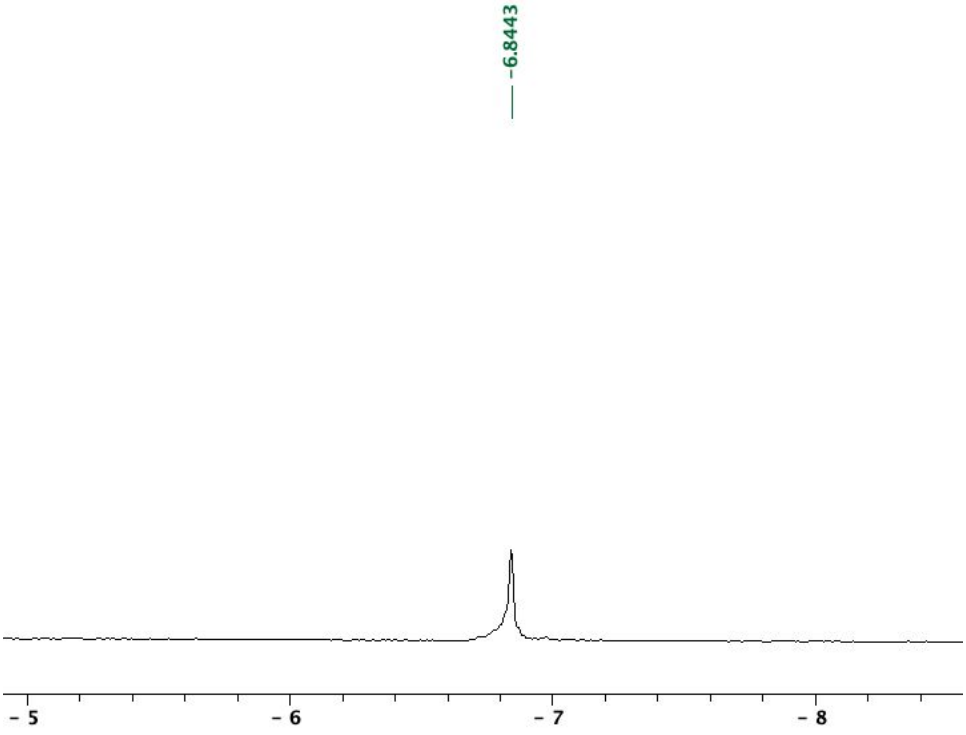


Figure S20. ^{1}H NMR spectrum of $\mathbf{5^{Cl}}$ (400 MHz, CD_2Cl_2).

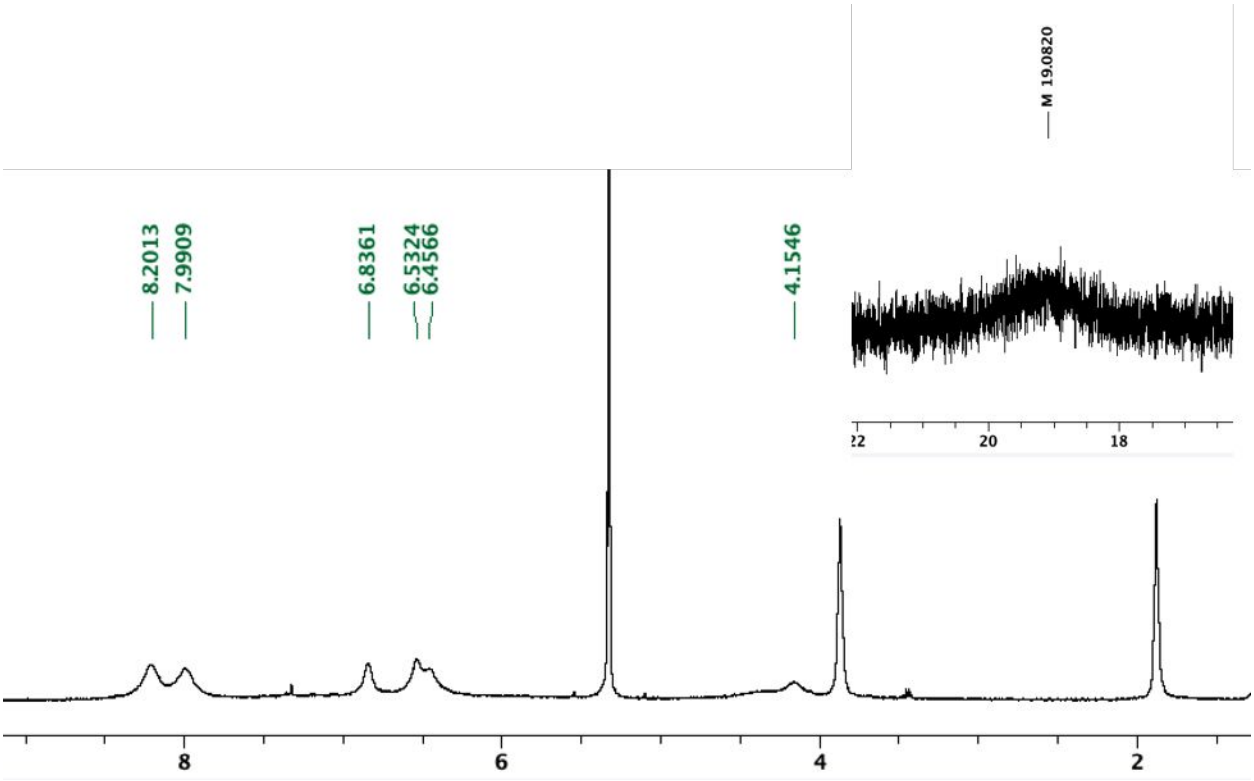


Figure S21. (top) ^{1}H NMR spectrum of **6** (600 MHz, C_6D_6). (bottom) Expansion of the aromatic region of the ^{1}H NMR spectrum of **6**. Stars denote residual solvent, in this case C_6D_5H and THF.

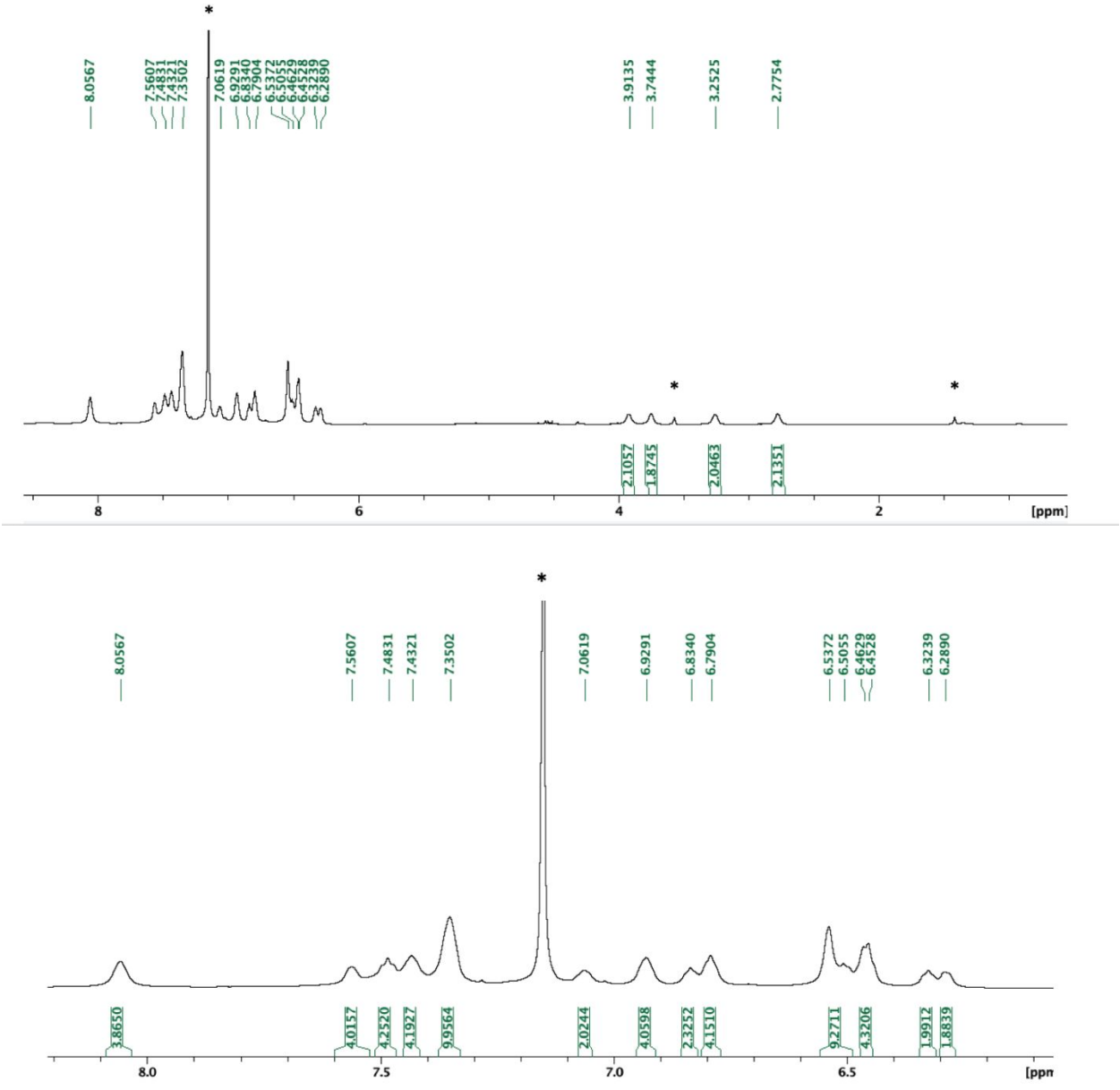


Figure S22. $^{31}P\{^{1}H\}$ NMR spectrum of **6** (242.8 MHz, C_6D_6).

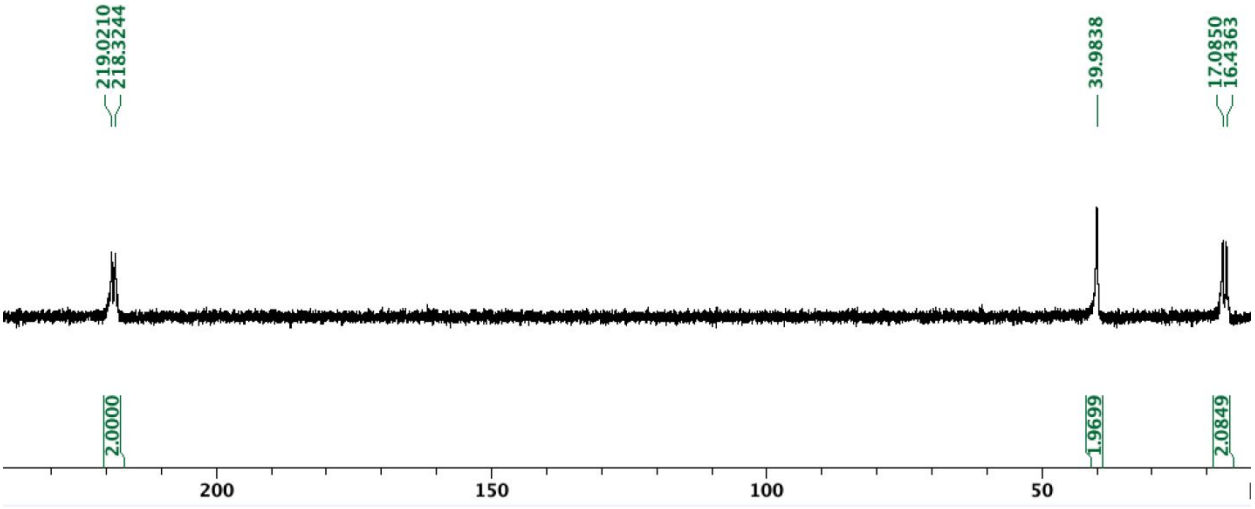


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of **6** (150.8 MHz, C_6D_6). Stars denote residual solvent, in this case C_6D_5H and THF.

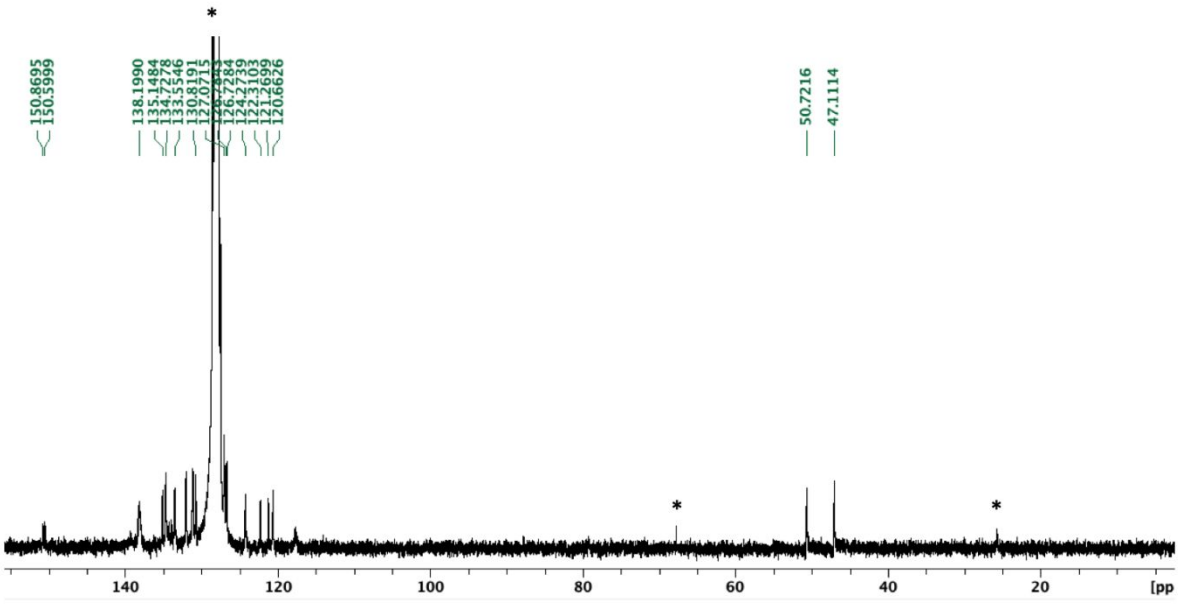
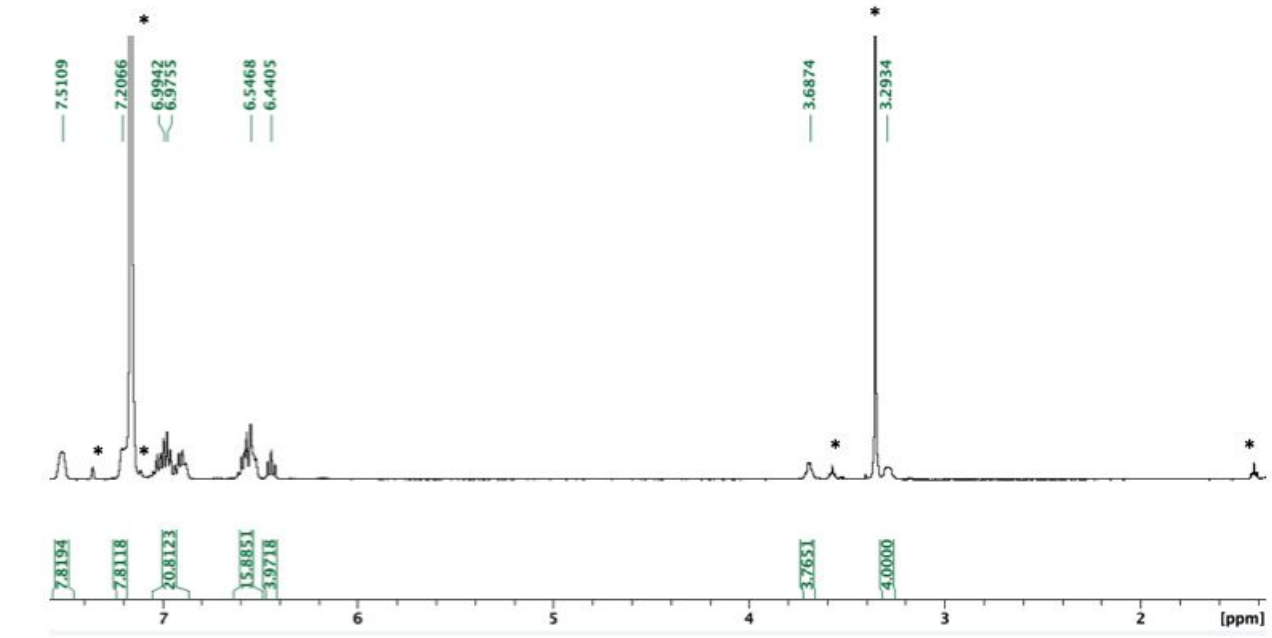


Figure S24. (top) ^{1}H NMR spectrum of **7** (400 MHz, C_6D_6). (bottom) Hydride region of the ^{1}H NMR spectrum of **7**. Stars denote residual solvent, in this case C_6D_5H, THF, and dioxane.



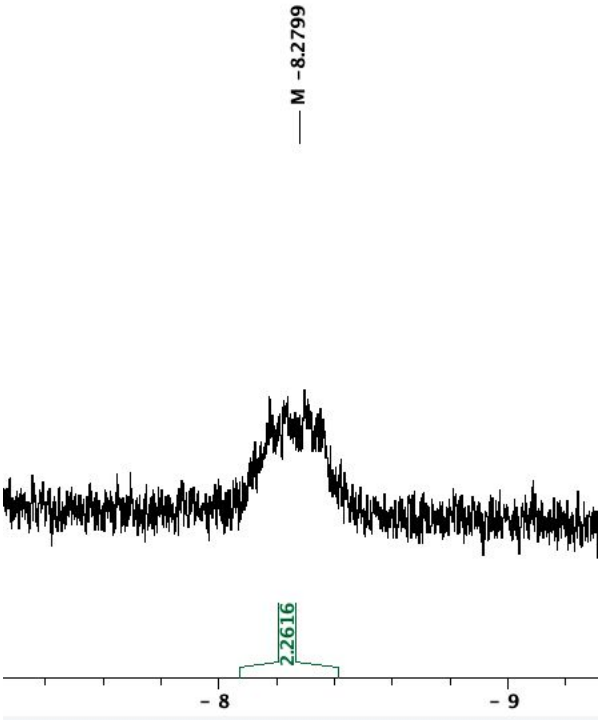


Figure S25. $^{31}P\{^{1}H\}$ NMR spectrum of **7** (161.8 MHz, C_6D_6).

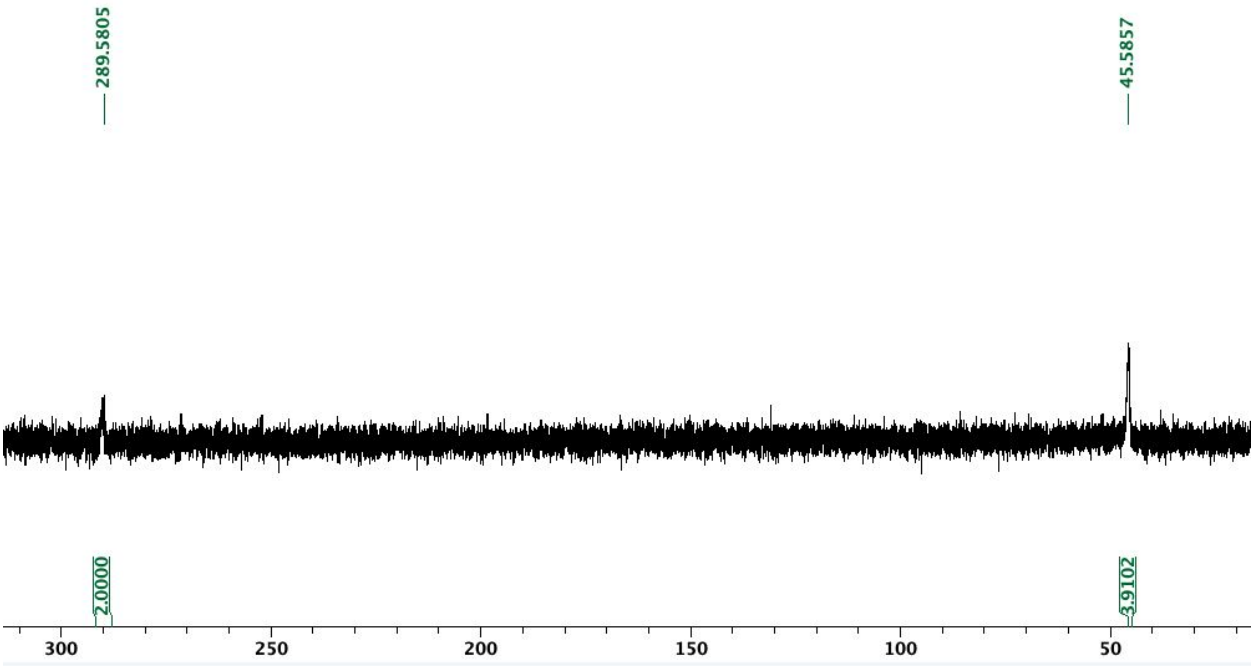


Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of **7** (100.5 MHz, C_6D_6). Stars denote residual solvent, in this case C_6D_5H, THF, and dioxane.

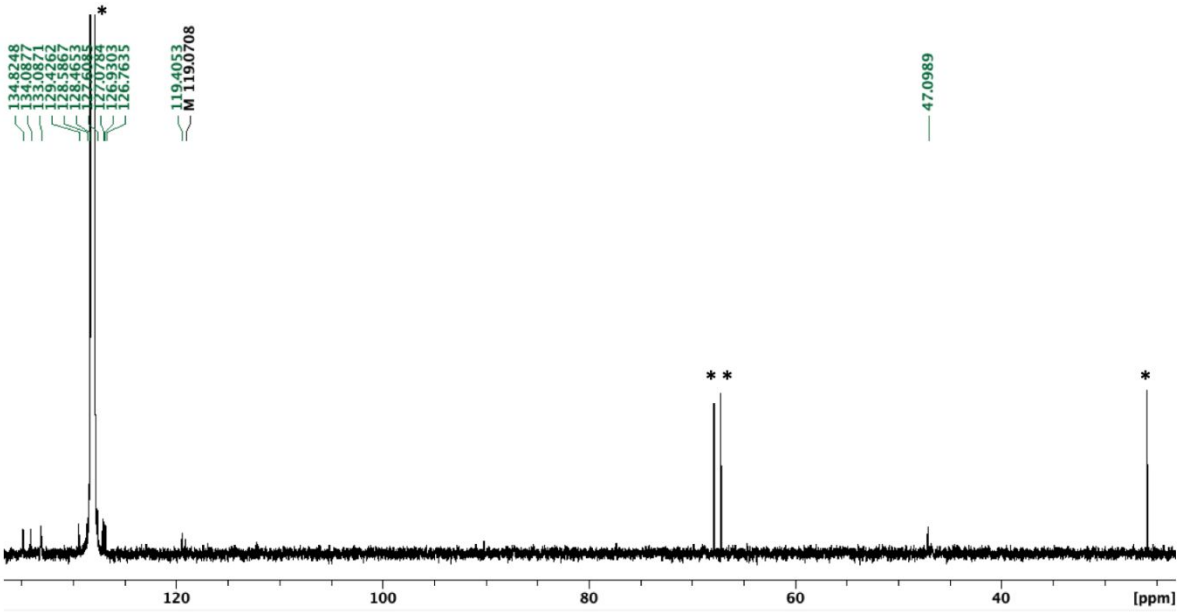


Figure S27. Cyclic Voltammogram of (PPP)CoPMe$_3$ (0.3 M [^{n}Bu$_4$N][PF$_6$] in THF, scan rate = 100 mV/s).

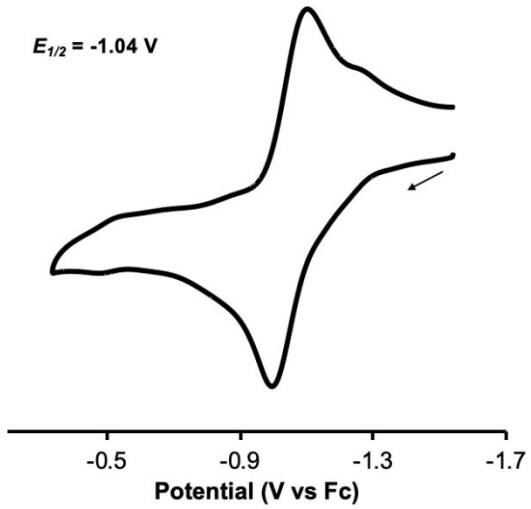


Figure S28. UV-visible absorption spectra of complexes **2**-**5** in THF.

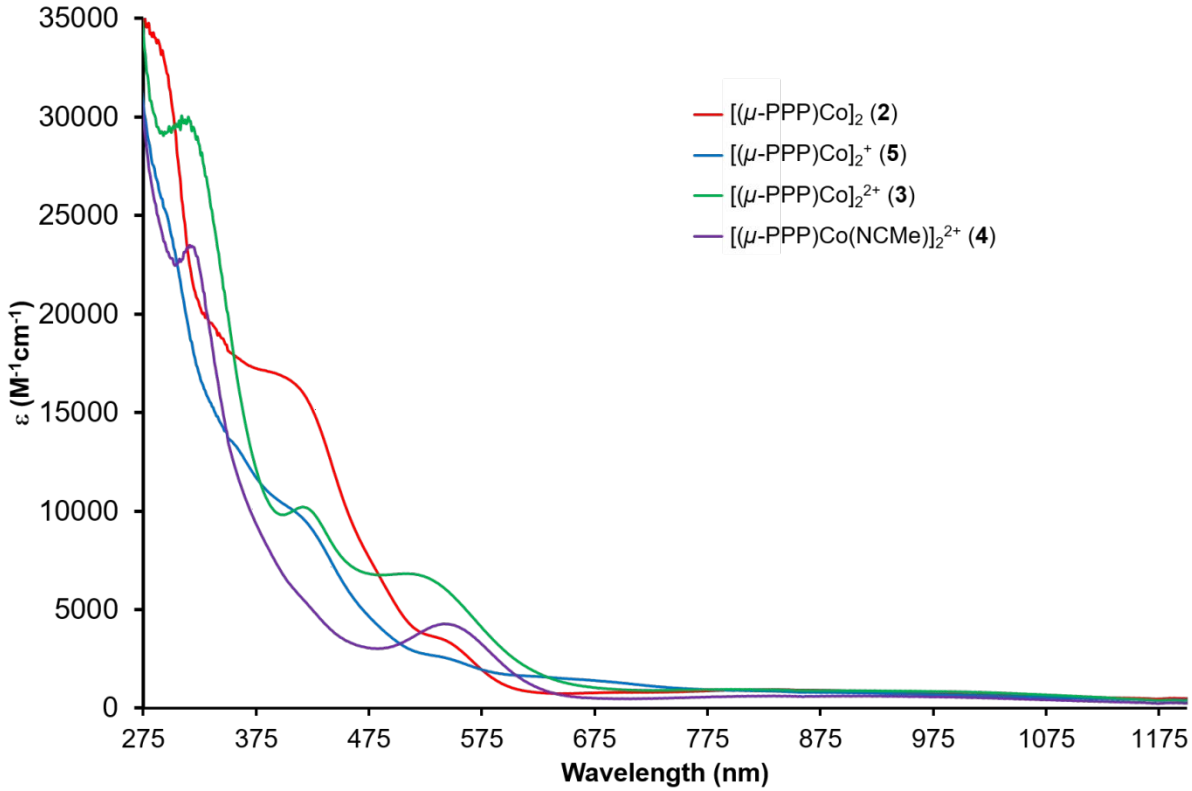


Figure S29. UV-visible absorption spectra of complexes **6**-**7** in THF.

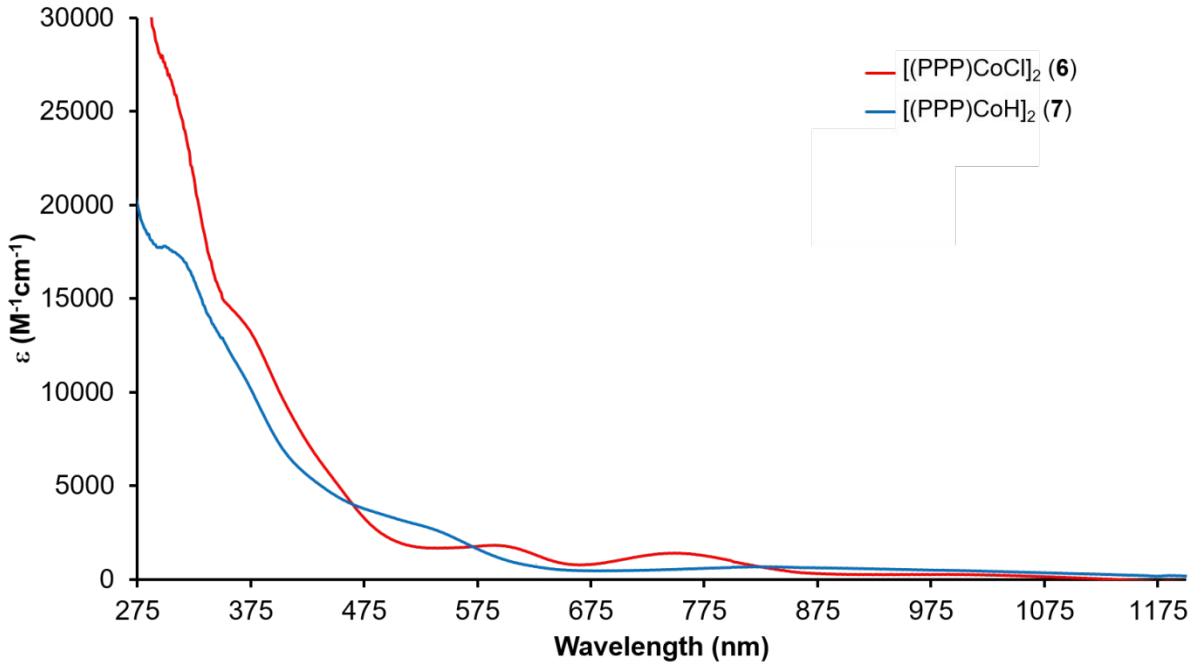


Table S1. X-Ray diffraction experimental details for **2**-**4**.

	2	**3**•CH_2Cl_2	**4**
Molecular formula	$C_{76}H_{64}Co_2N_4P_6$	$[C_{76}H_{64}Co_2N_4P_6]$ $[PF_6]_2 \bullet CH_2Cl_2$	$[C_{80}H_{70}Co_2N_6P_6]$ $[PF_6]_2$
Formula weight	1337.08	1711.85	1709.04
Temperature (K)	120	100	100
Wavelength (Å)	0.71073	0.71073	0.71073
a (Å)	16.846(3)	13.679(4)	13.7596(15)
b (Å)	16.846(3)	16.443(4)	26.248(6)
c (Å)	24.652(5)	17.518(4)	23.919(4)
α (°)	90	84.065(9)	90
β (°)	90	84.605(9)	100.580(7)
γ (°)	90	88.104(10)	90
Volume (Å^3)	6996(3)	3900.9(18)	8492(3)
Space group	$I\bar{4}c2$	*P*-1	P 1 2_1 1
Z	4	2	4
Density (calc) (g/cm^3)	1.269	1.457	1.337
μ (mm$^{-1)}$	0.656	0.732	0.612
R_1 [$I > 2\sigma(I)$], wR_2 (all data)	R_1 = 0.0615, wR_2 = 0.1581	R_1 = 0.0607, wR_2 = 0.1439	R_1 = 0.0659, wR_2 = 0.1660

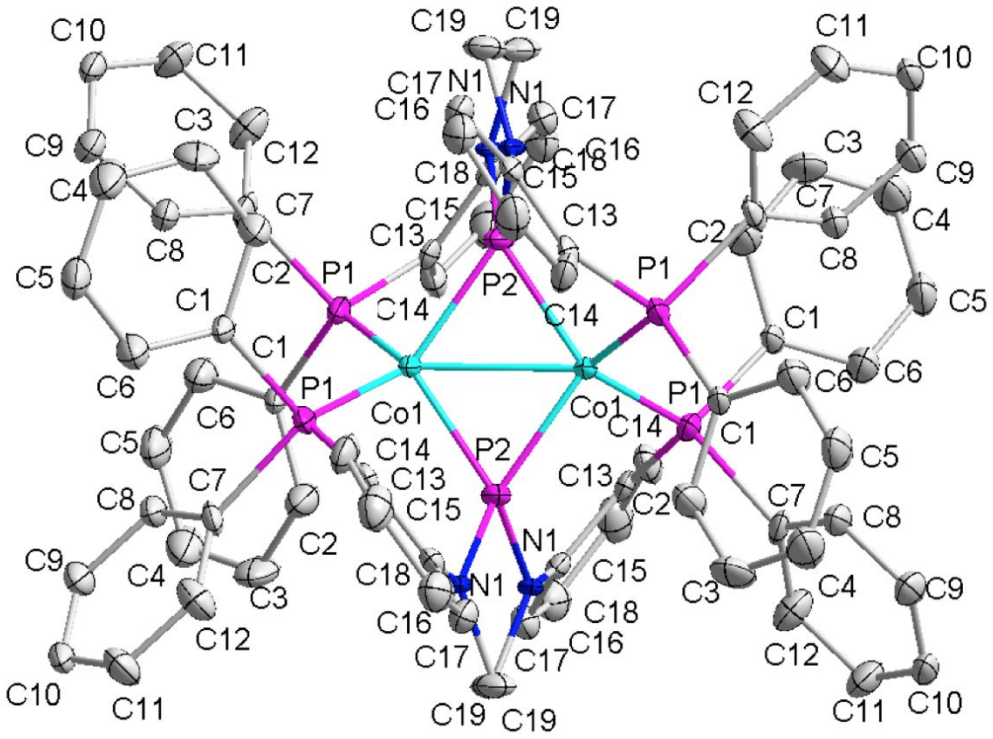
Table S2. X-Ray diffraction experimental details for **5**-**7**.

	$\mathbf{5}^{\mathbf{BPh4}} \bullet CH_2Cl_2$	**6** • 1.5 C_7H_8	**7** • 3 $C_4H_8O_2$
Molecular formula	$[C_{76}H_{64}Co_2N_4P_6]$ $[C_{24}H_{20}B] \bullet CH_2Cl_2$	$C_{86.5}H_{76}Cl_2Co_2N_4P_6$ • 1.5 C_7H_8	$[C_{76}H_{66}Co_2N_4P_6]_{0.5}$ • 1.5 $C_4H_8O_2$
Formula weight	1741.12	1592.26	801.66
Temperature (K)	100	120	150
Wavelength (Å)	0.71073	0.71073	0.71073
a (Å)	19.2394(15)	33.382(4)	11.9477(9)
b (Å)	19.3036(14)	20.153(2)	17.5946(13)
c (Å)	25.3126(17)	25.260(3)	19.6539(14)
α (°)	90	90	75.027(3)
β (°)	102.746(3)	112.473(2)	77.140(3)
γ (°)	90	90	75.016(3)
Volume (Å^3)	9169.2(12)	15703(3)	3801.5(5)
Space group	$P12_1/n1$	$C\,2/c$	P-1
Z	4	8	4
Density (calc) (g/cm^3)	1.261	1.308	1.401
μ (mm$^{-1)}$	0.573	0.660	0.622
R_1 [$I > 2\sigma(I)$], wR_2 (all data)	R_1 = 0.0478, wR_2 = 0.1213	R_1= 0.0506, wR_2= 0.1118	R_1 = 0.0317, wR_2 = 0.0820

X-ray data collection, solution and refinement details for 2.

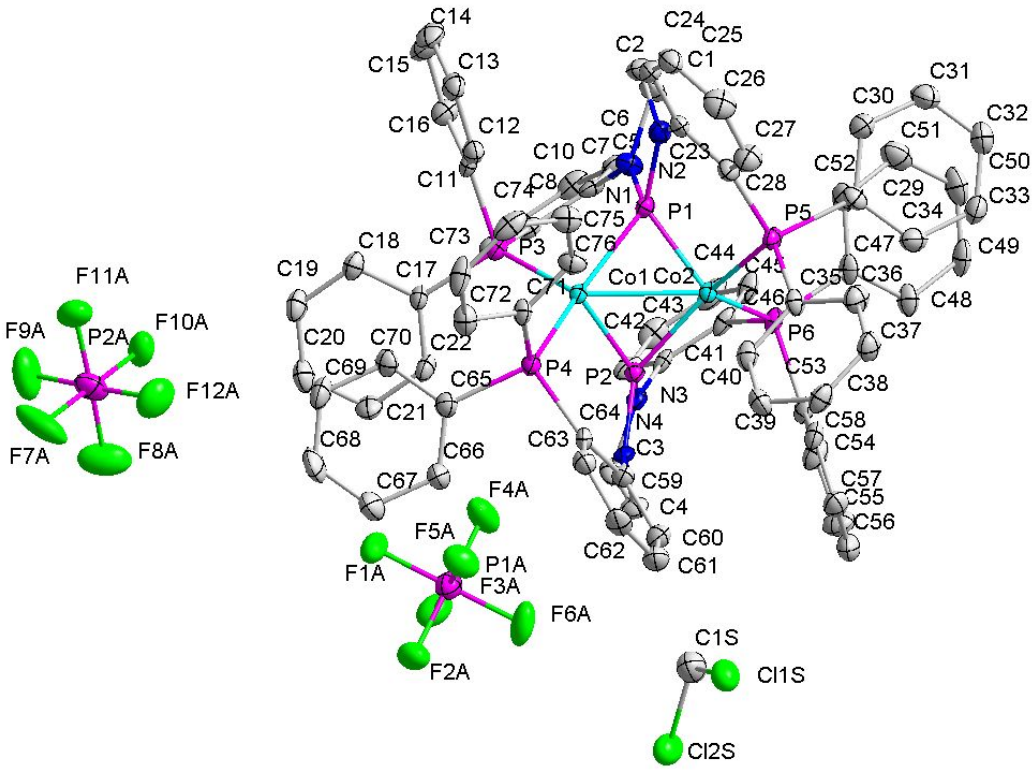
The structure of complex **2** was solved using *Sir-92*[1] and refined using the *Oxford University Crystals for Windows* program.[2-3] During the structure solution, electron density difference maps revealed that there were disordered species that could not be successfully modeled with or without restraints. Thus, the structure factors were modified using the PLATON SQUEEZE technique,[4-6] in order to produce a "solvate-free" structure factor set. PLATON reported a total electron density of 328 e^-, likely corresponding to eight THF molecules. Full X-Ray diffraction experimental details are available in Table S1.

Figure S30. Fully labelled displacement ellipsoid diagram of **2**.



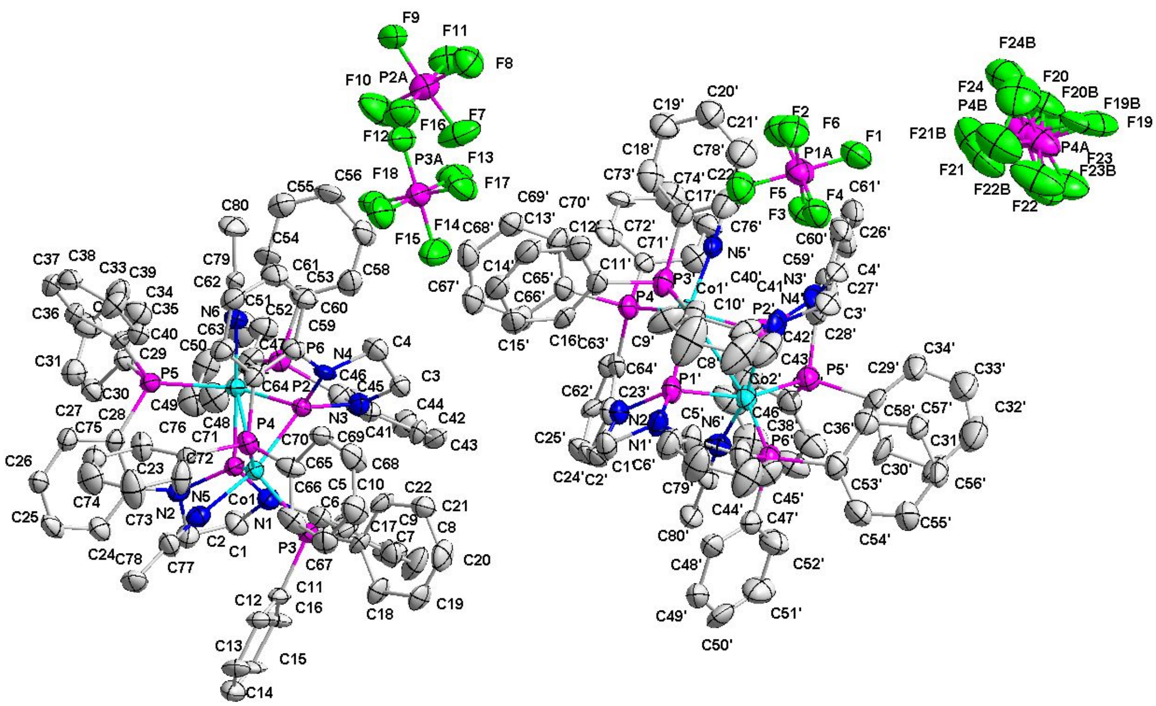
X-ray data collection, solution and refinement details for 3. The structure of complex **3** was solved using the Bruker SHELX Software package[7] within APEX3[8] and OLEX2.[9] During the structure solution, electron density difference maps revealed that there were disordered species that could not be successfully modeled with or without restraints. Due to unmodelable solvent disorder, PLATON SQUEEZE[4-6] was used to remove the electron density from the lattice due to the disordered solvent contribution. The solvent appeared to be dichloromethane. Two voids were found with approximately 59 electrons in each. During the refinement, it became clear that reflections were affected by the shadow of the beamstop, giving rise to a B Level checkcif Alert. Full X-Ray diffraction experimental details are available in Table S1.

Figure S31. Fully labelled displacement ellipsoid diagram of **3**.



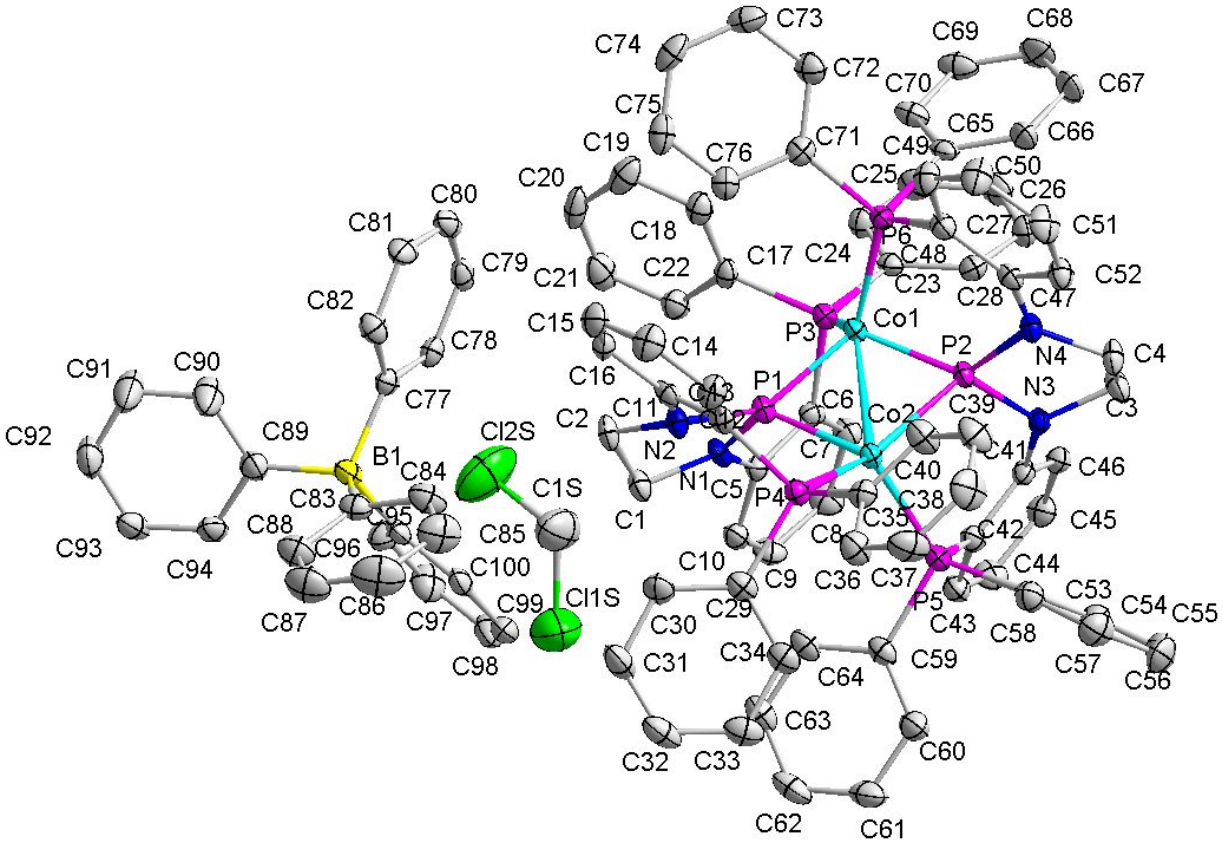
X-ray data collection, solution and refinement details for 4. The structure of complex **4** was solved using Bruker SHELX Software package[7] within APEX3[8] and OLEX2.[9] During the structure solution, electron density difference maps revealed that there were disordered species that could not be successfully modeled with or without restraints. Due to unmodelable solvent disorder, Olex2 SMBTX_Mask was used to remove the electron density from the lattice due to the disordered solvent contributions. The solvent appeared to be THF. Two major voids were found with approximately 184 electrons in each. During the refinement, it became clear that reflections were affected by the shadow of the beamstop, giving rise to the B Level checkcif Alert. Low bond precision on C-C bonds is due to the crystal not diffracting past 0.9 Å in some orientations. Full X-Ray diffraction experimental details are available in Table S1.

Figure S32. Fully labelled displacement ellipsoid diagram of **4**.



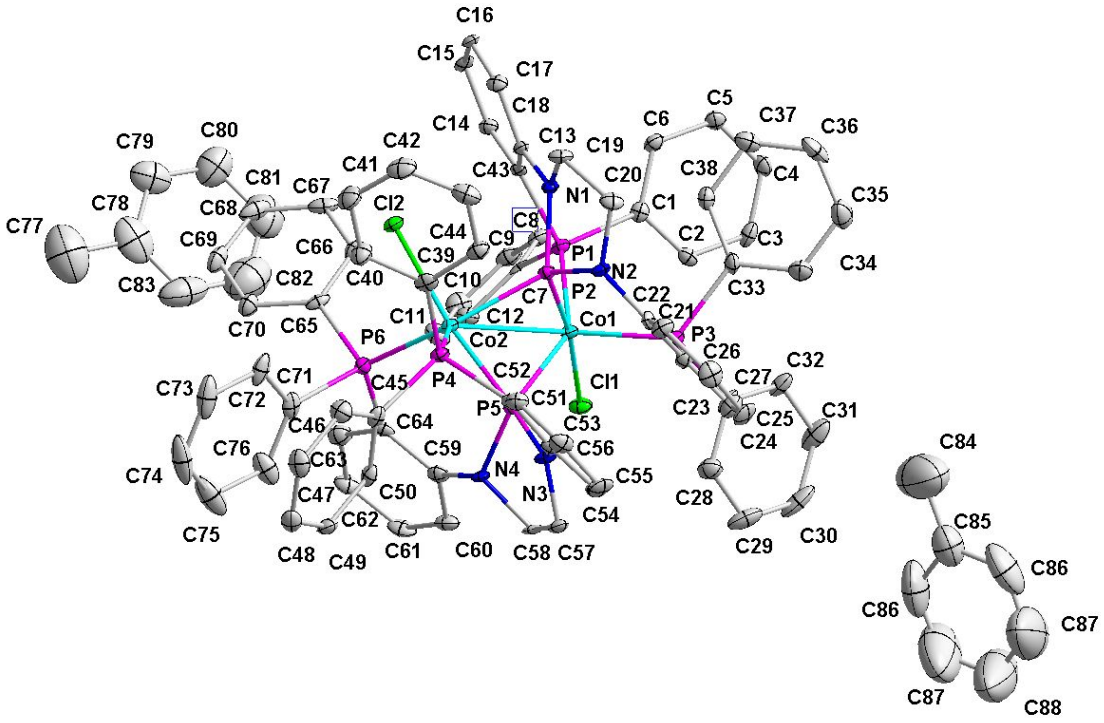
X-ray data collection, solution and refinement details for 5^{BPh4}. The structure of complex **5** was solved using Bruker SHELX Software package[7] within APEX3[8] and OLEX2.[9] During the structure solution, electron density difference maps revealed that there were disordered species that could not be successfully modeled with or without restraints. Due to unmodelable solvent disorder, PLATON SQUEEZE[4-6] was used to remove the electron density from the lattice due to the disordered solvent contribution. The solvent appeared to be dichloromethane. Four voids were found with approximately 66 electrons each. During the refinement, it became clear that reflections were affected by the shadow of the beamstop, giving rise to the B Level checkcif Alert. Full X-Ray diffraction experimental details are available in Table S2.

Figure S33. Fully labelled displacement ellipsoid diagram of 5^{BPh4}.



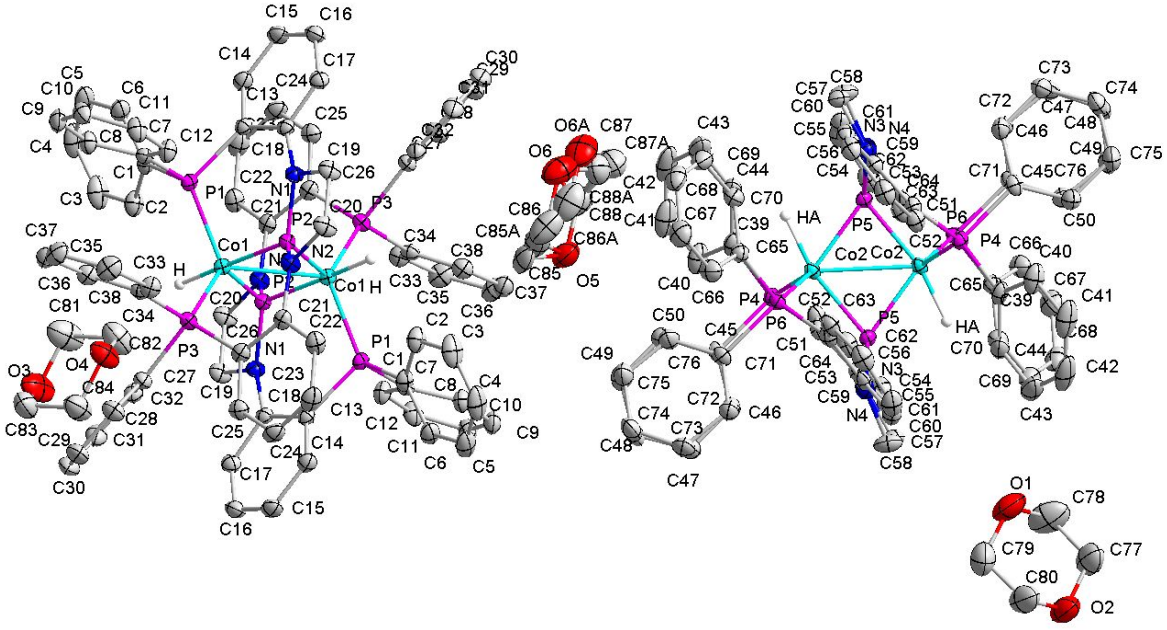
X-ray data collection, solution and refinement details for 6. The structure of complex **6** was solved using Bruker SHELX Software package[7] within APEX3[8] and OLEX2.[9] During the structure solution, electron density difference maps revealed that there were disordered species that could not be successfully modeled with or without restraints. Thus, the structure factors were modified using the PLATON SQUEEZE technique,[4-6] in order to produce a "solvate-free" structure factor set. PLATON reported a total electron density of 514 e^-, likely corresponding to one additional toluene molecule per asymmetric unit. Full X-Ray diffraction experimental details are available in Table S2.

Figure S34. Fully labelled displacement ellipsoid diagram of **6**.



X-ray data collection, solution and refinement details for 7. The structure of complex **7** was solved using Bruker SHELX Software package[7] within APEX3[8] and OLEX2.[9] During the structure solution, electron density difference maps revealed that there was a disorder dioxane solvent molecule, which was successfully modeled with two-component disorder, where the sum of the major and minor components was constrained to be one. During the refinement, it became clear that reflections were affected by the shadow of the beamstop, giving rise to the B Level checkcif Alert. Full X-Ray diffraction experimental details are available in Table S2.

Figure S35. Fully labelled displacement ellipsoid diagram of **7**.



Choice of Functional and Basis Set for DFT calculations. In order to choose the most effective and reliable computational method for the compounds described in this manuscript, geometry optimizations of dicationic complex **3** were carried out starting from X-ray derived experimental coordinates. Both functionals and basis sets were varied, for a total of 8 different combinations. Geometric parameters, specifically Co-Co and Co-P bond distances, for the resulting optimized geometries were then compared with the X-ray derived geometric parameters to determine which functional/basis set combination performed best for these complexes. The results are tabulated in Table S3. The B3LYP[10-11] functional gave the poorest match with experimental geometries regardless of the choice of basis set. The PBE0[12] functional reproduced the Co-P distances quite well, but overestimated the metal-metal distance. Both Head-Gordon's wB97XD functional[13] and Truhlar's M06 functional[14] performed much better, reproducing both the experimental Co-P and Co-Co distances relatively well. Using the def2SVP basis set[15] on all atoms led to a slight underestimation of Co-P^{NHP} distances. Using the LANL2DZ(p,d) basis set[16-19] on Co and P and the D95V basis set[20] on the C, H, and N atoms resulted in an excellent match with experimental Co-P distances while also minimizing the number of basis functionals (and therefore computational resources needed). Upgrading to a LANL2TZ basis set[16, 19] for Co did not lead to any noticeable change in geometry.

Based on these results, we narrowed down our choice of functional and basis sets to the top 3 methods highlighted in gray in Table S3, and benchmarked these methods with the monoanionic open shell complex **5** (Table S4). For comparison, a poorly performing functional and basis set combination (B3LYP/LANL2DZ) is also shown. In this case, the B3LYP functional again proved inferior to either the wB97XD or M06 functionals. The wB97XD functional with the LANL2DZ/D95V basis sets led to the poorest match in geometric parameters, particularly an overestimation of the Co-Co distance. The wB97XD functional with the def2SVP basis set, on the other hand, resulted in an optimized geometry in which the Co-Co and two of the Co-P^{NHP} distances were underestimated. The M06 functional with the LANL2DZ/D95V basis sets generally provided the best match with experiment while also minimizing the number of basis functions and therefore computational resources required. From these trials, the M06 functional with LANL2DZ(p,d) basis sets on Co and P and D95V basis sets on C, N, and H was chosen as the optimal method for all calculations reported in this paper.

Table S3. Comparison of experimental (X-ray) and computed interatomic distances (Å) for complex **3** using different basis set and functional combinations. The columns highlighted in light gray represent the closest matches with experimental geometric parameters.

Method	***Co-Co***	***Co-P^{Ar} (avg)***	***Co-P^{NHP} (avg)***	***Co-P^{NHP} (avg)***
X-ray	**2.5117(10)**	**2.1878(16)** **2.1997(17)** **2.1985(18)** **2.1905(17)**	**2.1878(17)** **2.1915(16)**	**2.0667(17)** **2.0711(16)**
B3LYP LANL2DZ(p,d) Co, P D95V C, N, H	2.75	2.28	2.20	2.11
B3LYP LANL2TZ(p,d) Co LANL2DZ(p,d) P D95V C, N, H	2.75	2.27	2.20	2.11
B3LYP Def2-tzvp Co, P Def2-svp C, N, H	2.71	2.25	2.18	2.08
wB97XD def2SVP on all atoms	2.59	2.20	2.16	2.05
wB97XD LANL2DZ(p,d) Co, P D95V C, N, H	2.62	2.21	2.17	2.08
wB97XD LANL2TZ(p,d) Co LANL2DZ(p,d) P D95V C, N, H	2.62	2.21	2.17	2.08
PBE1PBE LANL2DZ(p,d) Co, P D95V C, N, H	2.67	2.23	2.18	2.09
M06 LANL2DZ(p,d) Co, P D95V C, N, H	2.61	2.22	2.16	2.09

Table S4. Comparison of experimental (X-ray) and computed interatomic distances (Å) for complex **5** using different basis set and functional combinations.

Method	***Co-Co***	***Co-P^{Ar}***	***Co-P^{NHP}***	***Co-P^{NHP}***
X-ray	**2.4652(8)**	**2.1489(12)** **2.1502(11)** **2.2169(11)** **2.2029(11)**	**2.1878(17)** **2.1915(16)**	**2.0667(17)** **2.0711(16)**
B3LYP LANL2DZ(p,d) Co, P D95V C, N, H	2.62	2.24 2.23 2.40 2.38	2.34 2.41	2.06 2.08
wB97XD def2SVP on all atoms	2.45	2.15 2.16 2.26 2.28	2.25 2.31	2.03 2.00
wB97XD LANL2DZ(p,d) Co, P D95V C, N, H	2.52	2.16 2.18 2.29 2.31	2.26 2.31	2.04 2.03
M06 LANL2DZ(p,d) Co, P D95V C, N, H	2.49	2.17 2.19 2.26 2.26	2.26 2.31	2.04 2.03

Table S5. Comparison of selected bond distances (Å) determined experimentally (X-ray) with those in the DFT-optimized structures of **2**-**5** (Calc).

	2 (X-ray)	**2 (Calc)**	**3 (X-ray)**	**3 (Calc)**	**5 (X-ray)**	**5 (Calc)**
Co-Co	2.3867 (8)	2.39	2.5117(10)	2.61	2.4652 (8)	2.49
Co-P^{NHP}	2.0957 (12)	2.13	2.1878(17)	2.16	2.0594 (10)	2.04
Co-P^{NHP}	2.0957 (12)	2.11	2.0667(17)	2.09	2.1890 (12)	2.26
Co-P^{NHP}	2.0957 (12)	2.13	2.0711(16)	2.09	2.0215 (11)	2.03
Co-P^{NHP}	2.0957 (12)	2.11	2.1915(16)	2.16	2.2257 (10)	2.31
Co-P^{Ar}	2.1332 (13)	2.16	2.1878(16)	2.21	2.1489 (12)	2.17
Co-P^{Ar}	2.1332 (13)	2.15	2.1997(17)	2.22	2.1502 (11)	2.19
Co-P^{Ar}	2.1332 (13)	2.16	2.1985(18)	2.22	2.2169 (11)	2.26
Co-P^{Ar}	2.1332 (13)	2.15	2.1905(17)	2.21	2.2029 (11)	2.26

Table S6. Calculated relative free energies of **5** and **5'**.

Complex:	Energy (kcal/mol)
5	0
5'	8.8

Table S7. Computed Wiberg bond indices (WBI) and Mayer bond orders (MBO) for **2**, **3**, **5**, **6**$^{\text{monomer}}$, and **7**$^{\text{monomer}}$.

Complex	Co-P WBI	Co-Co WBI	Co-P MBO	Co-Co MBO
2	0.86 0.86	0.59	0.94 0.96	0.89
3	0.71 0.82	0.39	0.76 0.88	0.71
5	1.01 1.08 0.54 0.55	0.37	0.83 0.98 0.82 0.75	0.61
6$^{\text{monomer}}$	0.97	N/A	1.08	N/A
7$^{\text{monomer}}$	0.98	N/A	1.11	N/A

Table S8. Calculated relative free energies of **6**$^{\text{monomer}}$ and **7**$^{\text{monomer}}$ in the $S = 1/2$ and $S = 3/2$ spin states.

Complex:	*S*	multiplicity	Energy (kcal/mol)
6$^{\text{monomer}}$	1/2 3/2	doublet quartet	0 19.3
7$^{\text{monomer}}$	1/2 3/2	doublet quartet	0 39.3

Figure S36. Pictorial representations of the calculated frontier molecular orbitals of complex **2**.

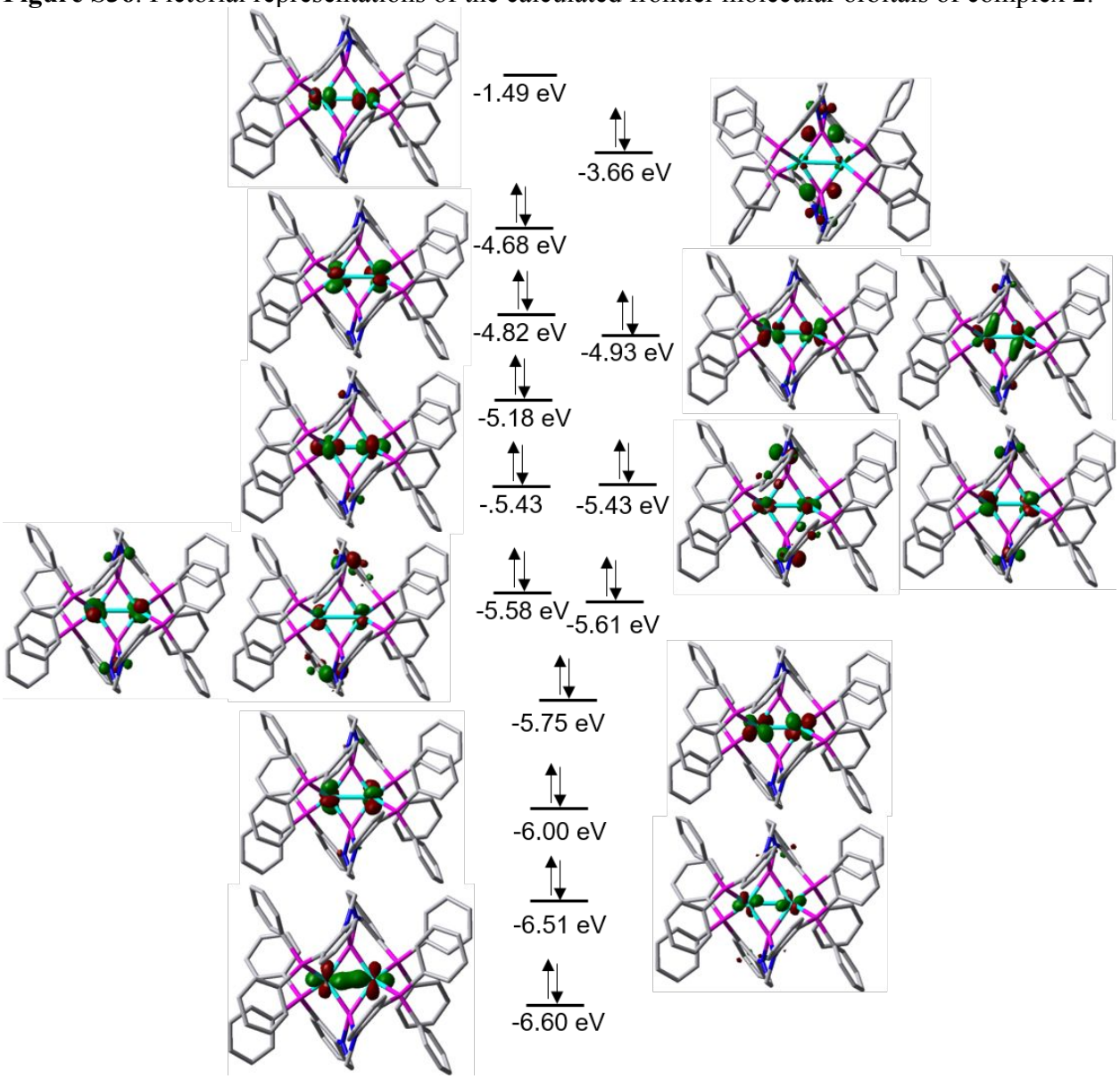


Figure S37. Pictorial representations of two representative Co-P^{NHP} natural bond orbitals of **3** associated with the long (left) and short (right) Co-P^{NHP} bonds to one Co atom.

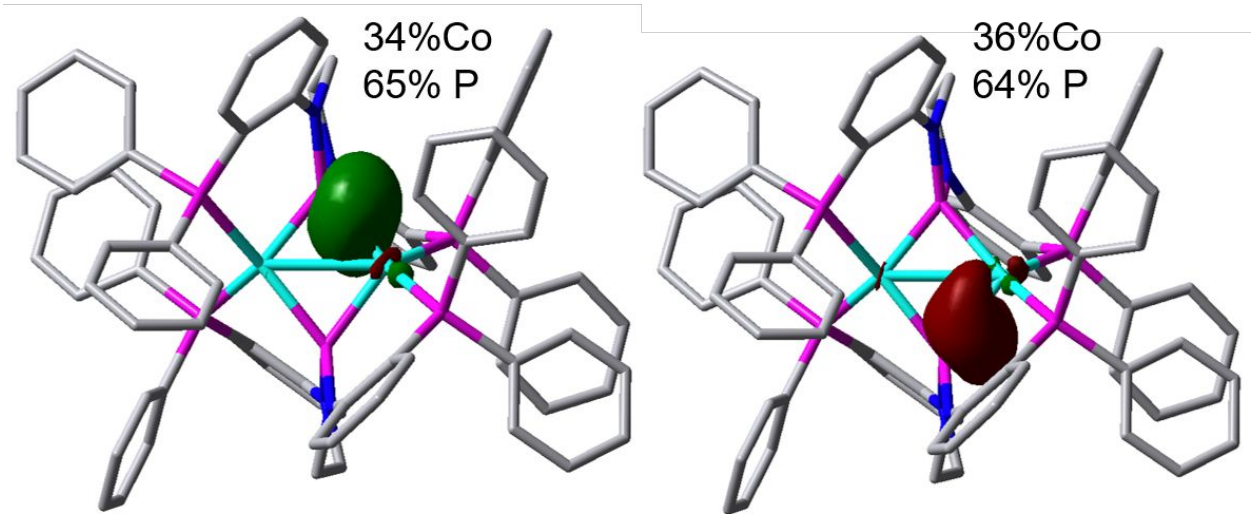


Table S9. DFT-optimized XYZ Coordinates for **2** (M06: LANL2DZ(p,d), Co, P; D95V, C, H, N). Note: The frequency calculation on **2** using this computational method revealed a small (-80 cm^{-1}) imaginary frequency. This imaginary frequency was not reproduced using any of the other basis set and functional combinations, so we have made the assumption that the small imaginary frequency is negligible.

Tag	Symbol	X	Y	Z
1	Co	-0.397164	1.126045	0.088186
2	P	-1.556613	2.042656	-1.478927
3	P	-1.637623	-0.595578	-0.042469
4	P	-0.035117	-2.588503	1.616702
5	N	-2.860348	-1.374266	0.967297
6	N	-2.75921	-0.761947	-1.400417
7	C	-0.870137	3.549712	-2.315689
8	C	0.531921	3.667789	-2.362977
9	C	1.131156	4.760057	-3.000034
10	C	0.335315	5.754845	-3.588136
11	C	-1.062482	5.648287	-3.538017
12	C	-1.663067	4.548671	-2.907658
13	C	-3.347841	2.480643	-1.216684
14	C	-3.76461	2.849653	0.074752
15	C	-5.105153	3.170994	0.330585
16	C	-6.050782	3.110671	-0.702926
17	C	-5.646949	2.732612	-1.993321
18	C	-4.304162	2.424223	-2.249982
19	C	-1.738444	0.876629	-2.910394
20	C	-1.344368	1.215057	-4.215094
21	C	-1.663067	0.399142	-5.309099
22	C	-2.394905	-0.778388	-5.102289
23	C	-2.757653	-1.159932	-3.806806
24	C	-2.419302	-0.358229	-2.697421
25	C	-3.92359	-1.606746	-1.127528
26	C	-4.197465	-1.38895	0.363075
27	C	-2.654439	-1.634083	2.323628
28	C	-3.713064	-1.442328	3.240828
29	C	-3.532882	-1.668771	4.607026
30	C	-2.280385	-2.069181	5.091914
31	C	-1.233665	-2.287809	4.187776
32	C	-1.391678	-2.105263	2.800824
33	C	-0.573866	-4.288533	1.101779
34	C	0.362629	-5.120396	0.45414
35	C	-0.008052	-6.383078	-0.019263

36	C	-1.330401	-6.829921	0.128903
37	C	-2.271495	-6.007286	0.762257
38	C	-1.895103	-4.746895	1.250695
39	C	1.346192	-2.952936	2.807995
40	C	1.610266	-4.225285	3.346874
41	C	2.670405	-4.408962	4.247349
42	C	3.463349	-3.319044	4.635028
43	C	3.192944	-2.042844	4.116366
44	C	2.146369	-1.86303	3.204145
45	H	1.140775	2.901775	-1.877288
46	H	2.214777	4.84606	-3.021292
47	H	0.800133	6.607108	-4.076073
48	H	-1.684531	6.415517	-3.990864
49	H	-2.748081	4.475312	-2.872595
50	H	-3.044001	2.856066	0.890314
51	H	-5.405201	3.455569	1.335575
52	H	-7.091907	3.350962	-0.505951
53	H	-6.374884	2.678279	-2.798215
54	H	-4.002645	2.123133	-3.252794
55	H	-0.80409	2.143285	-4.389092
56	H	-1.35606	0.692309	-6.308668
57	H	-2.666021	-1.410499	-5.943437
58	H	-3.289453	-2.095386	-3.647155
59	H	-3.719648	-2.677416	-1.312949
60	H	-4.77151	-1.289886	-1.747984
61	H	-4.732471	-0.434909	0.513508
62	H	-4.793683	-2.207113	0.787154
63	H	-4.673282	-1.086891	2.874712
64	H	-4.363583	-1.516215	5.291425
65	H	-2.121237	-2.227613	6.153693
66	H	-0.277433	-2.629715	4.574611
67	H	1.390001	-4.782611	0.316336
68	H	0.729717	-7.008423	-0.514346
69	H	-1.620629	-7.807367	-0.245928
70	H	-3.295867	-6.347081	0.888853
71	H	-2.630824	-4.13027	1.763134
72	H	0.988985	-5.073277	3.067934
73	H	2.868588	-5.398489	4.649755
74	H	4.279984	-3.461403	5.337374
75	H	3.788988	-1.184679	4.416559

76	H	1.947048	-0.8737	2.789176
77	Co	0.397164	-1.126045	0.088186
78	P	1.556613	-2.042656	-1.478927
79	P	1.637623	0.595578	-0.042469
80	P	0.035117	2.588503	1.616702
81	N	2.860348	1.374266	0.967297
82	N	2.75921	0.761947	-1.400417
83	C	0.870137	-3.549712	-2.315689
84	C	-0.531921	-3.667789	-2.362977
85	C	-1.131156	-4.760057	-3.000034
86	C	-0.335315	-5.754845	-3.588136
87	C	1.062482	-5.648287	-3.538017
88	C	1.663067	-4.548671	-2.907658
89	C	3.347841	-2.480643	-1.216684
90	C	3.76461	-2.849653	0.074752
91	C	5.105153	-3.170994	0.330585
92	C	6.050782	-3.110671	-0.702926
93	C	5.646949	-2.732612	-1.993321
94	C	4.304162	-2.424223	-2.249982
95	C	1.738444	-0.876629	-2.910394
96	C	1.344368	-1.215057	-4.215094
97	C	1.663067	-0.399142	-5.309099
98	C	2.394905	0.778388	-5.102289
99	C	2.757653	1.159932	-3.806806
100	C	2.419302	0.358229	-2.697421
101	C	3.92359	1.606746	-1.127528
102	C	4.197465	1.38895	0.363075
103	C	2.654439	1.634083	2.323628
104	C	3.713064	1.442328	3.240828
105	C	3.532882	1.668771	4.607026
106	C	2.280385	2.069181	5.091914
107	C	1.233665	2.287809	4.187776
108	C	1.391678	2.105263	2.800824
109	C	0.573866	4.288533	1.101779
110	C	-0.362629	5.120396	0.45414
111	C	0.008052	6.383078	-0.019263
112	C	1.330401	6.829921	0.128903
113	C	2.271495	6.007286	0.762257
114	C	1.895103	4.746895	1.250695
115	C	-1.346192	2.952936	2.807995

116	C	-1.610266	4.225285	3.346874
117	C	-2.670405	4.408962	4.247349
118	C	-3.463349	3.319044	4.635028
119	C	-3.192944	2.042844	4.116366
120	C	-2.146369	1.86303	3.204145
121	H	-1.140775	-2.901775	-1.877288
122	H	-2.214777	-4.84606	-3.021292
123	H	-0.800133	-6.607108	-4.076073
124	H	1.684531	-6.415517	-3.990864
125	H	2.748081	-4.475312	-2.872595
126	H	3.044001	-2.856066	0.890314
127	H	5.405201	-3.455569	1.335575
128	H	7.091907	-3.350962	-0.505951
129	H	6.374884	-2.678279	-2.798215
130	H	4.002645	-2.123133	-3.252794
131	H	0.80409	-2.143285	-4.389092
132	H	1.35606	-0.692309	-6.308668
133	H	2.666021	1.410499	-5.943437
134	H	3.289453	2.095386	-3.647155
135	H	3.719648	2.677416	-1.312949
136	H	4.77151	1.289886	-1.747984
137	H	4.732471	0.434909	0.513508
138	H	4.793683	2.207113	0.787154
139	H	4.673282	1.086891	2.874712
140	H	4.363583	1.516215	5.291425
141	H	2.121237	2.227613	6.153693
142	H	0.277433	2.629715	4.574611
143	H	-1.390001	4.782611	0.316336
144	H	-0.729717	7.008423	-0.514346
145	H	1.620629	7.807367	-0.245928
146	H	3.295867	6.347081	0.888853
147	H	2.630824	4.13027	1.763134
148	H	-0.988985	5.073277	3.067934
149	H	-2.868588	5.398489	4.649755
150	H	-4.279984	3.461403	5.337374
151	H	-3.788988	1.184679	4.416559
152	H	-1.947048	0.8737	2.789176

Table S10. DFT-optimized XYZ Coordinates for **3** (M06: LANL2DZ(p,d), Co, P; D95V, C, H, N).

Tag	Symbol	X	Y	Z
1	Co	1.258268	0.33072	0.196199
2	P	2.310792	1.459801	-1.394404
3	P	-0.468105	1.577377	-0.148008
4	P	-2.746823	0.538364	1.570064
5	N	-0.985255	2.955651	0.72548
6	N	-0.626273	2.44449	-1.613815
7	C	3.862037	0.746748	-2.070057
8	C	3.891983	-0.649638	-2.253429
9	C	4.99783	-1.25906	-2.853628
10	C	6.088558	-0.476714	-3.267806
11	C	6.068466	0.911991	-3.074309
12	C	4.95564	1.527117	-2.480556
13	C	2.640212	3.239965	-1.050028
14	C	2.808207	3.647411	0.288338
15	C	3.048848	4.994765	0.592651
16	C	3.11526	5.945482	-0.436759
17	C	2.943437	5.545969	-1.772231
18	C	2.707819	4.199661	-2.07993
19	C	1.264526	1.553008	-2.930078
20	C	1.788002	1.2406	-4.198381
21	C	1.046496	1.459879	-5.366561
22	C	-0.251572	1.977408	-5.282978
23	C	-0.807368	2.256232	-4.030713
24	C	-0.059232	2.055201	-2.860392
25	C	-1.329639	3.743415	-1.486018
26	C	-0.995412	4.208897	-0.069729
27	C	-1.370647	2.974124	2.091528
28	C	-1.037234	4.085444	2.885014
29	C	-1.480181	4.164451	4.209676
30	C	-2.226069	3.115348	4.766738
31	C	-2.551802	2.003832	3.979442
32	C	-2.149364	1.92418	2.633653
33	C	-4.432101	1.081592	1.09381
34	C	-5.35779	0.131913	0.616163
35	C	-6.63526	0.534812	0.215731
36	C	-6.992426	1.891637	0.261339
37	C	-6.068466	2.842966	0.714858

38	C	-4.792802	2.441541	1.134813
39	C	-2.939333	-0.830775	2.783068
40	C	-4.178122	-1.261903	3.292181
41	C	-4.228138	-2.305225	4.227119
42	C	-3.045691	-2.915109	4.670101
43	C	-1.806509	-2.476788	4.178471
44	C	-1.751046	-1.444364	3.235678
45	H	3.042414	-1.251808	-1.922925
46	H	5.019083	-2.336969	-2.989952
47	H	6.947798	-0.947053	-3.735169
48	H	6.910838	1.517203	-3.39381
49	H	4.945478	2.60614	-2.342991
50	H	2.750465	2.917721	1.096275
51	H	3.18828	5.294695	1.627082
52	H	3.304633	6.988316	-0.203181
53	H	2.999351	6.279586	-2.5701
54	H	2.573014	3.900738	-3.118376
55	H	2.799642	0.852913	-4.286389
56	H	1.487232	1.235291	-6.332292
57	H	-0.830139	2.156475	-6.18343
58	H	-1.822754	2.640344	-3.95729
59	H	-2.416655	3.626431	-1.61353
60	H	-0.95163	4.436861	-2.243545
61	H	-0.013707	4.703854	-0.037935
62	H	-1.756151	4.887526	0.329295
63	H	-0.43036	4.883105	2.463506
64	H	-1.236546	5.03737	4.806831
65	H	-2.56463	3.168492	5.795528
66	H	-3.149006	1.202905	4.409415
67	H	-5.088154	-0.921875	0.557438
68	H	-7.347378	-0.205993	-0.134632
69	H	-7.98534	2.201895	-0.047849
70	H	-6.34517	3.891408	0.760817
71	H	-4.097574	3.186574	1.51869
72	H	-5.100576	-0.779225	2.981703
73	H	-5.187106	-2.627057	4.620072
74	H	-3.088827	-3.711497	5.406089
75	H	-0.883655	-2.924596	4.535093
76	H	-0.780751	-1.099264	2.87104
77	Co	-1.258268	-0.33072	0.196199

78	P	-2.310792	-1.459801	-1.394404
79	P	0.468105	-1.577377	-0.148008
80	P	2.746823	-0.538364	1.570064
81	N	0.985255	-2.955651	0.72548
82	N	0.626273	-2.44449	-1.613815
83	C	-3.862037	-0.746748	-2.070057
84	C	-3.891983	0.649638	-2.253429
85	C	-4.99783	1.25906	-2.853628
86	C	-6.088558	0.476714	-3.267806
87	C	-6.068466	-0.911991	-3.074309
88	C	-4.95564	-1.527117	-2.480556
89	C	-2.640212	-3.239965	-1.050028
90	C	-2.808207	-3.647411	0.288338
91	C	-3.048848	-4.994765	0.592651
92	C	-3.11526	-5.945482	-0.436759
93	C	-2.943437	-5.545969	-1.772231
94	C	-2.707819	-4.199661	-2.07993
95	C	-1.264526	-1.553008	-2.930078
96	C	-1.788002	-1.2406	-4.198381
97	C	-1.046496	-1.459879	-5.366561
98	C	0.251572	-1.977408	-5.282978
99	C	0.807368	-2.256232	-4.030713
100	C	0.059232	-2.055201	-2.860392
101	C	1.329639	-3.743415	-1.486018
102	C	0.995412	-4.208897	-0.069729
103	C	1.370647	-2.974124	2.091528
104	C	1.037234	-4.085444	2.885014
105	C	1.480181	-4.164451	4.209676
106	C	2.226069	-3.115348	4.766738
107	C	2.551802	-2.003832	3.979442
108	C	2.149364	-1.92418	2.633653
109	C	4.432101	-1.081592	1.09381
110	C	5.35779	-0.131913	0.616163
111	C	6.63526	-0.534812	0.215731
112	C	6.992426	-1.891637	0.261339
113	C	6.068466	-2.842966	0.714858
114	C	4.792802	-2.441541	1.134813
115	C	2.939333	0.830775	2.783068
116	C	4.178122	1.261903	3.292181
117	C	4.228138	2.305225	4.227119

118	C	3.045691	2.915109	4.670101
119	C	1.806509	2.476788	4.178471
120	C	1.751046	1.444364	3.235678
121	H	-3.042414	1.251808	-1.922925
122	H	-5.019083	2.336969	-2.989952
123	H	-6.947798	0.947053	-3.735169
124	H	-6.910838	-1.517203	-3.39381
125	H	-4.945478	-2.60614	-2.342991
126	H	-2.750465	-2.917721	1.096275
127	H	-3.18828	-5.294695	1.627082
128	H	-3.304633	-6.988316	-0.203181
129	H	-2.999351	-6.279586	-2.5701
130	H	-2.573014	-3.900738	-3.118376
131	H	-2.799642	-0.852913	-4.286389
132	H	-1.487232	-1.235291	-6.332292
133	H	0.830139	-2.156475	-6.18343
134	H	1.822754	-2.640344	-3.95729
135	H	2.416655	-3.626431	-1.61353
136	H	0.95163	-4.436861	-2.243545
137	H	0.013707	-4.703854	-0.037935
138	H	1.756151	-4.887526	0.329295
139	H	0.43036	-4.883105	2.463506
140	H	1.236546	-5.03737	4.806831
141	H	2.56463	-3.168492	5.795528
142	H	3.149006	-1.202905	4.409415
143	H	5.088154	0.921875	0.557438
144	H	7.347378	0.205993	-0.134632
145	H	7.98534	-2.201895	-0.047849
146	H	6.34517	-3.891408	0.760817
147	H	4.097574	-3.186574	1.51869
148	H	5.100576	0.779225	2.981703
149	H	5.187106	2.627057	4.620072
150	H	3.088827	3.711497	5.406089
151	H	0.883655	2.924596	4.535093
152	H	0.780751	1.099264	2.87104

Table S11. DFT-optimized XYZ Coordinates for **5** (M06: LANL2DZ(p,d), Co, P; D95V, C, H, N).

Tag	Symbol	X	Y	Z
1	C	4.126095	0.793568	3.160846
2	H	3.357648	1.201772	3.81481
3	Co	1.264192	0.104792	-0.087216
4	N	-0.564138	1.442935	-2.919977
5	P	2.489239	1.595179	0.941363
6	C	5.261994	0.193904	3.726245
7	H	5.353854	0.130654	4.806671
8	Co	-1.208815	0.184346	0.218951
9	N	-0.073212	-0.939063	-2.904413
10	P	2.429165	-1.399872	-1.137649
11	C	6.282412	-0.300773	2.903562
12	H	7.165617	-0.756404	3.340993
13	N	0.579535	0.299538	3.164745
14	P	0.052645	0.335524	-1.716095
15	C	6.16044	-0.199922	1.50886
16	H	6.946016	-0.58086	0.862895
17	N	0.102869	-1.992841	2.492787
18	P	0.406053	-0.51306	1.640537
19	C	5.020793	0.381757	0.944699
20	H	4.937713	0.44227	-0.140882
21	P	-2.5718	1.762071	-0.664222
22	C	3.993435	0.893103	1.764248
23	P	-2.388937	-1.650185	0.817157
24	C	4.445215	3.580666	0.236069
25	H	5.085454	3.154479	1.005023
26	C	4.899711	4.672823	-0.516524
27	H	5.888526	5.080412	-0.329591
28	C	4.07886	5.24105	-1.501356
29	H	4.431685	6.089056	-2.080601
30	C	2.799385	4.712831	-1.732028
31	H	2.150762	5.15176	-2.485656
32	C	2.349628	3.613349	-0.990665
33	H	1.359026	3.196404	-1.180815
34	C	3.169356	3.0362	-0.001671
35	C	1.631045	2.41808	2.373949
36	C	1.810031	3.796896	2.595953
37	H	2.401872	4.374266	1.890931

38	C	1.277199	4.44832	3.714662
39	H	1.453422	5.508665	3.860266
40	C	0.543822	3.709285	4.649615
41	H	0.141992	4.189044	5.53757
42	C	0.313506	2.347268	4.436934
43	H	-0.290576	1.794356	5.150818
44	C	0.836553	1.683549	3.306499
45	C	0.216958	-0.521937	4.339382
46	H	-0.847865	-0.403916	4.598175
47	H	0.830952	-0.232545	5.199996
48	C	0.499343	-1.962121	3.907895
49	H	1.569472	-2.197736	4.039748
50	H	-0.098444	-2.68149	4.478908
51	C	-0.255857	-3.18973	1.832022
52	C	0.433429	-4.383595	2.096655
53	H	1.263301	-4.379315	2.799958
54	C	0.060918	-5.56988	1.453615
55	H	0.594076	-6.490343	1.670657
56	C	-0.983376	-5.561902	0.520591
57	H	-1.266039	-6.47409	0.004593
58	C	-1.683291	-4.374209	0.263926
59	H	-2.512014	-4.390606	-0.44047
60	C	-1.351249	-3.18386	0.930377
61	C	-3.371818	-2.77477	3.260578
62	H	-3.078343	-3.747868	2.868688
63	C	-3.937028	-2.682501	4.539205
64	H	-4.089077	-3.582579	5.127114
65	C	-4.309299	-1.432231	5.059006
66	H	-4.748341	-1.364966	6.049703
67	C	-4.114193	-0.272305	4.29562
68	H	-4.399194	0.699948	4.686967
69	C	-3.543794	-0.362661	3.018121
70	H	-3.382344	0.547281	2.439843
71	C	-3.171319	-1.613438	2.489181
72	C	-4.911003	-2.778706	0.049677
73	H	-5.13774	-2.892987	1.107759
74	C	-5.831121	-3.221344	-0.91237
75	H	-6.764683	-3.67625	-0.595472
76	C	-5.54184	-3.088681	-2.278592
77	H	-6.253303	-3.437256	-3.020951

78	C	-4.334118	-2.499862	-2.684916
79	H	-4.115781	-2.382385	-3.74324
80	C	-3.420589	-2.046634	-1.727399
81	H	-2.485715	-1.573257	-2.036033
82	C	-3.700389	-2.190874	-0.354716
83	C	-3.214388	2.643236	0.824732
84	C	-2.292622	2.902441	1.862441
85	H	-1.243313	2.613394	1.756128
86	C	-2.711024	3.554362	3.029363
87	H	-1.98703	3.756593	3.81261
88	C	-4.049025	3.949635	3.177143
89	H	-4.370574	4.456031	4.082095
90	C	-4.965327	3.705835	2.144464
91	H	-5.9982	4.024633	2.24462
92	C	-4.549753	3.061683	0.970709
93	H	-5.265499	2.894757	0.170125
94	C	-5.114847	0.670566	-1.124532
95	H	-5.056976	0.336105	-0.088857
96	C	-6.246626	0.355256	-1.882249
97	H	-7.056715	-0.208004	-1.428593
98	C	-6.327293	0.754943	-3.225542
99	H	-7.204556	0.506794	-3.815006
100	C	-5.275807	1.481527	-3.800275
101	H	-5.337874	1.802471	-4.83572
102	C	-4.149438	1.818724	-3.035722
103	H	-3.355785	2.414806	-3.482222
104	C	-4.061533	1.417304	-1.69101
105	C	-1.726196	3.124136	-1.58422
106	C	-1.995545	4.476877	-1.31626
107	H	-2.657865	4.742561	-0.495799
108	C	-1.444272	5.492841	-2.108289
109	H	-1.67061	6.531322	-1.891426
110	C	-0.619581	5.157393	-3.19112
111	H	-0.206055	5.937766	-3.823514
112	C	-0.314885	3.817355	-3.455553
113	H	0.351987	3.55766	-4.274462
114	C	-0.853699	2.796222	-2.652395
115	C	-0.371395	0.957013	-4.29745
116	H	0.661177	1.120663	-4.64691
117	H	-1.066398	1.466754	-4.974318

118	C	-0.664408	-0.536912	-4.195507
119	H	-1.753921	-0.707795	-4.216047
120	H	-0.196982	-1.101159	-5.010361
121	C	0.223932	-2.304773	-2.662104
122	C	-0.54991	-3.296183	-3.297546
123	H	-1.370692	-3.005995	-3.948607
124	C	-0.281969	-4.654089	-3.100973
125	H	-0.886904	-5.398583	-3.609728
126	C	0.751343	-5.046442	-2.24149
127	H	0.960006	-6.098089	-2.071382
128	C	1.533383	-4.069238	-1.61386
129	H	2.350332	-4.380608	-0.966412
130	C	1.308971	-2.699062	-1.830603
131	C	3.723029	-2.386186	-0.262319
132	C	3.549059	-2.616253	1.114775
133	H	2.687034	-2.179567	1.620895
134	C	4.483372	-3.369091	1.834275
135	H	4.344028	-3.528035	2.900632
136	C	5.610597	-3.894505	1.184894
137	H	6.34047	-4.473896	1.742277
138	C	5.796881	-3.660582	-0.185599
139	H	6.66969	-4.061222	-0.692315
140	C	4.857182	-2.911511	-0.907964
141	H	5.016315	-2.731797	-1.968811
142	C	3.254751	-0.818525	-2.69547
143	C	3.648324	0.53014	-2.779477
144	H	3.457853	1.200392	-1.942728
145	C	4.249304	1.028856	-3.942999
146	H	4.549702	2.072257	-3.984549
147	C	4.451004	0.184143	-5.044201
148	H	4.913089	0.56733	-5.949061
149	C	4.050828	-1.159711	-4.974409
150	H	4.201142	-1.816831	-5.825885
151	C	3.458542	-1.659916	-3.806709
152	H	3.14032	-2.701144	-3.768469

Table S12. DFT-optimized XYZ Coordinates for **5'** (M06: LANL2DZ(p,d), Co, P; D95V, C, H, N).

Tag	Symbol	X	Y	Z
1	Co	-1.328226	-0.058224	0.18476
2	P	-2.493889	-0.72911	-1.557573
3	P	0.146383	-1.630947	-0.228841
4	P	2.466263	-1.066779	1.748928
5	N	0.329613	-3.087667	0.696097
6	N	-0.016237	-2.599152	-1.656219
7	C	-3.792264	0.356321	-2.28889
8	C	-3.510357	1.734807	-2.342749
9	C	-4.422241	2.623861	-2.921322
10	C	-5.636475	2.14427	-3.43698
11	C	-5.931261	0.774526	-3.370408
12	C	-5.010896	-0.119287	-2.802928
13	C	-3.334841	-2.342479	-1.203622
14	C	-3.655877	-2.628	0.138266
15	C	-4.261203	-3.843525	0.485671
16	C	-4.545805	-4.791719	-0.508064
17	C	-4.224114	-4.518322	-1.847423
18	C	-3.621845	-3.301235	-2.194736
19	C	-1.493251	-1.1962	-3.05854
20	C	-1.833523	-0.747688	-4.346014
21	C	-1.158314	-1.210021	-5.484293
22	C	-0.114642	-2.131629	-5.346391
23	C	0.270771	-2.558455	-4.071512
24	C	-0.403161	-2.097878	-2.927466
25	C	0.358049	-4.016018	-1.487933
26	C	-0.005234	-4.32684	-0.038091
27	C	0.527453	-3.1264	2.100897
28	C	-0.176214	-4.079654	2.861574
29	C	0.022922	-4.180558	4.242543
30	C	0.906676	-3.307482	4.889182
31	C	1.609671	-2.357691	4.136798
32	C	1.453561	-2.26005	2.742865
33	C	3.895248	-2.108826	1.217642
34	C	4.995329	-1.460548	0.619196
35	C	6.093154	-2.197879	0.165594
36	C	6.093859	-3.597788	0.274899
37	C	4.995329	-4.251196	0.848827

38	C	3.902629	-3.510566	1.325431
39	C	3.179871	0.039795	3.042518
40	C	4.434188	-0.174928	3.642715
41	C	4.912898	0.71358	4.615509
42	C	4.139189	1.816307	5.00478
43	C	2.882186	2.028973	4.418847
44	C	2.40476	1.149212	3.439207
45	H	-2.576656	2.103157	-1.914053
46	H	-4.198789	3.687281	-2.952603
47	H	-6.349203	2.832633	-3.880969
48	H	-6.87144	0.400955	-3.764864
49	H	-5.24627	-1.180726	-2.759749
50	H	-3.425741	-1.899029	0.916349
51	H	-4.507018	-4.041945	1.525196
52	H	-5.015772	-5.734255	-0.243998
53	H	-4.445127	-5.249576	-2.619171
54	H	-3.367534	-3.102478	-3.235185
55	H	-2.654831	-0.045562	-4.471238
56	H	-1.453891	-0.854974	-6.466612
57	H	0.409387	-2.504281	-6.221201
58	H	1.103967	-3.248909	-3.957476
59	H	1.435194	-4.179229	-1.659222
60	H	-0.210814	-4.634876	-2.190307
61	H	-1.079125	-4.559033	0.043166
62	H	0.576826	-5.165143	0.361354
63	H	-0.888758	-4.737232	2.370093
64	H	-0.515989	-4.934669	4.808948
65	H	1.061392	-3.372467	5.96097
66	H	2.308986	-1.696089	4.642141
67	H	4.998626	-0.375481	0.512743
68	H	6.939243	-1.684014	-0.281171
69	H	6.944535	-4.170504	-0.081833
70	H	4.993708	-5.333062	0.944036
71	H	3.070593	-4.02724	1.800944
72	H	5.037022	-1.032606	3.352911
73	H	5.883242	0.540569	5.070703
74	H	4.510241	2.500598	5.761746
75	H	2.269989	2.873925	4.720886
76	H	1.423882	1.321721	2.988487
77	Co	1.328226	0.058224	0.18476

78	P	2.493889	0.72911	-1.557573
79	P	-0.146383	1.630947	-0.228841
80	P	-2.466263	1.066779	1.748928
81	N	-0.329613	3.087667	0.696097
82	N	0.016237	2.599152	-1.656219
83	C	3.792264	-0.356321	-2.28889
84	C	3.510357	-1.734807	-2.342749
85	C	4.422241	-2.623861	-2.921322
86	C	5.636475	-2.14427	-3.43698
87	C	5.931261	-0.774526	-3.370408
88	C	5.010896	0.119287	-2.802928
89	C	3.334841	2.342479	-1.203622
90	C	3.655877	2.628	0.138266
91	C	4.261203	3.843525	0.485671
92	C	4.545805	4.791719	-0.508064
93	C	4.224114	4.518322	-1.847423
94	C	3.621845	3.301235	-2.194736
95	C	1.493251	1.1962	-3.05854
96	C	1.833523	0.747688	-4.346014
97	C	1.158314	1.210021	-5.484293
98	C	0.114642	2.131629	-5.346391
99	C	-0.270771	2.558455	-4.071512
100	C	0.403161	2.097878	-2.927466
101	C	-0.358049	4.016018	-1.487933
102	C	0.005234	4.32684	-0.038091
103	C	-0.527453	3.1264	2.100897
104	C	0.176214	4.079654	2.861574
105	C	-0.022922	4.180558	4.242543
106	C	-0.906676	3.307482	4.889182
107	C	-1.609671	2.357691	4.136798
108	C	-1.453561	2.26005	2.742865
109	C	-3.895248	2.108826	1.217642
110	C	-4.995329	1.460548	0.619196
111	C	-6.093154	2.197879	0.165594
112	C	-6.093859	3.597788	0.274899
113	C	-4.995329	4.251196	0.848827
114	C	-3.902629	3.510566	1.325431
115	C	-3.179871	-0.039795	3.042518
116	C	-4.434188	0.174928	3.642715
117	C	-4.912898	-0.71358	4.615509

118	C	-4.139189	-1.816307	5.00478
119	C	-2.882186	-2.028973	4.418847
120	C	-2.40476	-1.149212	3.439207
121	H	2.576656	-2.103157	-1.914053
122	H	4.198789	-3.687281	-2.952603
123	H	6.349203	-2.832633	-3.880969
124	H	6.87144	-0.400955	-3.764864
125	H	5.24627	1.180726	-2.759749
126	H	3.425741	1.899029	0.916349
127	H	4.507018	4.041945	1.525196
128	H	5.015772	5.734255	-0.243998
129	H	4.445127	5.249576	-2.619171
130	H	3.367534	3.102478	-3.235185
131	H	2.654831	0.045562	-4.471238
132	H	1.453891	0.854974	-6.466612
133	H	-0.409387	2.504281	-6.221201
134	H	-1.103967	3.248909	-3.957476
135	H	-1.435194	4.179229	-1.659222
136	H	0.210814	4.634876	-2.190307
137	H	1.079125	4.559033	0.043166
138	H	-0.576826	5.165143	0.361354
139	H	0.888758	4.737232	2.370093
140	H	0.515989	4.934669	4.808948
141	H	-1.061392	3.372467	5.96097
142	H	-2.308986	1.696089	4.642141
143	H	-4.998626	0.375481	0.512743
144	H	-6.939243	1.684014	-0.281171
145	H	-6.944535	4.170504	-0.081833
146	H	-4.993708	5.333062	0.944036
147	H	-3.070593	4.02724	1.800944
148	H	-5.037022	1.032606	3.352911
149	H	-5.883242	-0.540569	5.070703
150	H	-4.510241	-2.500598	5.761746
151	H	-2.269989	-2.873925	4.720886
152	H	-1.423882	-1.321721	2.988487

Table S13. DFT-optimized XYZ Coordinates for **6**$^{\text{monomer}}$ in the S = 1/2 state (M06: LANL2DZ(p,d), Co, P; D95V, C, H, N).

Tag	Symbol	X	Y	Z
1	Co	-0.105893	0.4539	-1.319179
2	Cl	-0.225817	2.255686	-2.625878
3	P	-2.01128	0.184845	-0.135087
4	P	0.016237	-1.679801	-1.604842
5	P	1.788853	0.393182	-0.095371
6	N	-0.619056	-2.726448	-0.33325
7	N	1.596633	-2.357805	-1.326926
8	C	-1.8924	1.08965	1.470783
9	C	-1.227571	2.333549	1.413491
10	H	-0.880371	2.716887	0.452484
11	C	-0.995339	3.063545	2.584683
12	H	-0.470386	4.012891	2.52834
13	C	-1.4209	2.559184	3.824157
14	H	-1.229744	3.120388	4.734162
15	C	-2.087113	1.326956	3.885106
16	H	-2.41744	0.933207	4.842104
17	C	-2.324003	0.593667	2.712967
18	H	-2.824734	-0.370995	2.772909
19	C	-3.443462	0.97654	-0.984283
20	C	-4.294068	1.905622	-0.362153
21	H	-4.124634	2.195164	0.673325
22	C	-5.355856	2.476137	-1.078705
23	H	-6.005179	3.199458	-0.593904
24	C	-5.574914	2.119361	-2.415864
25	H	-6.394978	2.565408	-2.971002
26	C	-4.723403	1.195605	-3.041906
27	H	-4.878026	0.929971	-4.083221
28	C	-3.658551	0.631683	-2.332487
29	H	-2.980359	-0.060642	-2.830638
30	C	-2.682477	-1.48459	0.295192
31	C	-4.000686	-1.550808	0.789837
32	H	-4.584771	-0.632779	0.84086
33	C	-4.58261	-2.749816	1.207056
34	H	-5.60087	-2.766097	1.581164
35	C	-3.82682	-3.927857	1.121964
36	H	-4.255094	-4.875946	1.434998
37	C	-2.530294	-3.900375	0.609577

38	H	-1.987519	-4.83518	0.515275
39	C	-1.927069	-2.691552	0.177882
40	C	0.216757	-3.924702	-0.131442
41	H	-0.095607	-4.73851	-0.805835
42	H	0.120145	-4.277203	0.902524
43	C	1.667539	-3.513055	-0.416905
44	H	2.183643	-3.225215	0.512324
45	H	2.222406	-4.344103	-0.871465
46	C	2.798596	-1.67962	-1.692115
47	C	3.736038	-2.322698	-2.513257
48	H	3.507505	-3.319254	-2.884074
49	C	4.92789	-1.679227	-2.869181
50	H	5.645581	-2.184001	-3.508902
51	C	5.18047	-0.37723	-2.415958
52	H	6.096167	0.132366	-2.699769
53	C	4.249709	0.27135	-1.591828
54	H	4.456767	1.277989	-1.234724
55	C	3.062045	-0.369742	-1.208492
56	C	2.531592	2.005023	0.413066
57	C	2.488585	3.062455	-0.520261
58	H	2.03438	2.904873	-1.498699
59	C	2.987437	4.324971	-0.177146
60	H	2.946166	5.130486	-0.903944
61	C	3.519128	4.551884	1.101862
62	H	3.898924	5.534251	1.367762
63	C	3.547915	3.509001	2.038164
64	H	3.948033	3.679948	3.033477
65	C	3.057786	2.24061	1.697102
66	H	3.073878	1.445549	2.438307
67	C	1.990954	-0.672279	1.404003
68	C	3.261012	-1.10577	1.834005
69	H	4.151047	-0.807729	1.281299
70	C	3.383926	-1.927966	2.961188
71	H	4.367396	-2.255559	3.285398
72	C	2.23852	-2.327637	3.670806
73	H	2.335927	-2.965406	4.544638
74	C	0.972521	-1.898298	3.248713
75	H	0.078305	-2.197426	3.789429
76	C	0.852802	-1.076232	2.119135
77	H	-0.130873	-0.752383	1.791344

Table S14. DFT-optimized XYZ Coordinates for **7**$^{\text{monomer}}$ in the S = 1/2 state (M06: LANL2DZ(p,d), Co, P; D95V, C, H, N).

Tag	Symbol	X	Y	Z
1	Co	0.010221	0.422992	-0.616139
2	P	0.075908	-1.647871	-1.2093
3	P	2.165189	0.438458	-0.236919
4	P	-2.150065	0.318367	-0.311336
5	N	1.49039	-2.58483	-0.632821
6	N	-0.967629	-2.7529	-0.282223
7	C	2.807274	-2.242812	-0.951121
8	C	3.270914	-0.889665	-0.879975
9	C	4.60159	-0.603639	-1.231675
10	H	4.949898	0.42551	-1.194149
11	C	-2.31479	-2.567949	-0.005908
12	C	-4.395776	-1.267035	0.021747
13	H	-4.906511	-0.315829	-0.12251
14	C	2.149023	0.153487	1.587673
15	C	-2.996114	-1.314489	-0.157524
16	C	3.137787	1.990156	-0.436509
17	C	-3.147856	1.210701	-1.579093
18	C	-2.54521	1.145059	1.295934
19	C	-3.090332	-3.677592	0.444552
20	H	-2.608157	-4.629632	0.635748
21	C	2.942136	-0.814152	2.227739
22	H	3.636859	-1.417967	1.646143
23	C	2.782752	2.864419	-1.477996
24	H	1.928686	2.62267	-2.107574
25	C	-0.307282	-4.02021	0.067984
26	H	-0.850123	-4.883589	-0.341896
27	H	-0.273496	-4.124484	1.162338
28	C	4.203152	2.325822	0.420187
29	H	4.469995	1.660658	1.240267
30	C	-3.107312	1.055737	3.665431
31	H	-3.409571	0.477429	4.53362
32	C	-4.46531	-3.586175	0.635688
33	H	-5.012484	-4.464891	0.966768
34	C	2.836065	-1.006021	3.612477
35	H	3.454475	-1.753858	4.10091
36	C	-2.891911	2.435623	3.777901
37	H	-3.029981	2.934031	4.733208

38	C	1.2416	0.921817	2.347799
39	H	0.623636	1.674499	1.85515
40	C	1.106354	-3.994025	-0.526848
41	H	1.804656	-4.534191	0.122914
42	H	1.10791	-4.484429	-1.51783
43	C	-2.934628	0.41195	2.43124
44	H	-3.10431	-0.660254	2.356026
45	C	-5.146085	-2.381423	0.392698
46	H	-6.222457	-2.312048	0.50817
47	C	5.497356	-1.60496	-1.625307
48	H	6.517389	-1.350978	-1.894121
49	C	3.73071	-3.24527	-1.337811
50	H	3.404413	-4.278038	-1.408119
51	C	-4.249912	2.029302	-1.277028
52	H	-4.54495	2.188881	-0.241402
53	C	5.052678	-2.93245	-1.660126
54	H	5.730257	-3.72847	-1.956878
55	C	-2.311443	2.530956	1.419475
56	H	-1.969469	3.096804	0.555158
57	C	4.910104	3.519838	0.228692
58	H	5.72555	3.778363	0.897894
59	C	1.933859	-0.239858	4.364746
60	H	1.851265	-0.394093	5.436898
61	C	3.499174	4.0521	-1.676618
62	H	3.219647	4.723141	-2.483299
63	C	-4.96474	2.657201	-2.306407
64	H	-5.812106	3.292063	-2.063906
65	C	4.563255	4.38066	-0.824438
66	H	5.112861	5.305859	-0.972397
67	C	-2.768377	1.030801	-2.922652
68	H	-1.906531	0.407567	-3.161982
69	C	-2.493097	3.172207	2.650115
70	H	-2.317149	4.240957	2.730596
71	C	1.135622	0.723948	3.729562
72	H	0.429094	1.317527	4.302869
73	C	-4.58869	2.466666	-3.643368
74	H	-5.144001	2.95319	-4.439993
75	C	-3.488939	1.650728	-3.949735
76	H	-3.189675	1.504062	-4.983276
77	H	-0.128017	1.98985	-0.599981

Table S15. DFT-optimized XYZ Coordinates for **6**$^{\text{monomer}}$ in the S = 3/2 state (M06: LANL2DZ(p,d), Co, P; D95V, C, H, N).

Tag	Symbol	X	Y	Z
1	Co	-0.159684	0.552772	-1.451301
2	Cl	-0.087235	2.258755	-2.885924
3	P	-2.053371	0.183524	-0.155978
4	P	0.104327	-1.694057	-1.678731
5	P	1.767477	0.452111	-0.053863
6	N	-0.521835	-2.71395	-0.389835
7	N	1.701769	-2.289212	-1.388128
8	C	-1.929178	1.015441	1.489596
9	C	-1.278375	2.267665	1.484414
10	H	-0.944257	2.701145	0.540033
11	C	-1.04216	2.949135	2.683622
12	H	-0.523962	3.903586	2.664126
13	C	-1.453455	2.386731	3.90271
14	H	-1.258282	2.907991	4.835228
15	C	-2.11044	1.148077	3.913539
16	H	-2.430741	0.71008	4.854533
17	C	-2.349682	0.46411	2.712322
18	H	-2.841499	-0.506829	2.733628
19	C	-3.533571	0.967242	-0.926378
20	C	-4.428875	1.797738	-0.230035
21	H	-4.271082	2.006492	0.826747
22	C	-5.51943	2.371955	-0.897929
23	H	-6.204256	3.017354	-0.355486
24	C	-5.723075	2.118105	-2.261453
25	H	-6.566064	2.56715	-2.778459
26	C	-4.827387	1.295523	-2.961774
27	H	-4.970302	1.111595	-4.022141
28	C	-3.733396	0.728192	-2.299915
29	H	-3.022404	0.115275	-2.853702
30	C	-2.638324	-1.532227	0.224225
31	C	-3.959194	-1.656085	0.703665
32	H	-4.58487	-0.765283	0.736484
33	C	-4.493164	-2.87167	1.134448
34	H	-5.514586	-2.927348	1.495656
35	C	-3.680138	-4.013013	1.084446
36	H	-4.064459	-4.974098	1.414504
37	C	-2.382202	-3.934088	0.583785

38	H	-1.798809	-4.845934	0.518224
39	C	-1.825541	-2.708395	0.12843
40	C	0.322002	-3.918413	-0.236599
41	H	-0.051714	-4.735425	-0.874299
42	H	0.293374	-4.252777	0.807702
43	C	1.768588	-3.549798	-0.633392
44	H	2.391784	-3.392416	0.260066
45	H	2.214716	-4.362955	-1.22238
46	C	2.883775	-1.553734	-1.6798
47	C	3.895273	-2.151233	-2.450268
48	H	3.737434	-3.158486	-2.828983
49	C	5.067877	-1.450355	-2.753719
50	H	5.838658	-1.921842	-3.356119
51	C	5.233063	-0.133931	-2.300801
52	H	6.131903	0.422284	-2.548032
53	C	4.236357	0.464314	-1.51708
54	H	4.381433	1.476688	-1.146454
55	C	3.067151	-0.234226	-1.180251
56	C	2.483778	2.044158	0.547201
57	C	2.371083	3.157545	-0.313428
58	H	1.902331	3.044463	-1.292601
59	C	2.835014	4.413751	0.096301
60	H	2.744345	5.262027	-0.575323
61	C	3.40003	4.576981	1.370826
62	H	3.753744	5.553548	1.688914
63	C	3.497479	3.477296	2.235266
64	H	3.925235	3.599121	3.226329
65	C	3.042527	2.215501	1.827036
66	H	3.111505	1.373478	2.511511
67	C	1.966315	-0.701751	1.380323
68	C	3.232018	-1.176923	1.778727
69	H	4.124455	-0.856971	1.242279
70	C	3.348054	-2.068457	2.85311
71	H	4.328842	-2.425703	3.153475
72	C	2.200242	-2.498994	3.540393
73	H	2.292527	-3.191021	4.372566
74	C	0.938466	-2.028674	3.150374
75	H	0.041131	-2.350788	3.672795
76	C	0.826357	-1.135782	2.075249
77	H	-0.154866	-0.779873	1.77622

Table S16. DFT-optimized XYZ Coordinates for **7**^{monomer} in the S = 3/2 state (M06: LANL2DZ(p,d), Co, P; D95V, C, H, N).

Tag	Symbol	X	Y	Z
1	Co	-0.06403	0.451825	-1.604389
2	P	0.016915	-1.812238	-1.609312
3	P	1.944971	0.433013	-0.358961
4	P	-2.017336	0.372569	-0.277752
5	N	1.294886	-2.592733	-0.698713
6	N	-1.16575	-2.646702	-0.606711
7	C	2.656661	-2.27612	-0.876485
8	C	3.100135	-0.921375	-0.888419
9	C	4.454745	-0.657111	-1.160353
10	H	4.8014	0.372924	-1.191758
11	C	-2.550312	-2.42224	-0.718315
12	C	-4.476025	-0.945674	-0.871559
13	H	-4.904096	0.052393	-0.886149
14	C	2.003171	0.235834	1.482337
15	C	-3.092652	-1.101556	-0.676314
16	C	2.950803	1.967036	-0.598391
17	C	-3.10116	1.82169	-0.65847
18	C	-1.995654	0.322546	1.575149
19	C	-3.422868	-3.521107	-0.874683
20	H	-3.010545	-4.525897	-0.909357
21	C	2.692623	-0.794704	2.145658
22	H	3.237747	-1.544321	1.574626
23	C	2.722495	2.716343	-1.76822
24	H	1.959892	2.381407	-2.473531
25	C	-0.624119	-3.942306	-0.170857
26	H	-0.657984	-4.691615	-0.980967
27	H	-1.196031	-4.323699	0.684333
28	C	3.924392	2.401485	0.323011
29	H	4.105077	1.830904	1.232604
30	C	-1.743698	-0.942238	3.645281
31	H	-1.60583	-1.894893	4.148538
32	C	-4.798414	-3.335784	-1.025391
33	H	-5.446906	-4.198207	-1.15042
34	C	2.708502	-0.850024	3.547674
35	H	3.248038	-1.65026	4.046707
36	C	-1.85505	0.237791	4.394234
37	H	-1.812811	0.203103	5.479085

38	C	1.327115	1.207611	2.247079
39	H	0.785514	2.00919	1.743926
40	C	0.831988	-3.648427	0.218389
41	H	0.882653	-3.279479	1.255943
42	H	1.441403	-4.557285	0.143018
43	C	-1.815678	-0.9028	2.247356
44	H	-1.73431	-1.826754	1.677887
45	C	-5.330268	-2.040943	-1.048555
46	H	-6.393537	-1.880665	-1.195238
47	C	5.375432	-1.690843	-1.367802
48	H	6.415637	-1.45786	-1.572055
49	C	3.596808	-3.310569	-1.067353
50	H	3.253715	-4.342234	-1.070468
51	C	-4.229508	2.18299	0.107095
52	H	-4.495525	1.602693	0.988677
53	C	4.943829	-3.024013	-1.297427
54	H	5.649018	-3.836287	-1.448798
55	C	-2.064576	1.508618	2.333135
56	H	-2.174267	2.469471	1.834666
57	C	4.65838	3.568247	0.07582
58	H	5.40521	3.897806	0.792524
59	C	2.050864	0.131898	4.300468
60	H	2.072794	0.095757	5.38596
61	C	3.463958	3.880515	-2.015428
62	H	3.28119	4.451451	-2.920999
63	C	-5.00667	3.288927	-0.254253
64	H	-5.872229	3.559147	0.343714
65	C	4.431175	4.308513	-1.095471
66	H	5.002101	5.213046	-1.285463
67	C	-2.767587	2.588451	-1.790889
68	H	-1.892229	2.321036	-2.387157
69	C	-2.011908	1.463426	3.732004
70	H	-2.092482	2.38543	4.301595
71	C	1.362895	1.164431	3.644427
72	H	0.848385	1.92907	4.219255
73	C	-4.669867	4.045201	-1.38898
74	H	-5.274582	4.902816	-1.669401
75	C	-3.55137	3.693127	-2.155328
76	H	-3.283428	4.275238	-3.031776
77	H	0.222128	1.192099	-3.033727

Table S17. DFT-optimized XYZ Coordinates for **3** (B3LYP: LANL2DZ (p,d), Co, P; D95V, C, H, N).

Tag	Symbol	X	Y	Z
1	Co	1.36895	-0.139278	0.15276
2	P	2.835704	0.480459	-1.470408
3	P	0.09207	1.580026	-0.358856
4	P	-2.36786	1.531706	1.651425
5	N	0.080187	3.099717	0.459315
6	N	0.321429	2.375905	-1.866073
7	C	4.11862	-0.716214	-2.058102
8	C	3.725183	-2.053235	-2.302297
9	C	4.636679	-2.980257	-2.832627
10	C	5.960185	-2.587201	-3.115669
11	C	6.364583	-1.264394	-2.857474
12	C	5.449218	-0.330736	-2.335021
13	C	3.764906	2.035359	-1.068797
14	C	4.095354	2.303365	0.280781
15	C	4.826684	3.456364	0.622521
16	C	5.22841	4.361139	-0.379033
17	C	4.894521	4.107157	-1.724604
18	C	4.168956	2.952204	-2.068989
19	C	1.966558	0.922114	-3.062451
20	C	2.462656	0.468302	-4.306525
21	C	1.892657	0.878371	-5.523485
22	C	0.787863	1.746263	-5.517237
23	C	0.258812	2.186996	-4.295278
24	C	0.837872	1.793288	-3.070328
25	C	0.074936	3.848919	-1.813213
26	C	0.502073	4.251489	-0.395014
27	C	-0.144819	3.313493	1.855659
28	C	0.658374	4.255941	2.538528
29	C	0.431903	4.542596	3.893208
30	C	-0.580321	3.86374	4.597267
31	C	-1.377217	2.922441	3.925351
32	C	-1.192764	2.647463	2.550647
33	C	-3.773649	2.662638	1.237819
34	C	-5.023322	2.110594	0.866586
35	C	-6.114333	2.94642	0.580712
36	C	-5.970594	4.346605	0.641364
37	C	-4.726852	4.903707	0.98996

38	C	-3.634604	4.068368	1.289948
39	C	-3.021394	0.433909	2.993182
40	C	-4.221869	0.703198	3.692774
41	C	-4.636679	-0.135917	4.742531
42	C	-3.858429	-1.250005	5.110687
43	C	-2.661798	-1.523658	4.421145
44	C	-2.246365	-0.690928	3.367077
45	H	2.70797	-2.365981	-2.078651
46	H	4.323769	-4.004264	-3.019282
47	H	6.665657	-3.303175	-3.528538
48	H	7.383884	-0.953924	-3.071182
49	H	5.778086	0.688372	-2.155534
50	H	3.787953	1.620565	1.068879
51	H	5.084305	3.642436	1.661938
52	H	5.797479	5.249071	-0.116986
53	H	5.205533	4.799368	-2.502577
54	H	3.925467	2.770276	-3.112287
55	H	3.322195	-0.191524	-4.334278
56	H	2.315717	0.530302	-6.461251
57	H	0.337672	2.073353	-6.450298
58	H	-0.607136	2.843407	-4.287895
59	H	-0.982528	4.088041	-1.989187
60	H	0.679908	4.348755	-2.573902
61	H	1.588088	4.403407	-0.345033
62	H	-0.003323	5.1621	-0.059744
63	H	1.459784	4.764405	2.011332
64	H	1.045804	5.285599	4.395093
65	H	-0.759299	4.074494	5.647337
66	H	-2.165972	2.415959	4.472676
67	H	-5.15801	1.033804	0.81192
68	H	-7.071018	2.507331	0.312173
69	H	-6.817682	4.992201	0.426012
70	H	-4.609206	5.9826	1.047512
71	H	-2.695233	4.520546	1.592308
72	H	-4.82955	1.564122	3.434763
73	H	-5.557512	0.086869	5.274646
74	H	-4.176896	-1.891108	5.928311
75	H	-2.050521	-2.374198	4.704453
76	H	-1.309203	-0.905682	2.858019
77	Co	-1.36895	0.139278	0.15276

78	P	-2.835704	-0.480459	-1.470408
79	P	-0.09207	-1.580026	-0.358856
80	P	2.36786	-1.531706	1.651425
81	N	-0.080187	-3.099717	0.459315
82	N	-0.321429	-2.375905	-1.866073
83	C	-4.11862	0.716214	-2.058102
84	C	-3.725183	2.053235	-2.302297
85	C	-4.636679	2.980257	-2.832627
86	C	-5.960185	2.587201	-3.115669
87	C	-6.364583	1.264394	-2.857474
88	C	-5.449218	0.330736	-2.335021
89	C	-3.764906	-2.035359	-1.068797
90	C	-4.095354	-2.303365	0.280781
91	C	-4.826684	-3.456364	0.622521
92	C	-5.22841	-4.361139	-0.379033
93	C	-4.894521	-4.107157	-1.724604
94	C	-4.168956	-2.952204	-2.068989
95	C	-1.966558	-0.922114	-3.062451
96	C	-2.462656	-0.468302	-4.306525
97	C	-1.892657	-0.878371	-5.523485
98	C	-0.787863	-1.746263	-5.517237
99	C	-0.258812	-2.186996	-4.295278
100	C	-0.837872	-1.793288	-3.070328
101	C	-0.074936	-3.848919	-1.813213
102	C	-0.502073	-4.251489	-0.395014
103	C	0.144819	-3.313493	1.855659
104	C	-0.658374	-4.255941	2.538528
105	C	-0.431903	-4.542596	3.893208
106	C	0.580321	-3.86374	4.597267
107	C	1.377217	-2.922441	3.925351
108	C	1.192764	-2.647463	2.550647
109	C	3.773649	-2.662638	1.237819
110	C	5.023322	-2.110594	0.866586
111	C	6.114333	-2.94642	0.580712
112	C	5.970594	-4.346605	0.641364
113	C	4.726852	-4.903707	0.98996
114	C	3.634604	-4.068368	1.289948
115	C	3.021394	-0.433909	2.993182
116	C	4.221869	-0.703198	3.692774
117	C	4.636679	0.135917	4.742531

118	C	3.858429	1.250005	5.110687
119	C	2.661798	1.523658	4.421145
120	C	2.246365	0.690928	3.367077
121	H	-2.70797	2.365981	-2.078651
122	H	-4.323769	4.004264	-3.019282
123	H	-6.665657	3.303175	-3.528538
124	H	-7.383884	0.953924	-3.071182
125	H	-5.778086	-0.688372	-2.155534
126	H	-3.787953	-1.620565	1.068879
127	H	-5.084305	-3.642436	1.661938
128	H	-5.797479	-5.249071	-0.116986
129	H	-5.205533	-4.799368	-2.502577
130	H	-3.925467	-2.770276	-3.112287
131	H	-3.322195	0.191524	-4.334278
132	H	-2.315717	-0.530302	-6.461251
133	H	-0.337672	-2.073353	-6.450298
134	H	0.607136	-2.843407	-4.287895
135	H	0.982528	-4.088041	-1.989187
136	H	-0.679908	-4.348755	-2.573902
137	H	-1.588088	-4.403407	-0.345033
138	H	0.003323	-5.1621	-0.059744
139	H	-1.459784	-4.764405	2.011332
140	H	-1.045804	-5.285599	4.395093
141	H	0.759299	-4.074494	5.647337
142	H	2.165972	-2.415959	4.472676
143	H	5.15801	-1.033804	0.81192
144	H	7.071018	-2.507331	0.312173
145	H	6.817682	-4.992201	0.426012
146	H	4.609206	-5.9826	1.047512
147	H	2.695233	-4.520546	1.592308
148	H	4.82955	-1.564122	3.434763
149	H	5.557512	-0.086869	5.274646
150	H	4.176896	1.891108	5.928311
151	H	2.050521	2.374198	4.704453
152	H	1.309203	0.905682	2.858019

Table S18. DFT-optimized XYZ Coordinates for **3** (B3LYP: LANL2TZ (p,d), Co; LANL2DZ(p,d), P; D95V, C, H, N).

Tag	Symbol	X	Y	Z
1	Co	1.366731	-0.137282	0.154209
2	P	2.82016	0.465274	-1.477454
3	P	0.088326	1.578384	-0.355133
4	P	-2.359978	1.518806	1.657358
5	N	0.082244	3.092553	0.475633
6	N	0.318572	2.386278	-1.856793
7	C	4.085461	-0.744803	-2.077325
8	C	3.677734	-2.078513	-2.315271
9	C	4.57533	-3.013548	-2.855072
10	C	5.89818	-2.631429	-3.155249
11	C	6.316573	-1.311464	-2.9045
12	C	5.415427	-0.37	-2.371427
13	C	3.772707	2.004474	-1.070208
14	C	4.136667	2.245992	0.27586
15	C	4.889276	3.384057	0.619946
16	C	5.279843	4.300648	-0.375247
17	C	4.913084	4.07317	-1.716907
18	C	4.16596	2.932769	-2.063935
19	C	1.950121	0.925448	-3.063641
20	C	2.440578	0.475589	-4.311243
21	C	1.875069	0.90064	-5.524986
22	C	0.780773	1.781795	-5.512073
23	C	0.257279	2.219423	-4.286772
24	C	0.831248	1.809578	-3.064642
25	C	0.078056	3.85917	-1.79142
26	C	0.506202	4.24932	-0.369649
27	C	-0.134807	3.292862	1.874873
28	C	0.6715	4.227945	2.563723
29	C	0.449943	4.501339	3.922048
30	C	-0.560208	3.816198	4.622826
31	C	-1.359984	2.881696	3.944616
32	C	-1.180022	2.619962	2.567161
33	C	-3.749935	2.666233	1.233866
34	C	-4.9987	2.127619	0.840879
35	C	-6.079548	2.974609	0.549487
36	C	-5.9261	4.372927	0.626225
37	C	-4.68278	4.91699	0.996455

38	C	-3.600936	4.070196	1.302186
39	C	-3.039176	0.429656	2.993564
40	C	-4.249287	0.706881	3.673237
41	C	-4.68278	-0.125507	4.720835
42	C	-3.913922	-1.240085	5.1068
43	C	-2.707399	-1.520911	4.437647
44	C	-2.273104	-0.695375	3.385779
45	H	2.660774	-2.382259	-2.07952
46	H	4.252704	-4.035695	-3.035438
47	H	6.592712	-3.353826	-3.57539
48	H	7.335544	-1.009638	-3.131671
49	H	5.75462	0.64638	-2.196152
50	H	3.840674	1.55327	1.059546
51	H	5.171592	3.549829	1.656369
52	H	5.865076	5.177357	-0.111162
53	H	5.215239	4.774344	-2.490327
54	H	3.897983	2.770697	-3.104413
55	H	3.292846	-0.19326	-4.344352
56	H	2.293748	0.554325	-6.465317
57	H	0.334432	2.121153	-6.442611
58	H	-0.600805	2.885939	-4.274502
59	H	-0.978378	4.104685	-1.965092
60	H	0.685181	4.363439	-2.54753
61	H	1.592545	4.399947	-0.319507
62	H	0.002912	5.158737	-0.027727
63	H	1.470812	4.741835	2.038688
64	H	1.065678	5.239384	4.428983
65	H	-0.735895	4.017113	5.675375
66	H	-2.147706	2.371054	4.489329
67	H	-5.141049	1.052501	0.773388
68	H	-7.036023	2.545685	0.264265
69	H	-6.765573	5.026995	0.406673
70	H	-4.557812	5.994304	1.066651
71	H	-2.662226	4.511847	1.621681
72	H	-4.849714	1.56877	3.402096
73	H	-5.610558	0.103445	5.238047
74	H	-4.246849	-1.875737	5.92291
75	H	-2.103008	-2.371445	4.735104
76	H	-1.327823	-0.914735	2.893857
77	Co	-1.366731	0.137282	0.154209

78	P	-2.82016	-0.465274	-1.477454
79	P	-0.088326	-1.578384	-0.355133
80	P	2.359978	-1.518806	1.657358
81	N	-0.082244	-3.092553	0.475633
82	N	-0.318572	-2.386278	-1.856793
83	C	-4.085461	0.744803	-2.077325
84	C	-3.677734	2.078513	-2.315271
85	C	-4.57533	3.013548	-2.855072
86	C	-5.89818	2.631429	-3.155249
87	C	-6.316573	1.311464	-2.9045
88	C	-5.415427	0.37	-2.371427
89	C	-3.772707	-2.004474	-1.070208
90	C	-4.136667	-2.245992	0.27586
91	C	-4.889276	-3.384057	0.619946
92	C	-5.279843	-4.300648	-0.375247
93	C	-4.913084	-4.07317	-1.716907
94	C	-4.16596	-2.932769	-2.063935
95	C	-1.950121	-0.925448	-3.063641
96	C	-2.440578	-0.475589	-4.311243
97	C	-1.875069	-0.90064	-5.524986
98	C	-0.780773	-1.781795	-5.512073
99	C	-0.257279	-2.219423	-4.286772
100	C	-0.831248	-1.809578	-3.064642
101	C	-0.078056	-3.85917	-1.79142
102	C	-0.506202	-4.24932	-0.369649
103	C	0.134807	-3.292862	1.874873
104	C	-0.6715	-4.227945	2.563723
105	C	-0.449943	-4.501339	3.922048
106	C	0.560208	-3.816198	4.622826
107	C	1.359984	-2.881696	3.944616
108	C	1.180022	-2.619962	2.567161
109	C	3.749935	-2.666233	1.233866
110	C	4.9987	-2.127619	0.840879
111	C	6.079548	-2.974609	0.549487
112	C	5.9261	-4.372927	0.626225
113	C	4.68278	-4.91699	0.996455
114	C	3.600936	-4.070196	1.302186
115	C	3.039176	-0.429656	2.993564
116	C	4.249287	-0.706881	3.673237
117	C	4.68278	0.125507	4.720835

118	C	3.913922	1.240085	5.1068
119	C	2.707399	1.520911	4.437647
120	C	2.273104	0.695375	3.385779
121	H	-2.660774	2.382259	-2.07952
122	H	-4.252704	4.035695	-3.035438
123	H	-6.592712	3.353826	-3.57539
124	H	-7.335544	1.009638	-3.131671
125	H	-5.75462	-0.64638	-2.196152
126	H	-3.840674	-1.55327	1.059546
127	H	-5.171592	-3.549829	1.656369
128	H	-5.865076	-5.177357	-0.111162
129	H	-5.215239	-4.774344	-2.490327
130	H	-3.897983	-2.770697	-3.104413
131	H	-3.292846	0.19326	-4.344352
132	H	-2.293748	-0.554325	-6.465317
133	H	-0.334432	-2.121153	-6.442611
134	H	0.600805	-2.885939	-4.274502
135	H	0.978378	-4.104685	-1.965092
136	H	-0.685181	-4.363439	-2.54753
137	H	-1.592545	-4.399947	-0.319507
138	H	-0.002912	-5.158737	-0.027727
139	H	-1.470812	-4.741835	2.038688
140	H	-1.065678	-5.239384	4.428983
141	H	0.735895	-4.017113	5.675375
142	H	2.147706	-2.371054	4.489329
143	H	5.141049	-1.052501	0.773388
144	H	7.036023	-2.545685	0.264265
145	H	6.765573	-5.026995	0.406673
146	H	4.557812	-5.994304	1.066651
147	H	2.662226	-4.511847	1.621681
148	H	4.849714	-1.56877	3.402096
149	H	5.610558	-0.103445	5.238047
150	H	4.246849	1.875737	5.92291
151	H	2.103008	2.371445	4.735104
152	H	1.327823	0.914735	2.893857

Table S19. DFT-optimized XYZ Coordinates for **3** (B3LYP: Def2-tzvp, Co, P; Def2-svp, C, H, N).

Tag	Symbol	X	Y	Z
1	Co	1.348778	-0.136919	0.146844
2	P	2.792152	0.509074	-1.462115
3	P	0.081344	1.575486	-0.323828
4	P	-2.36187	1.503499	1.63378
5	N	0.086314	3.049524	0.514574
6	N	0.278826	2.379464	-1.798746
7	C	4.058479	-0.663446	-2.073617
8	C	3.66173	-1.981571	-2.361034
9	C	4.563101	-2.889501	-2.917604
10	C	5.880974	-2.497433	-3.178913
11	C	6.290211	-1.195893	-2.877625
12	C	5.384622	-0.280061	-2.330516
13	C	3.717392	2.040366	-1.048589
14	C	4.114824	2.25516	0.283047
15	C	4.84433	3.395751	0.632682
16	C	5.178314	4.340666	-0.342572
17	C	4.783179	4.13878	-1.669564
18	C	4.058479	2.996702	-2.022648
19	C	1.913005	0.966375	-3.021058
20	C	2.401498	0.544938	-4.270214
21	C	1.821333	0.965255	-5.468627
22	C	0.714552	1.813285	-5.438643
23	C	0.195389	2.226851	-4.212534
24	C	0.782329	1.822856	-3.002628
25	C	0.034719	3.829946	-1.715358
26	C	0.482642	4.20376	-0.309389
27	C	-0.13714	3.227878	1.900915
28	C	0.667172	4.137016	2.610904
29	C	0.430082	4.395453	3.961172
30	C	-0.59651	3.727006	4.632742
31	C	-1.395587	2.819808	3.935414
32	C	-1.197773	2.569019	2.567009
33	C	-3.707248	2.661709	1.184845
34	C	-4.948792	2.149847	0.764462
35	C	-6.004096	3.009745	0.458851
36	C	-5.829419	4.395382	0.541983
37	C	-4.594748	4.914747	0.937409

38	C	-3.541406	4.054873	1.264856
39	C	-3.07462	0.430735	2.938984
40	C	-4.302318	0.700372	3.570642
41	C	-4.764909	-0.126078	4.598827
42	C	-4.008409	-1.225524	5.01412
43	C	-2.783371	-1.497394	4.397159
44	C	-2.319669	-0.677826	3.365188
45	H	2.635131	-2.292895	-2.157455
46	H	4.242082	-3.909207	-3.143258
47	H	6.587859	-3.20746	-3.614628
48	H	7.318323	-0.884362	-3.077366
49	H	5.718052	0.736104	-2.115322
50	H	3.857971	1.529822	1.057764
51	H	5.152725	3.543548	1.670334
52	H	5.74926	5.231779	-0.070862
53	H	5.046477	4.871298	-2.436488
54	H	3.764127	2.85061	-3.063523
55	H	3.274149	-0.10519	-4.313983
56	H	2.242408	0.634725	-6.420478
57	H	0.248897	2.152099	-6.366826
58	H	-0.678697	2.880181	-4.18839
59	H	-1.031118	4.074371	-1.869308
60	H	0.622734	4.349173	-2.483632
61	H	1.573405	4.36684	-0.275462
62	H	-0.019269	5.110937	0.056386
63	H	1.487409	4.644838	2.101864
64	H	1.05689	5.117753	4.489603
65	H	-0.785922	3.919759	5.690744
66	H	-2.207866	2.31662	4.461211
67	H	-5.106475	1.072607	0.693152
68	H	-6.9671	2.595433	0.153239
69	H	-6.657054	5.06785	0.30443
70	H	-4.452749	5.995519	1.012292
71	H	-2.597755	4.480671	1.607588
72	H	-4.900037	1.562172	3.274454
73	H	-5.718195	0.099008	5.082894
74	H	-4.369699	-1.865222	5.822844
75	H	-2.18028	-2.346938	4.720495
76	H	-1.352258	-0.892562	2.904101
77	Co	-1.348778	0.136919	0.146844

78	P	-2.792152	-0.509074	-1.462115
79	P	-0.081344	-1.575486	-0.323828
80	P	2.36187	-1.503499	1.63378
81	N	-0.086314	-3.049524	0.514574
82	N	-0.278826	-2.379464	-1.798746
83	C	-4.058479	0.663446	-2.073617
84	C	-3.66173	1.981571	-2.361034
85	C	-4.563101	2.889501	-2.917604
86	C	-5.880974	2.497433	-3.178913
87	C	-6.290211	1.195893	-2.877625
88	C	-5.384622	0.280061	-2.330516
89	C	-3.717392	-2.040366	-1.048589
90	C	-4.114824	-2.25516	0.283047
91	C	-4.84433	-3.395751	0.632682
92	C	-5.178314	-4.340666	-0.342572
93	C	-4.783179	-4.13878	-1.669564
94	C	-4.058479	-2.996702	-2.022648
95	C	-1.913005	-0.966375	-3.021058
96	C	-2.401498	-0.544938	-4.270214
97	C	-1.821333	-0.965255	-5.468627
98	C	-0.714552	-1.813285	-5.438643
99	C	-0.195389	-2.226851	-4.212534
100	C	-0.782329	-1.822856	-3.002628
101	C	-0.034719	-3.829946	-1.715358
102	C	-0.482642	-4.20376	-0.309389
103	C	0.13714	-3.227878	1.900915
104	C	-0.667172	-4.137016	2.610904
105	C	-0.430082	-4.395453	3.961172
106	C	0.59651	-3.727006	4.632742
107	C	1.395587	-2.819808	3.935414
108	C	1.197773	-2.569019	2.567009
109	C	3.707248	-2.661709	1.184845
110	C	4.948792	-2.149847	0.764462
111	C	6.004096	-3.009745	0.458851
112	C	5.829419	-4.395382	0.541983
113	C	4.594748	-4.914747	0.937409
114	C	3.541406	-4.054873	1.264856
115	C	3.07462	-0.430735	2.938984
116	C	4.302318	-0.700372	3.570642
117	C	4.764909	0.126078	4.598827

118	C	4.008409	1.225524	5.01412
119	C	2.783371	1.497394	4.397159
120	C	2.319669	0.677826	3.365188
121	H	-2.635131	2.292895	-2.157455
122	H	-4.242082	3.909207	-3.143258
123	H	-6.587859	3.20746	-3.614628
124	H	-7.318323	0.884362	-3.077366
125	H	-5.718052	-0.736104	-2.115322
126	H	-3.857971	-1.529822	1.057764
127	H	-5.152725	-3.543548	1.670334
128	H	-5.74926	-5.231779	-0.070862
129	H	-5.046477	-4.871298	-2.436488
130	H	-3.764127	-2.85061	-3.063523
131	H	-3.274149	0.10519	-4.313983
132	H	-2.242408	-0.634725	-6.420478
133	H	-0.248897	-2.152099	-6.366826
134	H	0.678697	-2.880181	-4.18839
135	H	1.031118	-4.074371	-1.869308
136	H	-0.622734	-4.349173	-2.483632
137	H	-1.573405	-4.36684	-0.275462
138	H	0.019269	-5.110937	0.056386
139	H	-1.487409	-4.644838	2.101864
140	H	-1.05689	-5.117753	4.489603
141	H	0.785922	-3.919759	5.690744
142	H	2.207866	-2.31662	4.461211
143	H	5.106475	-1.072607	0.693152
144	H	6.9671	-2.595433	0.153239
145	H	6.657054	-5.06785	0.30443
146	H	4.452749	-5.995519	1.012292
147	H	2.597755	-4.480671	1.607588
148	H	4.900037	-1.562172	3.274454
149	H	5.718195	-0.099008	5.082894
150	H	4.369699	1.865222	5.822844
151	H	2.18028	2.346938	4.720495
152	H	1.352258	0.892562	2.904101

Table S20. DFT-optimized XYZ Coordinates for **3** (wB97XD: def2SVP on all atoms).

Tag	Symbol	X	Y	Z
1	Co	1.047742	0.759259	0.177237
2	P	1.77101	2.145126	-1.364802
3	P	-0.970021	1.192283	-0.454282
4	P	-2.665807	-0.321386	1.601258
5	N	-1.988379	2.365769	0.235079
6	N	-1.265789	1.799095	-2.006735
7	C	3.53667	2.203962	-1.800429
8	C	4.200015	0.980243	-1.955992
9	C	5.523256	0.94803	-2.379609
10	C	6.198976	2.142224	-2.638008
11	C	5.549349	3.362697	-2.467807
12	C	4.218093	3.397136	-2.051342
13	C	1.253727	3.857465	-0.978389
14	C	1.121074	4.214392	0.369945
15	C	0.677948	5.487768	0.722162
16	C	0.356709	6.412114	-0.272091
17	C	0.485054	6.062752	-1.617526
18	C	0.930897	4.7904	-1.971842
19	C	0.994707	1.839892	-3.005756
20	C	1.763078	1.851974	-4.17648
21	C	1.174486	1.75364	-5.433927
22	C	-0.205042	1.612669	-5.537788
23	C	-0.984322	1.564562	-4.387706
24	C	-0.403933	1.693278	-3.122881
25	C	-2.394924	2.730221	-2.057186
26	C	-2.384123	3.418282	-0.702802
27	C	-2.348398	2.472323	1.591737
28	C	-2.466616	3.745142	2.169624
29	C	-2.933579	3.891531	3.470996
30	C	-3.255968	2.770419	4.235216
31	C	-3.109891	1.503971	3.679478
32	C	-2.673603	1.337229	2.359202
33	C	-4.428025	-0.640802	1.272097
34	C	-4.856527	-1.958975	1.061808
35	C	-6.197236	-2.228997	0.814762
36	C	-7.11956	-1.18366	0.748596
37	C	-6.696613	0.13012	0.93232
38	C	-5.355166	0.403396	1.19912

39	C	-2.203705	-1.454352	2.956399
40	C	-3.136599	-2.111704	3.768703
41	C	-2.701051	-2.966082	4.779295
42	C	-1.337223	-3.172338	4.986049
43	C	-0.403933	-2.517396	4.184628
44	C	-0.83428	-1.661451	3.174918
45	H	3.670672	0.047936	-1.741628
46	H	6.036368	-0.008071	-2.49816
47	H	7.239401	2.119472	-2.968112
48	H	6.078733	4.296824	-2.665332
49	H	3.714172	4.358409	-1.929662
50	H	1.354461	3.494056	1.159362
51	H	0.583602	5.754718	1.776666
52	H	0.008912	7.41062	0.000612
53	H	0.237701	6.787065	-2.396121
54	H	1.02023	4.521177	-3.027279
55	H	2.844674	1.972936	-4.111327
56	H	1.797562	1.791459	-6.328936
57	H	-0.680751	1.527851	-6.516544
58	H	-2.064995	1.432943	-4.464227
59	H	-3.34949	2.203404	-2.230133
60	H	-2.244717	3.44705	-2.874699
61	H	-1.666923	4.256711	-0.692865
62	H	-3.378011	3.799922	-0.430356
63	H	-2.195974	4.628282	1.589787
64	H	-3.037547	4.892449	3.894364
65	H	-3.619964	2.881142	5.257665
66	H	-3.362606	0.624408	4.275614
67	H	-4.142361	-2.785447	1.098881
68	H	-6.52349	-3.259578	0.665358
69	H	-8.172539	-1.396656	0.554216
70	H	-7.416341	0.949513	0.884237
71	H	-5.041245	1.435582	1.368113
72	H	-4.206703	-1.958654	3.617572
73	H	-3.433717	-3.470497	5.412132
74	H	-1.001062	-3.841143	5.780811
75	H	0.663275	-2.663981	4.346483
76	H	-0.09531	-1.138588	2.560131
77	Co	-1.047742	-0.759259	0.177237
78	P	-1.77101	-2.145126	-1.364802

79	P	0.970021	-1.192283	-0.454282
80	P	2.665807	0.321386	1.601258
81	N	1.988379	-2.365769	0.235079
82	N	1.265789	-1.799095	-2.006735
83	C	-3.53667	-2.203962	-1.800429
84	C	-4.200015	-0.980243	-1.955992
85	C	-5.523256	-0.94803	-2.379609
86	C	-6.198976	-2.142224	-2.638008
87	C	-5.549349	-3.362697	-2.467807
88	C	-4.218093	-3.397136	-2.051342
89	C	-1.253727	-3.857465	-0.978389
90	C	-1.121074	-4.214392	0.369945
91	C	-0.677948	-5.487768	0.722162
92	C	-0.356709	-6.412114	-0.272091
93	C	-0.485054	-6.062752	-1.617526
94	C	-0.930897	-4.7904	-1.971842
95	C	-0.994707	-1.839892	-3.005756
96	C	-1.763078	-1.851974	-4.17648
97	C	-1.174486	-1.75364	-5.433927
98	C	0.205042	-1.612669	-5.537788
99	C	0.984322	-1.564562	-4.387706
100	C	0.403933	-1.693278	-3.122881
101	C	2.394924	-2.730221	-2.057186
102	C	2.384123	-3.418282	-0.702802
103	C	2.348398	-2.472323	1.591737
104	C	2.466616	-3.745142	2.169624
105	C	2.933579	-3.891531	3.470996
106	C	3.255968	-2.770419	4.235216
107	C	3.109891	-1.503971	3.679478
108	C	2.673603	-1.337229	2.359202
109	C	4.428025	0.640802	1.272097
110	C	4.856527	1.958975	1.061808
111	C	6.197236	2.228997	0.814762
112	C	7.11956	1.18366	0.748596
113	C	6.696613	-0.13012	0.93232
114	C	5.355166	-0.403396	1.19912
115	C	2.203705	1.454352	2.956399
116	C	3.136599	2.111704	3.768703
117	C	2.701051	2.966082	4.779295
118	C	1.337223	3.172338	4.986049

119	C	0.403933	2.517396	4.184628
120	C	0.83428	1.661451	3.174918
121	H	-3.670672	-0.047936	-1.741628
122	H	-6.036368	0.008071	-2.49816
123	H	-7.239401	-2.119472	-2.968112
124	H	-6.078733	-4.296824	-2.665332
125	H	-3.714172	-4.358409	-1.929662
126	H	-1.354461	-3.494056	1.159362
127	H	-0.583602	-5.754718	1.776666
128	H	-0.008912	-7.41062	0.000612
129	H	-0.237701	-6.787065	-2.396121
130	H	-1.02023	-4.521177	-3.027279
131	H	-2.844674	-1.972936	-4.111327
132	H	-1.797562	-1.791459	-6.328936
133	H	0.680751	-1.527851	-6.516544
134	H	2.064995	-1.432943	-4.464227
135	H	3.34949	-2.203404	-2.230133
136	H	2.244717	-3.44705	-2.874699
137	H	1.666923	-4.256711	-0.692865
138	H	3.378011	-3.799922	-0.430356
139	H	2.195974	-4.628282	1.589787
140	H	3.037547	-4.892449	3.894364
141	H	3.619964	-2.881142	5.257665
142	H	3.362606	-0.624408	4.275614
143	H	4.142361	2.785447	1.098881
144	H	6.52349	3.259578	0.665358
145	H	8.172539	1.396656	0.554216
146	H	7.416341	-0.949513	0.884237
147	H	5.041245	-1.435582	1.368113
148	H	4.206703	1.958654	3.617572
149	H	3.433717	3.470497	5.412132
150	H	1.001062	3.841143	5.780811
151	H	-0.663275	2.663981	4.346483
152	H	0.09531	1.138588	2.560131

Table S21. DFT-optimized XYZ Coordinates for **3** (wB97XD: LANL2DZ(p,d), Co, P; D95V, C, H, N).

Tag	Symbol	X	Y	Z
1	Co	1.055962	0.779057	0.173831
2	P	1.747099	2.203985	-1.373142
3	P	-0.983135	1.211679	-0.431515
4	P	-2.69405	-0.354884	1.594641
5	N	-2.006028	2.37684	0.277193
6	N	-1.297759	1.827388	-1.982768
7	C	3.51636	2.280008	-1.826283
8	C	4.190622	1.055385	-2.001977
9	C	5.517634	1.035775	-2.439788
10	C	6.187219	2.243714	-2.698442
11	C	5.525713	3.465301	-2.510662
12	C	4.190622	3.486104	-2.078591
13	C	1.219633	3.920575	-0.98505
14	C	1.09517	4.284461	0.370671
15	C	0.658678	5.5684	0.724189
16	C	0.335296	6.498817	-0.276037
17	C	0.454583	6.141936	-1.629696
18	C	0.895506	4.859342	-1.984066
19	C	0.960156	1.893937	-3.017802
20	C	1.718255	1.911301	-4.203814
21	C	1.111253	1.789886	-5.459419
22	C	-0.274696	1.614874	-5.547001
23	C	-1.042924	1.561528	-4.380124
24	C	-0.442012	1.7187	-3.122869
25	C	-2.438974	2.775819	-2.02934
26	C	-2.430777	3.451191	-0.654478
27	C	-2.378672	2.456883	1.647988
28	C	-2.495882	3.724861	2.248222
29	C	-2.962261	3.846719	3.560556
30	C	-3.280886	2.70141	4.306584
31	C	-3.137915	1.438704	3.721772
32	C	-2.705802	1.297941	2.388975
33	C	-4.464439	-0.664184	1.255758
34	C	-4.905428	-1.985782	1.041123
35	C	-6.252962	-2.244909	0.776861
36	C	-7.172137	-1.185826	0.701594
37	C	-6.735664	0.132064	0.891793

38	C	-5.386759	0.394027	1.17145
39	C	-2.236076	-1.505091	2.946756
40	C	-3.175005	-2.181622	3.749496
41	C	-2.740214	-3.035896	4.771303
42	C	-1.368185	-3.219914	5.003355
43	C	-0.428597	-2.543982	4.21163
44	C	-0.859132	-1.69277	3.188079
45	H	3.674983	0.122492	-1.787896
46	H	6.03414	0.091133	-2.567886
47	H	7.216922	2.230522	-3.037681
48	H	6.041358	4.398603	-2.706824
49	H	3.686767	4.437974	-1.945229
50	H	1.330508	3.570721	1.156372
51	H	0.577897	5.839431	1.771207
52	H	0.001729	7.494545	-0.00576
53	H	0.213498	6.861764	-2.403841
54	H	0.982353	4.593583	-3.033345
55	H	2.791357	2.051877	-4.156475
56	H	1.717124	1.836058	-6.35672
57	H	-0.755544	1.510356	-6.512797
58	H	-2.114801	1.40502	-4.440024
59	H	-3.385331	2.253028	-2.209071
60	H	-2.277398	3.499114	-2.830362
61	H	-1.726547	4.290994	-0.635735
62	H	-3.424141	3.807529	-0.372379
63	H	-2.229795	4.613256	1.686751
64	H	-3.069012	4.831209	4.001773
65	H	-3.640852	2.790585	5.324387
66	H	-3.387299	0.555021	4.299855
67	H	-4.205589	-2.815181	1.084243
68	H	-6.583921	-3.265517	0.6231
69	H	-8.217802	-1.388843	0.499534
70	H	-7.442996	0.952223	0.840891
71	H	-5.071419	1.417724	1.346598
72	H	-4.238605	-2.043867	3.588451
73	H	-3.469777	-3.54801	5.388395
74	H	-1.036427	-3.875912	5.800391
75	H	0.631237	-2.667435	4.396088
76	H	-0.119953	-1.158519	2.593523
77	27	-1.055962	-0.779057	0.173831

78	P	-1.747099	-2.203985	-1.373142
79	P	0.983135	-1.211679	-0.431515
80	P	2.69405	0.354884	1.594641
81	N	2.006028	-2.37684	0.277193
82	N	1.297759	-1.827388	-1.982768
83	C	-3.51636	-2.280008	-1.826283
84	C	-4.190622	-1.055385	-2.001977
85	C	-5.517634	-1.035775	-2.439788
86	C	-6.187219	-2.243714	-2.698442
87	C	-5.525713	-3.465301	-2.510662
88	C	-4.190622	-3.486104	-2.078591
89	C	-1.219633	-3.920575	-0.98505
90	C	-1.09517	-4.284461	0.370671
91	C	-0.658678	-5.5684	0.724189
92	C	-0.335296	-6.498817	-0.276037
93	C	-0.454583	-6.141936	-1.629696
94	C	-0.895506	-4.859342	-1.984066
95	C	-0.960156	-1.893937	-3.017802
96	C	-1.718255	-1.911301	-4.203814
97	C	-1.111253	-1.789886	-5.459419
98	C	0.274696	-1.614874	-5.547001
99	C	1.042924	-1.561528	-4.380124
100	C	0.442012	-1.7187	-3.122869
101	C	2.438974	-2.775819	-2.02934
102	C	2.430777	-3.451191	-0.654478
103	C	2.378672	-2.456883	1.647988
104	C	2.495882	-3.724861	2.248222
105	C	2.962261	-3.846719	3.560556
106	C	3.280886	-2.70141	4.306584
107	C	3.137915	-1.438704	3.721772
108	C	2.705802	-1.297941	2.388975
109	C	4.464439	0.664184	1.255758
110	C	4.905428	1.985782	1.041123
111	C	6.252962	2.244909	0.776861
112	C	7.172137	1.185826	0.701594
113	C	6.735664	-0.132064	0.891793
114	C	5.386759	-0.394027	1.17145
115	C	2.236076	1.505091	2.946756
116	C	3.175005	2.181622	3.749496
117	C	2.740214	3.035896	4.771303

118	C	1.368185	3.219914	5.003355
119	C	0.428597	2.543982	4.21163
120	C	0.859132	1.69277	3.188079
121	H	-3.674983	-0.122492	-1.787896
122	H	-6.03414	-0.091133	-2.567886
123	H	-7.216922	-2.230522	-3.037681
124	H	-6.041358	-4.398603	-2.706824
125	H	-3.686767	-4.437974	-1.945229
126	H	-1.330508	-3.570721	1.156372
127	H	-0.577897	-5.839431	1.771207
128	H	-0.001729	-7.494545	-0.00576
129	H	-0.213498	-6.861764	-2.403841
130	H	-0.982353	-4.593583	-3.033345
131	H	-2.791357	-2.051877	-4.156475
132	H	-1.717124	-1.836058	-6.35672
133	H	0.755544	-1.510356	-6.512797
134	H	2.114801	-1.40502	-4.440024
135	H	3.385331	-2.253028	-2.209071
136	H	2.277398	-3.499114	-2.830362
137	H	1.726547	-4.290994	-0.635735
138	H	3.424141	-3.807529	-0.372379
139	H	2.229795	-4.613256	1.686751
140	H	3.069012	-4.831209	4.001773
141	H	3.640852	-2.790585	5.324387
142	H	3.387299	-0.555021	4.299855
143	H	4.205589	2.815181	1.084243
144	H	6.583921	3.265517	0.6231
145	H	8.217802	1.388843	0.499534
146	H	7.442996	-0.952223	0.840891
147	H	5.071419	-1.417724	1.346598
148	H	4.238605	2.043867	3.588451
149	H	3.469777	3.54801	5.388395
150	H	1.036427	3.875912	5.800391
151	H	-0.631237	2.667435	4.396088
152	H	0.119953	1.158519	2.593523

Table S22. DFT-optimized XYZ Coordinates for **3** (wB97XD: LANL2TZ(p,d), Co; LANL2DZ(p,d), P; D95V, C, H, N).

Tag	Symbol	X	Y	Z
1	Co	-1.050423	-0.779193	0.170103
2	P	-1.750951	-2.19615	-1.37461
3	P	0.986204	-1.204691	-0.448224
4	P	2.677745	0.359561	1.601806
5	N	2.01317	-2.368612	0.258763
6	N	1.293357	-1.82341	-2.000335
7	C	-3.521892	-2.275509	-1.820585
8	C	-4.200762	-1.052619	-1.989739
9	C	-5.529254	-1.036019	-2.422848
10	C	-6.195589	-2.245247	-2.683698
11	C	-5.529254	-3.465223	-2.5028
12	C	-4.192779	-3.482967	-2.075173
13	C	-1.219847	-3.912177	-0.987892
14	C	-1.088494	-4.277113	0.366917
15	C	-0.652337	-5.561711	0.717458
16	C	-0.336336	-6.492309	-0.284861
17	C	-0.462166	-6.134484	-1.637661
18	C	-0.90261	-4.850955	-1.989054
19	C	-0.970753	-1.885642	-3.022497
20	C	-1.735433	-1.900943	-4.204221
21	C	-1.135095	-1.785484	-5.463458
22	C	0.251421	-1.619417	-5.559172
23	C	1.026238	-1.567221	-4.396707
24	C	0.431782	-1.71727	-3.135477
25	C	2.437937	-2.766929	-2.050255
26	C	2.436885	-3.441551	-0.674837
27	C	2.379989	-2.455051	1.630602
28	C	2.502437	-3.726442	2.222822
29	C	2.964692	-3.855249	3.535885
30	C	3.274727	-2.713714	4.291072
31	C	3.125114	-1.447894	3.714992
32	C	2.69601	-1.299688	2.382174
33	C	4.44807	0.67566	1.265385
34	C	4.883063	1.999978	1.055371
35	C	6.230104	2.266919	0.797235
36	C	7.155382	1.212945	0.72446
37	C	6.725238	-0.107524	0.910663

38	C	5.376434	-0.377251	1.183671
39	C	2.224284	1.500759	2.963584
40	C	3.167789	2.162449	3.773399
41	C	2.738937	3.01098	4.802286
42	C	1.368177	3.204722	5.033854
43	C	0.424126	2.543891	4.234808
44	C	0.848728	1.697551	3.204763
45	H	-3.687775	-0.11865	-1.774446
46	H	-6.049411	-0.092685	-2.545738
47	H	-7.226469	-2.234266	-3.019415
48	H	-6.042338	-4.39957	-2.700633
49	H	-3.685526	-4.433665	-1.946669
50	H	-1.319412	-3.564338	1.154947
51	H	-0.566226	-5.833216	1.763927
52	H	-0.00326	-7.488792	-0.016802
53	H	-0.226468	-6.854248	-2.413518
54	H	-0.994471	-4.584492	-3.037722
55	H	-2.80896	-2.035769	-4.150849
56	H	-1.746397	-1.829873	-6.357143
57	H	0.727601	-1.520311	-6.527857
58	H	2.098466	-1.416012	-4.463188
59	H	3.381913	-2.241079	-2.233677
60	H	2.276683	-3.49186	-2.849897
61	H	1.734649	-4.283061	-0.654049
62	H	3.432185	-3.795796	-0.39677
63	H	2.244289	-4.612758	1.654499
64	H	3.075497	-4.842379	3.970166
65	H	3.632705	-2.808061	5.309109
66	H	3.366678	-0.567018	4.300572
67	H	4.178797	2.825737	1.098222
68	H	6.556379	3.28957	0.647018
69	H	8.200834	1.422001	0.52748
70	H	7.437222	-0.923767	0.861724
71	H	5.065909	-1.402957	1.355383
72	H	4.230442	2.018245	3.611776
73	H	3.471978	3.511628	5.424646
74	H	1.040709	3.856848	5.835829
75	H	-0.63481	2.675441	4.418583
76	H	0.10605	1.173952	2.605342
77	Co	1.050423	0.779193	0.170103

78	P	1.750951	2.19615	-1.37461
79	P	-0.986204	1.204691	-0.448224
80	P	-2.677745	-0.359561	1.601806
81	N	-2.01317	2.368612	0.258763
82	N	-1.293357	1.82341	-2.000335
83	C	3.521892	2.275509	-1.820585
84	C	4.200762	1.052619	-1.989739
85	C	5.529254	1.036019	-2.422848
86	C	6.195589	2.245247	-2.683698
87	C	5.529254	3.465223	-2.5028
88	C	4.192779	3.482967	-2.075173
89	C	1.219847	3.912177	-0.987892
90	C	1.088494	4.277113	0.366917
91	C	0.652337	5.561711	0.717458
92	C	0.336336	6.492309	-0.284861
93	C	0.462166	6.134484	-1.637661
94	C	0.90261	4.850955	-1.989054
95	C	0.970753	1.885642	-3.022497
96	C	1.735433	1.900943	-4.204221
97	C	1.135095	1.785484	-5.463458
98	C	-0.251421	1.619417	-5.559172
99	C	-1.026238	1.567221	-4.396707
100	C	-0.431782	1.71727	-3.135477
101	C	-2.437937	2.766929	-2.050255
102	C	-2.436885	3.441551	-0.674837
103	C	-2.379989	2.455051	1.630602
104	C	-2.502437	3.726442	2.222822
105	C	-2.964692	3.855249	3.535885
106	C	-3.274727	2.713714	4.291072
107	C	-3.125114	1.447894	3.714992
108	C	-2.69601	1.299688	2.382174
109	C	-4.44807	-0.67566	1.265385
110	C	-4.883063	-1.999978	1.055371
111	C	-6.230104	-2.266919	0.797235
112	C	-7.155382	-1.212945	0.72446
113	C	-6.725238	0.107524	0.910663
114	C	-5.376434	0.377251	1.183671
115	C	-2.224284	-1.500759	2.963584
116	C	-3.167789	-2.162449	3.773399
117	C	-2.738937	-3.01098	4.802286

118	C	-1.368177	-3.204722	5.033854
119	C	-0.424126	-2.543891	4.234808
120	C	-0.848728	-1.697551	3.204763
121	H	3.687775	0.11865	-1.774446
122	H	6.049411	0.092685	-2.545738
123	H	7.226469	2.234266	-3.019415
124	H	6.042338	4.39957	-2.700633
125	H	3.685526	4.433665	-1.946669
126	H	1.319412	3.564338	1.154947
127	H	0.566226	5.833216	1.763927
128	H	0.00326	7.488792	-0.016802
129	H	0.226468	6.854248	-2.413518
130	H	0.994471	4.584492	-3.037722
131	H	2.80896	2.035769	-4.150849
132	H	1.746397	1.829873	-6.357143
133	H	-0.727601	1.520311	-6.527857
134	H	-2.098466	1.416012	-4.463188
135	H	-3.381913	2.241079	-2.233677
136	H	-2.276683	3.49186	-2.849897
137	H	-1.734649	4.283061	-0.654049
138	H	-3.432185	3.795796	-0.39677
139	H	-2.244289	4.612758	1.654499
140	H	-3.075497	4.842379	3.970166
141	H	-3.632705	2.808061	5.309109
142	H	-3.366678	0.567018	4.300572
143	H	-4.178797	-2.825737	1.098222
144	H	-6.556379	-3.28957	0.647018
145	H	-8.200834	-1.422001	0.52748
146	H	-7.437222	0.923767	0.861724
147	H	-5.065909	1.402957	1.355383
148	H	-4.230442	-2.018245	3.611776
149	H	-3.471978	-3.511628	5.424646
150	H	-1.040709	-3.856848	5.835829
151	H	0.63481	-2.675441	4.418583
152	H	-0.10605	-1.173952	2.605342

Table S23. DFT-optimized XYZ Coordinates for **3** (PBE0: LANL2DZ(p,d), Co, P; D95V, C, H, N).

Tag	Symbol	X	Y	Z
1	Co	-1.023787	-0.859043	0.16288
2	P	-1.626698	-2.317472	-1.410625
3	P	1.057824	-1.148725	-0.411159
4	P	2.700658	0.564265	1.601685
5	N	2.173378	-2.226363	0.329679
6	N	1.426619	-1.8088	-1.947404
7	C	-3.385911	-2.469825	-1.925171
8	C	-4.120119	-1.285307	-2.135024
9	C	-5.430913	-1.341027	-2.620887
10	C	-6.026919	-2.583338	-2.892699
11	C	-5.307834	-3.766075	-2.668677
12	C	-3.990203	-3.71261	-2.189662
13	C	-1.083677	-4.034613	-1.012123
14	C	-1.051678	-4.431943	0.340065
15	C	-0.663307	-5.733619	0.688135
16	C	-0.29467	-6.647964	-0.310715
17	C	-0.31608	-6.256081	-1.659338
18	C	-0.709248	-4.957103	-2.010529
19	C	-0.797757	-1.994443	-3.037139
20	C	-1.524633	-2.054669	-4.242234
21	C	-0.893077	-1.928715	-5.485404
22	C	0.489192	-1.713053	-5.542332
23	C	1.226066	-1.620637	-4.357979
24	C	0.601639	-1.770982	-3.108216
25	C	2.649064	-2.648566	-1.957423
26	C	2.670997	-3.292245	-0.57355
27	C	2.526468	-2.263736	1.704239
28	C	2.702377	-3.512499	2.332666
29	C	3.125663	-3.585824	3.663102
30	C	3.346169	-2.411806	4.39946
31	C	3.158451	-1.169061	3.784177
32	C	2.769675	-1.075092	2.433658
33	C	4.471395	0.912946	1.250243
34	C	4.874834	2.234635	0.968178
35	C	6.22252	2.526348	0.733743
36	C	7.181162	1.500787	0.756211
37	C	6.783553	0.181837	1.014473

38	C	5.435629	-0.112666	1.264668
39	C	2.251857	1.718148	2.964219
40	C	3.20283	2.442294	3.711461
41	C	2.788491	3.267067	4.765933
42	C	1.426619	3.375753	5.086488
43	C	0.475708	2.655467	4.348478
44	C	0.883894	1.832532	3.291165
45	H	-3.663273	-0.323636	-1.914014
46	H	-5.991341	-0.424594	-2.779882
47	H	-7.043348	-2.627677	-3.271721
48	H	-5.765261	-4.729026	-2.874889
49	H	-3.442562	-4.636574	-2.030749
50	H	-1.32759	-3.731006	1.12485
51	H	-0.654535	-6.03216	1.732316
52	H	0.000879	-7.657906	-0.043022
53	H	-0.037114	-6.962717	-2.435262
54	H	-0.726024	-4.667085	-3.057635
55	H	-2.593755	-2.232791	-4.215707
56	H	-1.476742	-2.008142	-6.396866
57	H	0.991911	-1.611585	-6.49905
58	H	2.295334	-1.434239	-4.398372
59	H	3.551783	-2.048222	-2.129384
60	H	2.569615	-3.397786	-2.748754
61	H	2.018831	-4.174304	-0.54393
62	H	3.682392	-3.582651	-0.274673
63	H	2.508706	-4.426515	1.780542
64	H	3.275359	-4.556852	4.125176
65	H	3.672967	-2.462201	5.432826
66	H	3.34046	-0.261668	4.352031
67	H	4.146734	3.040807	0.942042
68	H	6.52341	3.549689	0.532426
69	H	8.227586	1.730123	0.579771
70	H	7.521245	-0.614517	1.04078
71	H	5.150866	-1.13408	1.498047
72	H	4.260653	2.360362	3.484119
73	H	3.529212	3.814328	5.34097
74	H	1.111498	4.009302	5.910071
75	H	-0.57728	2.725219	4.598341
76	H	0.1412	1.259492	2.737427
77	Co	1.023787	0.859043	0.16288

78	P	1.626698	2.317472	-1.410625
79	P	-1.057824	1.148725	-0.411159
80	P	-2.700658	-0.564265	1.601685
81	N	-2.173378	2.226363	0.329679
82	N	-1.426619	1.8088	-1.947404
83	C	3.385911	2.469825	-1.925171
84	C	4.120119	1.285307	-2.135024
85	C	5.430913	1.341027	-2.620887
86	C	6.026919	2.583338	-2.892699
87	C	5.307834	3.766075	-2.668677
88	C	3.990203	3.71261	-2.189662
89	C	1.083677	4.034613	-1.012123
90	C	1.051678	4.431943	0.340065
91	C	0.663307	5.733619	0.688135
92	C	0.29467	6.647964	-0.310715
93	C	0.31608	6.256081	-1.659338
94	C	0.709248	4.957103	-2.010529
95	C	0.797757	1.994443	-3.037139
96	C	1.524633	2.054669	-4.242234
97	C	0.893077	1.928715	-5.485404
98	C	-0.489192	1.713053	-5.542332
99	C	-1.226066	1.620637	-4.357979
100	C	-0.601639	1.770982	-3.108216
101	C	-2.649064	2.648566	-1.957423
102	C	-2.670997	3.292245	-0.57355
103	C	-2.526468	2.263736	1.704239
104	C	-2.702377	3.512499	2.332666
105	C	-3.125663	3.585824	3.663102
106	C	-3.346169	2.411806	4.39946
107	C	-3.158451	1.169061	3.784177
108	C	-2.769675	1.075092	2.433658
109	C	-4.471395	-0.912946	1.250243
110	C	-4.874834	-2.234635	0.968178
111	C	-6.22252	-2.526348	0.733743
112	C	-7.181162	-1.500787	0.756211
113	C	-6.783553	-0.181837	1.014473
114	C	-5.435629	0.112666	1.264668
115	C	-2.251857	-1.718148	2.964219
116	C	-3.20283	-2.442294	3.711461
117	C	-2.788491	-3.267067	4.765933

118	C	-1.426619	-3.375753	5.086488
119	C	-0.475708	-2.655467	4.348478
120	C	-0.883894	-1.832532	3.291165
121	H	3.663273	0.323636	-1.914014
122	H	5.991341	0.424594	-2.779882
123	H	7.043348	2.627677	-3.271721
124	H	5.765261	4.729026	-2.874889
125	H	3.442562	4.636574	-2.030749
126	H	1.32759	3.731006	1.12485
127	H	0.654535	6.03216	1.732316
128	H	-0.000879	7.657906	-0.043022
129	H	0.037114	6.962717	-2.435262
130	H	0.726024	4.667085	-3.057635
131	H	2.593755	2.232791	-4.215707
132	H	1.476742	2.008142	-6.396866
133	H	-0.991911	1.611585	-6.49905
134	H	-2.295334	1.434239	-4.398372
135	H	-3.551783	2.048222	-2.129384
136	H	-2.569615	3.397786	-2.748754
137	H	-2.018831	4.174304	-0.54393
138	H	-3.682392	3.582651	-0.274673
139	H	-2.508706	4.426515	1.780542
140	H	-3.275359	4.556852	4.125176
141	H	-3.672967	2.462201	5.432826
142	H	-3.34046	0.261668	4.352031
143	H	-4.146734	-3.040807	0.942042
144	H	-6.52341	-3.549689	0.532426
145	H	-8.227586	-1.730123	0.579771
146	H	-7.521245	0.614517	1.04078
147	H	-5.150866	1.13408	1.498047
148	H	-4.260653	-2.360362	3.484119
149	H	-3.529212	-3.814328	5.34097
150	H	-1.111498	-4.009302	5.910071
151	H	0.57728	-2.725219	4.598341
152	H	-0.1412	-1.259492	2.737427

Table S24. DFT-optimized XYZ Coordinates for **5** (B3LYP: LANL2DZ(p,d), Co, P; D95V (C, H, N).

Tag	Symbol	X	Y	Z
1	C	3.99022	1.053787	3.491928
2	H	3.201384	1.54878	4.049415
3	Co	1.34433	0.059869	-0.064931
4	N	-0.433095	1.60685	-2.852863
5	P	2.487773	1.616917	1.077346
6	C	5.103191	0.54584	4.190432
7	H	5.146974	0.643332	5.272719
8	Co	-1.267307	0.112435	0.165174
9	N	0.156526	-0.771636	-3.066112
10	P	2.575102	-1.428441	-1.175955
11	C	6.159607	-0.068392	3.493387
12	H	7.02208	-0.45343	4.031741
13	N	0.469633	0.274923	3.170155
14	P	0.171524	0.386238	-1.745374
15	C	6.093127	-0.175874	2.090275
16	H	6.901171	-0.649636	1.538789
17	N	0.036844	-2.057496	2.523997
18	P	0.40186	-0.592278	1.648178
19	C	4.977786	0.320707	1.396277
20	H	4.948125	0.222773	0.314947
21	P	-2.650261	1.836166	-0.731532
22	C	3.9115	0.946592	2.085318
23	P	-2.490508	-1.865212	0.763715
24	C	4.472462	3.682792	0.754244
25	H	4.926173	3.311824	1.66823
26	C	5.056244	4.778777	0.094451
27	H	5.951131	5.239345	0.505471
28	C	4.483233	5.280229	-1.090886
29	H	4.934195	6.128966	-1.599238
30	C	3.32494	4.673954	-1.612559
31	H	2.873265	5.055113	-2.524831
32	C	2.746968	3.570783	-0.957761
33	H	1.862005	3.101241	-1.375319
34	C	3.310122	3.063858	0.233941
35	C	1.452459	2.445842	2.39654
36	C	1.503257	3.847811	2.571139
37	H	2.113173	4.442829	1.900817

38	C	0.814495	4.502172	3.606354
39	H	0.893655	5.580028	3.714347
40	C	0.052269	3.742158	4.508902
41	H	-0.464689	4.222546	5.336325
42	C	-0.048907	2.353444	4.341367
43	H	-0.664626	1.786448	5.031438
44	C	0.624594	1.684468	3.28687
45	C	0.033761	-0.521501	4.348615
46	H	-1.040739	-0.390817	4.543585
47	H	0.595679	-0.215503	5.237832
48	C	0.328375	-1.983309	3.976333
49	H	1.377507	-2.232801	4.197929
50	H	-0.321205	-2.673115	4.524802
51	C	-0.307088	-3.293715	1.903115
52	C	0.417351	-4.461649	2.22389
53	H	1.244661	-4.399729	2.925655
54	C	0.08885	-5.694895	1.639095
55	H	0.65691	-6.584347	1.898922
56	C	-0.961009	-5.766791	0.707392
57	H	-1.216774	-6.71175	0.236298
58	C	-1.700789	-4.611022	0.398932
59	H	-2.52807	-4.693639	-0.297355
60	C	-1.408712	-3.368016	1.000964
61	C	-3.564673	-2.907633	3.223306
62	H	-3.206362	-3.882564	2.904347
63	C	-4.238297	-2.79108	4.452492
64	H	-4.395172	-3.675016	5.065737
65	C	-4.714145	-1.536933	4.88572
66	H	-5.238399	-1.449556	5.834033
67	C	-4.508953	-0.399714	4.082182
68	H	-4.872544	0.572936	4.403676
69	C	-3.831091	-0.515486	2.853418
70	H	-3.679555	0.375032	2.250561
71	C	-3.35415	-1.769494	2.408542
72	C	-5.106214	-2.837227	0.030626
73	H	-5.393554	-2.729227	1.071959
74	C	-6.050705	-3.320478	-0.896235
75	H	-7.05227	-3.573985	-0.557752
76	C	-5.697136	-3.489841	-2.247943
77	H	-6.42331	-3.874988	-2.959356

78	C	-4.395203	-3.157781	-2.673073
79	H	-4.115498	-3.283409	-3.716117
80	C	-3.457341	-2.659869	-1.75386
81	H	-2.458519	-2.403195	-2.096091
82	C	-3.798009	-2.506148	-0.388399
83	C	-3.548618	2.664284	0.668727
84	C	-2.811286	2.957946	1.843183
85	H	-1.750623	2.722367	1.903248
86	C	-3.433171	3.580452	2.939591
87	H	-2.846709	3.811617	3.824007
88	C	-4.802553	3.907806	2.887038
89	H	-5.282326	4.391551	3.734189
90	C	-5.543289	3.613029	1.727043
91	H	-6.598917	3.86691	1.673894
92	C	-4.921318	2.99858	0.623547
93	H	-5.50659	2.791434	-0.266513
94	C	-4.929227	0.587384	-1.836334
95	H	-4.878579	-0.060672	-0.966954
96	C	-5.967874	0.399761	-2.765122
97	H	-6.698663	-0.386463	-2.597418
98	C	-6.055384	1.220617	-3.905884
99	H	-6.857756	1.07506	-4.624734
100	C	-5.098515	2.233353	-4.106519
101	H	-5.160537	2.877476	-4.980213
102	C	-4.064573	2.42903	-3.172192
103	H	-3.35262	3.23125	-3.33608
104	C	-3.967573	1.607652	-2.024793
105	C	-1.645932	3.232145	-1.442061
106	C	-1.874635	4.578421	-1.082394
107	H	-2.578012	4.811869	-0.289914
108	C	-1.235247	5.634456	-1.755709
109	H	-1.436032	6.661642	-1.465005
110	C	-0.35918	5.351699	-2.819245
111	H	0.120561	6.160973	-3.363913
112	C	-0.091267	4.018958	-3.170094
113	H	0.605427	3.801218	-3.975307
114	C	-0.710086	2.952673	-2.479331
115	C	-0.276402	1.241825	-4.283255
116	H	0.726018	1.494092	-4.661688
117	H	-1.02573	1.763106	-4.887905

118	C	-0.488354	-0.276498	-4.309445
119	H	-1.564667	-0.506313	-4.323281
120	H	-0.016124	-0.732522	-5.185919
121	C	0.443908	-2.160205	-2.929063
122	C	-0.297391	-3.093647	-3.695258
123	H	-1.06688	-2.74406	-4.376605
124	C	-0.059993	-4.472719	-3.590958
125	H	-0.641161	-5.16461	-4.195555
126	C	0.914941	-4.951585	-2.699977
127	H	1.099793	-6.017404	-2.600183
128	C	1.67283	-4.033839	-1.952628
129	H	2.44452	-4.410448	-1.289192
130	C	1.479752	-2.640272	-2.065106
131	C	3.799487	-2.521589	-0.291814
132	C	3.532226	-2.885741	1.047066
133	H	2.642328	-2.501454	1.535035
134	C	4.414332	-3.717988	1.757318
135	H	4.195758	-3.984248	2.78889
136	C	5.590395	-4.18993	1.144719
137	H	6.277675	-4.827499	1.695316
138	C	5.875857	-3.820626	-0.183642
139	H	6.784738	-4.17329	-0.66499
140	C	4.98741	-2.99553	-0.897872
141	H	5.231862	-2.721655	-1.919215
142	C	3.573262	-0.773152	-2.613217
143	C	4.137261	0.519236	-2.529646
144	H	3.944457	1.140077	-1.661647
145	C	4.930423	1.029676	-3.573996
146	H	5.357278	2.025753	-3.485289
147	C	5.163302	0.257447	-4.72745
148	H	5.775685	0.649775	-5.535606
149	C	4.59344	-1.027193	-4.829145
150	H	4.762795	-1.630263	-5.718053
151	C	3.807461	-1.539059	-3.780679
152	H	3.374045	-2.530602	-3.879793

Table S25. DFT-optimized XYZ Coordinates for **5** (wB97XD: def2SVP on all atoms).

Tag	Symbol	X	Y	Z
1	C	4.053166	0.878536	3.049226
2	H	3.270616	1.245409	3.715437
3	Co	1.231037	0.117755	-0.088653
4	N	-0.643644	1.241451	-2.947133
5	P	2.406009	1.67112	0.856625
6	C	5.197117	0.294626	3.595971
7	H	5.288741	0.200333	4.680249
8	Co	-1.200513	0.19642	0.235517
9	N	-0.027379	-1.097019	-2.841804
10	P	2.430907	-1.397611	-1.04025
11	C	6.223465	-0.15048	2.767254
12	H	7.11951	-0.602805	3.197167
13	N	0.616387	0.394647	3.147759
14	P	0.027689	0.216851	-1.716531
15	C	6.103018	-0.01425	1.384338
16	H	6.899166	-0.365083	0.725102
17	N	0.134994	-1.898428	2.529342
18	P	0.425904	-0.448927	1.657339
19	C	4.955686	0.550062	0.838745
20	H	4.868848	0.635679	-0.247671
21	P	-2.578664	1.717588	-0.682456
22	C	3.919952	1.009218	1.664336
23	P	-2.343138	-1.653873	0.833751
24	C	4.286711	3.695829	0.158175
25	H	4.90011	3.340904	0.988732
26	C	4.73318	4.763828	-0.61783
27	H	5.693536	5.23199	-0.39229
28	C	3.956542	5.233449	-1.676469
29	H	4.308509	6.070049	-2.283872
30	C	2.730069	4.632154	-1.956304
31	H	2.112213	4.994655	-2.779629
32	C	2.287067	3.559032	-1.18683
33	H	1.33345	3.079441	-1.417489
34	C	3.059919	3.081091	-0.123483
35	C	1.532682	2.510921	2.25221
36	C	1.625668	3.900654	2.397789
37	H	2.171844	4.476234	1.649756
38	C	1.069764	4.574495	3.480949

39	H	1.178874	5.656682	3.565674
40	C	0.401525	3.846114	4.45852
41	H	-0.025029	4.349011	5.329436
42	C	0.252688	2.470779	4.323055
43	H	-0.312677	1.924396	5.077585
44	C	0.796155	1.780105	3.225797
45	C	0.219684	-0.38366	4.314415
46	H	-0.855231	-0.258334	4.54374
47	H	0.805519	-0.077881	5.193639
48	C	0.508257	-1.827891	3.929437
49	H	1.577662	-2.063857	4.091494
50	H	-0.097918	-2.531975	4.518002
51	C	-0.191114	-3.104292	1.895257
52	C	0.517805	-4.273394	2.186719
53	H	1.359097	-4.231226	2.880557
54	C	0.157873	-5.481462	1.596772
55	H	0.714451	-6.388627	1.840695
56	C	-0.892737	-5.52551	0.686435
57	H	-1.168619	-6.465248	0.205436
58	C	-1.602394	-4.363579	0.388746
59	H	-2.435743	-4.416078	-0.313087
60	C	-1.282703	-3.149435	1.00059
61	C	-3.242549	-2.643319	3.348592
62	H	-2.931172	-3.636228	3.014978
63	C	-3.762571	-2.475646	4.630725
64	H	-3.867229	-3.340127	5.289693
65	C	-4.145939	-1.208954	5.074236
66	H	-4.549681	-1.082372	6.080982
67	C	-4.011539	-0.10726	4.230648
68	H	-4.305534	0.889203	4.566899
69	C	-3.488918	-0.273945	2.949477
70	H	-3.366713	0.599301	2.305906
71	C	-3.102208	-1.540623	2.496936
72	C	-4.83026	-2.838614	0.107379
73	H	-5.050946	-2.941935	1.172414
74	C	-5.738977	-3.312093	-0.839314
75	H	-6.669228	-3.779869	-0.510288
76	C	-5.458621	-3.196234	-2.200087
77	H	-6.17112	-3.571383	-2.93767
78	C	-4.273782	-2.590695	-2.618987

79	H	-4.061454	-2.480563	-3.684584
80	C	-3.37385	-2.104224	-1.677208
81	H	-2.455649	-1.606173	-1.996597
82	C	-3.639203	-2.238715	-0.30909
83	C	-3.251329	2.688813	0.719539
84	C	-2.374698	2.980676	1.775547
85	H	-1.330982	2.651114	1.740284
86	C	-2.819412	3.707478	2.876982
87	H	-2.122758	3.928752	3.685683
88	C	-4.141179	4.147563	2.938492
89	H	-4.489134	4.715033	3.80417
90	C	-5.013721	3.871709	1.8875
91	H	-6.046322	4.224585	1.9239
92	C	-4.571009	3.150723	0.779532
93	H	-5.261614	2.952278	-0.041586
94	C	-5.079715	0.555593	-1.045192
95	H	-5.030137	0.342957	0.025686
96	C	-6.19248	0.143103	-1.768934
97	H	-7.00305	-0.382236	-1.260969
98	C	-6.259521	0.382357	-3.141796
99	H	-7.129276	0.051215	-3.712893
100	C	-5.216064	1.046889	-3.781242
101	H	-5.267379	1.243239	-4.854202
102	C	-4.109868	1.485054	-3.052209
103	H	-3.313508	2.033489	-3.558507
104	C	-4.034404	1.243315	-1.677908
105	C	-1.733713	3.003449	-1.680727
106	C	-1.966625	4.3668	-1.476099
107	H	-2.607063	4.688527	-0.653143
108	C	-1.416455	5.32524	-2.323329
109	H	-1.617629	6.383762	-2.151998
110	C	-0.632171	4.919631	-3.399942
111	H	-0.214089	5.661333	-4.084149
112	C	-0.361897	3.569857	-3.602813
113	H	0.281841	3.261725	-4.427943
114	C	-0.892961	2.601168	-2.740717
115	C	-0.404676	0.717426	-4.281971
116	H	0.62668	0.914265	-4.63193
117	H	-1.110289	1.166157	-4.996718
118	C	-0.629258	-0.775195	-4.126037

119	H	-1.713509	-0.997075	-4.143231
120	H	-0.142242	-1.348665	-4.928157
121	C	0.285331	-2.427566	-2.522462
122	C	-0.450898	-3.4675	-3.109408
123	H	-1.283652	-3.233754	-3.773389
124	C	-0.139153	-4.798617	-2.856103
125	H	-0.723753	-5.587048	-3.334691
126	C	0.899853	-5.119747	-1.989225
127	H	1.145021	-6.161457	-1.776509
128	C	1.635204	-4.097394	-1.39604
129	H	2.460578	-4.351034	-0.728292
130	C	1.363417	-2.753477	-1.664462
131	C	3.735697	-2.278835	-0.099989
132	C	3.538714	-2.467999	1.272599
133	H	2.640868	-2.065933	1.742773
134	C	4.485608	-3.139039	2.039442
135	H	4.322208	-3.270713	3.111216
136	C	5.652521	-3.617891	1.445059
137	H	6.402143	-4.136059	2.046824
138	C	5.86463	-3.421279	0.081977
139	H	6.780172	-3.786132	-0.388308
140	C	4.911662	-2.755929	-0.688561
141	H	5.096682	-2.603358	-1.753223
142	C	3.237846	-0.87185	-2.611057
143	C	3.532887	0.483598	-2.789541
144	H	3.278936	1.197759	-2.005593
145	C	4.108653	0.936299	-3.975429
146	H	4.334049	1.998553	-4.093117
147	C	4.382567	0.035934	-5.003923
148	H	4.829352	0.38703	-5.936642
149	C	4.077897	-1.316161	-4.841408
150	H	4.282185	-2.023792	-5.647777
151	C	3.507203	-1.768485	-3.652938
152	H	3.255533	-2.826506	-3.543642

Table S26. DFT-optimized XYZ Coordinates for **5** (wB97XD: LANL2DZ(p,d) Co, P; D95V, C, H, N).

Tag	Symbol	X	Y	Z
1	C	4.071767	1.029575	3.082045
2	H	3.292523	1.403345	3.737733
3	Co	1.274674	0.12322	-0.087129
4	N	-0.61671	1.220399	-2.966799
5	P	2.398059	1.738624	0.860189
6	C	5.233038	0.477098	3.645526
7	H	5.329591	0.419304	4.72484
8	Co	-1.218646	0.2072	0.258479
9	N	-0.025701	-1.135995	-2.83473
10	P	2.476235	-1.408162	-1.035531
11	C	6.269433	0.018922	2.821475
12	H	7.168149	-0.404599	3.256807
13	N	0.591969	0.434977	3.161112
14	P	0.052367	0.200355	-1.732587
15	C	6.139273	0.112503	1.426671
16	H	6.932373	-0.244655	0.778998
17	N	0.195947	-1.89348	2.570382
18	P	0.48744	-0.452423	1.683973
19	C	4.977076	0.650089	0.866518
20	H	4.889396	0.702095	-0.215061
21	P	-2.637465	1.731101	-0.703838
22	C	3.930106	1.119645	1.686863
23	P	-2.318092	-1.736647	0.851181
24	C	4.244705	3.815809	0.156898
25	H	4.856261	3.488645	0.991261
26	C	4.673726	4.891553	-0.632282
27	H	5.611854	5.385539	-0.403526
28	C	3.891086	5.330581	-1.711707
29	H	4.223343	6.165217	-2.31997
30	C	2.678493	4.686191	-1.999702
31	H	2.063556	5.021287	-2.82764
32	C	2.255594	3.603627	-1.217476
33	H	1.323818	3.097667	-1.45055
34	C	3.032394	3.158816	-0.131974
35	C	1.50436	2.576009	2.257981
36	C	1.5777	3.975154	2.399538
37	H	2.133723	4.551587	1.669874

38	C	0.974893	4.652678	3.465575
39	H	1.068013	5.729313	3.545775
40	C	0.274773	3.920155	4.429882
41	H	-0.182009	4.421058	5.277294
42	C	0.151534	2.533962	4.299808
43	H	-0.423323	1.989168	5.038968
44	C	0.748876	1.842644	3.22386
45	C	0.166044	-0.328072	4.353609
46	H	-0.907768	-0.196195	4.546038
47	H	0.730739	-0.002625	5.231508
48	C	0.46253	-1.795074	4.014217
49	H	1.506315	-2.042808	4.252321
50	H	-0.198256	-2.47051	4.563781
51	C	-0.119969	-3.130371	1.947232
52	C	0.635298	-4.2743	2.244617
53	H	1.483159	-4.194142	2.917083
54	C	0.304023	-5.508695	1.673995
55	H	0.888616	-6.389035	1.917387
56	C	-0.765366	-5.59532	0.774697
57	H	-1.016774	-6.542348	0.311243
58	C	-1.518472	-4.45318	0.470338
59	H	-2.349076	-4.540146	-0.220725
60	C	-1.228249	-3.215376	1.067109
61	C	-3.222223	-2.679469	3.403486
62	H	-2.882484	-3.668286	3.109967
63	C	-3.773523	-2.48685	4.677819
64	H	-3.867492	-3.328194	5.356034
65	C	-4.206417	-1.211165	5.076243
66	H	-4.6334	-1.066118	6.062725
67	C	-4.086659	-0.126957	4.193673
68	H	-4.417658	0.862938	4.489311
69	C	-3.530795	-0.320026	2.92159
70	H	-3.430304	0.532239	2.255469
71	C	-3.095576	-1.595789	2.513344
72	C	-4.789461	-3.008815	0.15227
73	H	-4.993991	-3.121816	1.212537
74	C	-5.704523	-3.504228	-0.788788
75	H	-6.610194	-3.99636	-0.451033
76	C	-5.445556	-3.373368	-2.161711
77	H	-6.153012	-3.76112	-2.886759

78	C	-4.276547	-2.728677	-2.595072
79	H	-4.086286	-2.604759	-3.656074
80	C	-3.370937	-2.22223	-1.657658
81	H	-2.479143	-1.696253	-1.986466
82	C	-3.614192	-2.369883	-0.278576
83	C	-3.352515	2.736504	0.661187
84	C	-2.505822	3.034962	1.750166
85	H	-1.47178	2.693629	1.757985
86	C	-2.979643	3.793882	2.827782
87	H	-2.312882	4.021753	3.650793
88	C	-4.303847	4.258074	2.834341
89	H	-4.670667	4.844937	3.669563
90	C	-5.149119	3.970077	1.752182
91	H	-6.170588	4.334351	1.746691
92	C	-4.675201	3.217904	0.668233
93	H	-5.335713	3.010581	-0.166835
94	C	-5.111713	0.48282	-1.044882
95	H	-5.053535	0.290085	0.022815
96	C	-6.218054	0.018193	-1.761258
97	H	-7.003018	-0.523061	-1.24529
98	C	-6.300886	0.235766	-3.146031
99	H	-7.157378	-0.128456	-3.702887
100	C	-5.274826	0.927265	-3.80417
101	H	-5.337459	1.106642	-4.872237
102	C	-4.172485	1.411069	-3.08281
103	H	-3.402585	1.974021	-3.600132
104	C	-4.08424	1.195339	-1.697279
105	C	-1.807458	2.99965	-1.753522
106	C	-2.079183	4.370762	-1.597831
107	H	-2.739693	4.70168	-0.804099
108	C	-1.530055	5.322966	-2.465365
109	H	-1.760759	6.373231	-2.331064
110	C	-0.699341	4.905973	-3.513981
111	H	-0.284904	5.632815	-4.20458
112	C	-0.389169	3.550326	-3.665107
113	H	0.281222	3.233543	-4.457008
114	C	-0.924751	2.591749	-2.78575
115	C	-0.46172	0.662994	-4.324182
116	H	0.539215	0.859736	-4.732275
117	H	-1.211959	1.091557	-4.993838

118	C	-0.667987	-0.839854	-4.129206
119	H	-1.742767	-1.071351	-4.112468
120	H	-0.191418	-1.418354	-4.924787
121	C	0.323629	-2.4768	-2.515313
122	C	-0.416059	-3.527632	-3.091239
123	H	-1.259075	-3.307052	-3.736369
124	C	-0.081902	-4.862672	-2.84328
125	H	-0.6608	-5.653812	-3.307512
126	C	0.983116	-5.170381	-1.989489
127	H	1.24282	-6.201675	-1.779938
128	C	1.720737	-4.132051	-1.40787
129	H	2.551606	-4.376442	-0.755083
130	C	1.427815	-2.784622	-1.673942
131	C	3.800045	-2.274611	-0.089519
132	C	3.629964	-2.428205	1.29934
133	H	2.752286	-2.008504	1.778401
134	C	4.597703	-3.080158	2.070873
135	H	4.459323	-3.174929	3.14289
136	C	5.75991	-3.580206	1.464916
137	H	6.516458	-4.077621	2.062461
138	C	5.945641	-3.420396	0.083867
139	H	6.84529	-3.796581	-0.391366
140	C	4.971313	-2.773422	-0.689703
141	H	5.137664	-2.651	-1.754433
142	C	3.295811	-0.878207	-2.60862
143	C	3.614303	0.48185	-2.778346
144	H	3.365927	1.194572	-1.99941
145	C	4.215843	0.935131	-3.960351
146	H	4.458018	1.987428	-4.068026
147	C	4.495081	0.031625	-4.996579
148	H	4.959261	0.378799	-5.913641
149	C	4.167055	-1.325426	-4.843474
150	H	4.373711	-2.028393	-5.643593
151	C	3.572251	-1.777421	-3.657639
152	H	3.309497	-2.826797	-3.55938

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