sp^2 C-H Activation of Dimethyl Fumarates by a [(Cp*Co)$_2$-μ-(η^4:η^4-toluene)] Complex

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-Supplementary Information-

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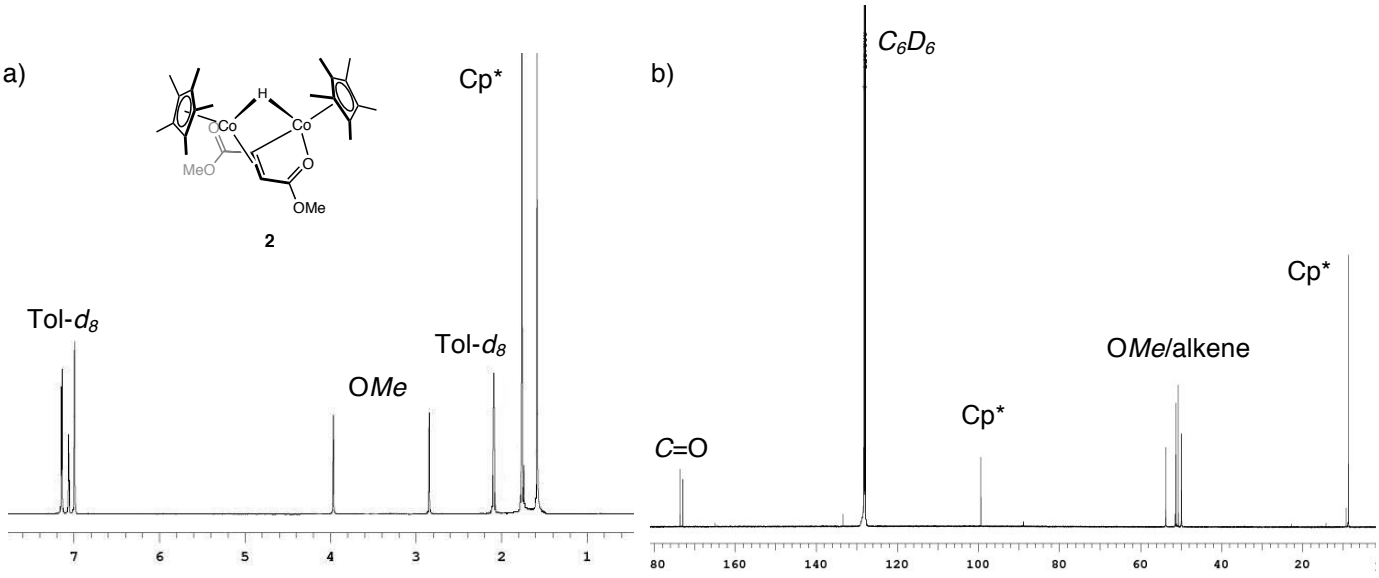


Figure S1. a) ^{1}H (toluene-d_8) and b) ^{13}C NMR spectra (benzene-d_6) of **2** recorded at 25 ºC.

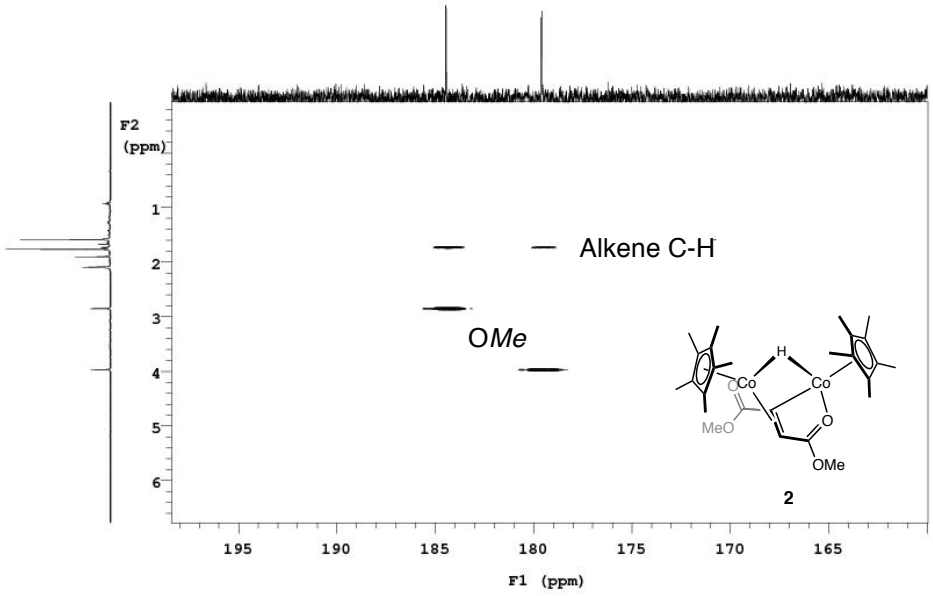
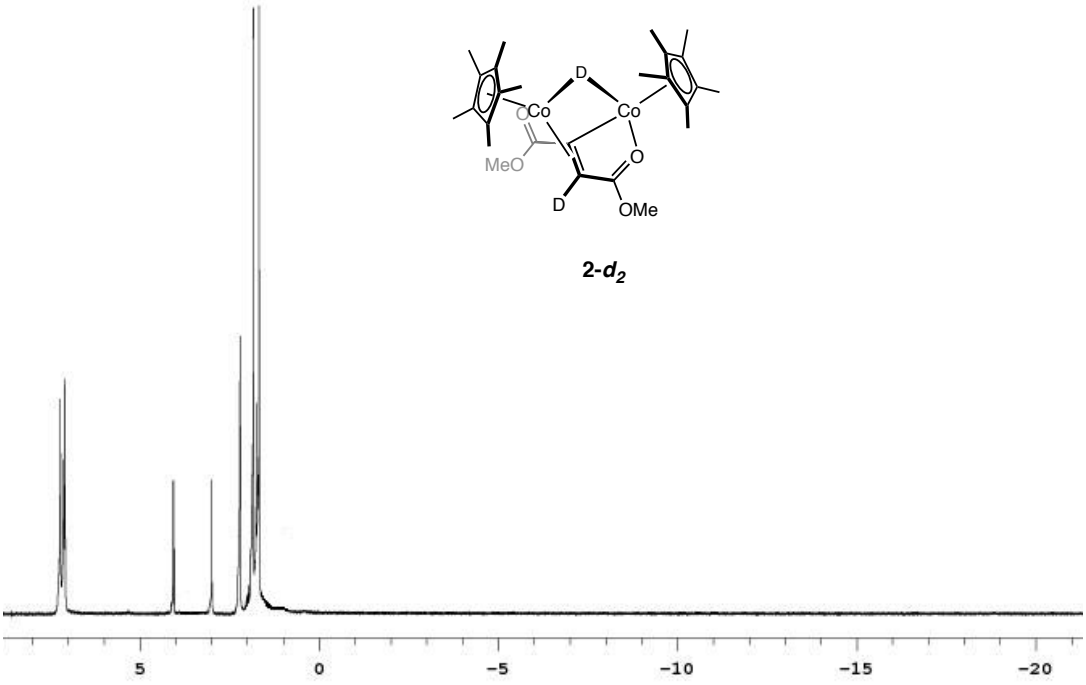
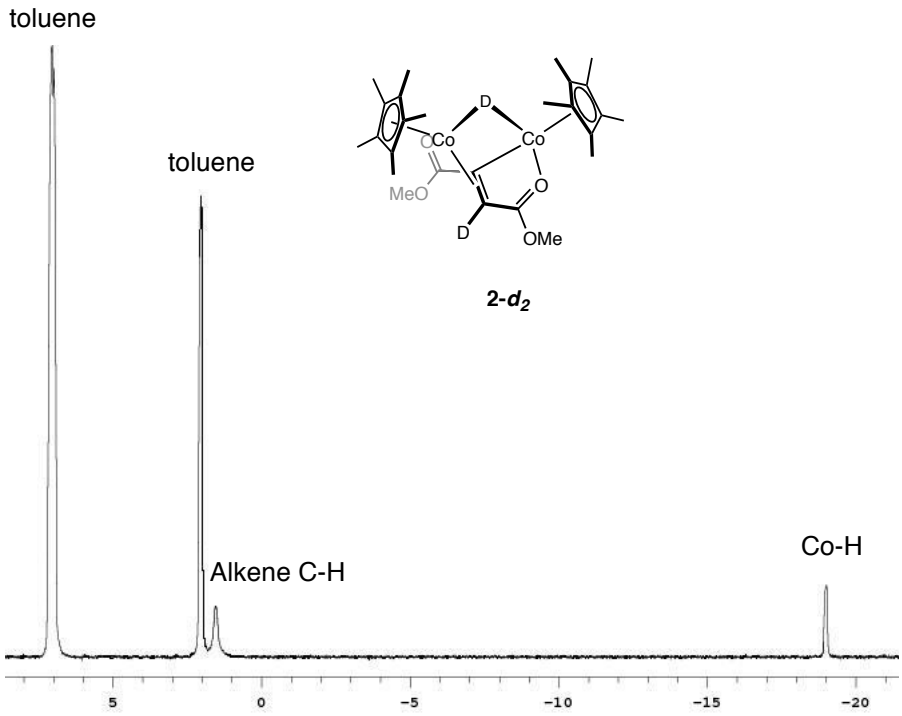


Figure S2. HMBC NMR spectrum of **2** in toluene-d_8 at –45 ºC. Two and three bond coupling to the alkenyl and C=O carbons identify the vinylic C-H while lack of correlation supports assignment of the Co-H.



2-*d*$_2$

Figure S3. ^{1}H NMR spectrum of **2-*d*$_2$** in toluene-d_8 at –45 ºC.



2-*d*$_2$

Figure S4. ^{2}H NMR spectrum of **2-*d*$_2$** in toluene at –45 ºC.

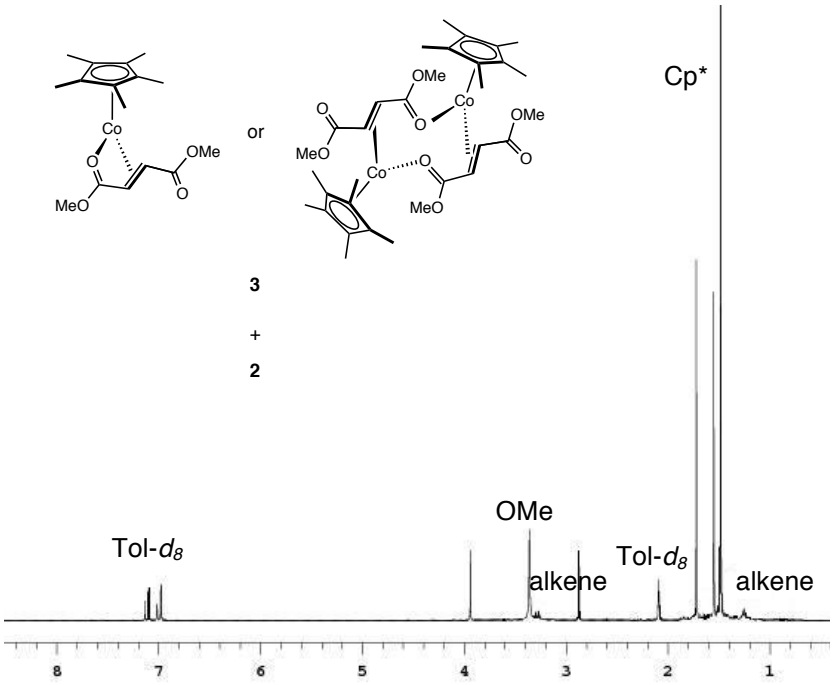


Figure S5. ^{1}H NMR spectrum of a mixture of **2** and **3** in toluene-d_8 at 25 ºC. Only resonances for **3** are noted; the other peaks belong to **2**.

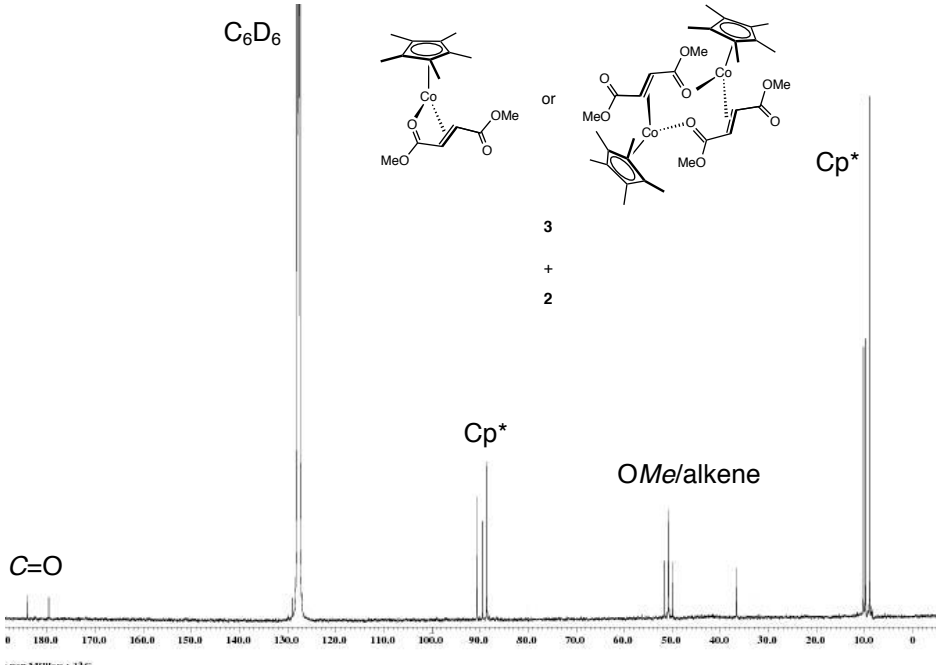


Figure S6. ^{13}C NMR spectrum of a mixture of **2** and **3** in benzene-d_6 at 25 ºC.

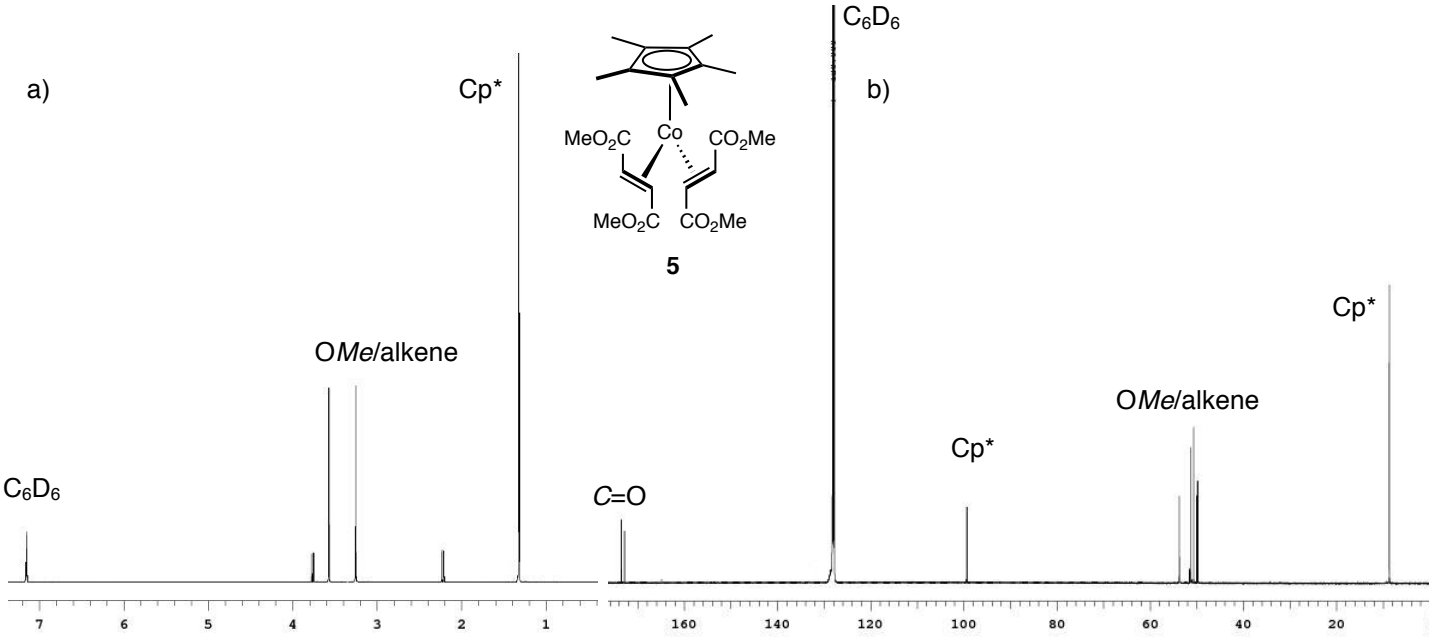


Figure S7. a) ^{1}H and b) ^{13}C NMR spectrum of **5** in benzene-d_6 at 25 ºC.

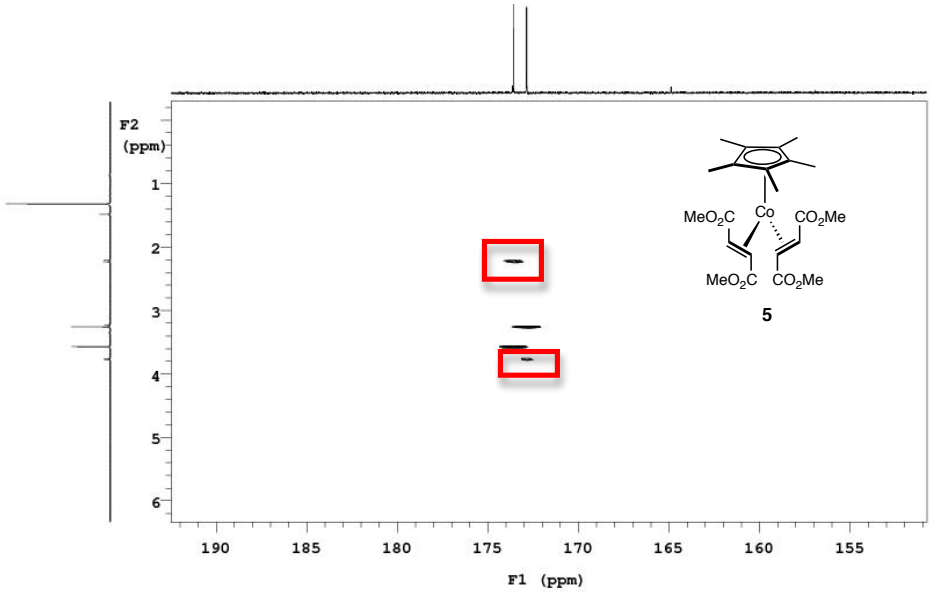


Figure S8. HMBC NMR spectrum of **5** in benzene-d_6 at 25 ºC. Two and three bond coupling of the alkenyl hydrogens to the C=O carbons identify the presence of two vinylic hydrogens (shown in red).

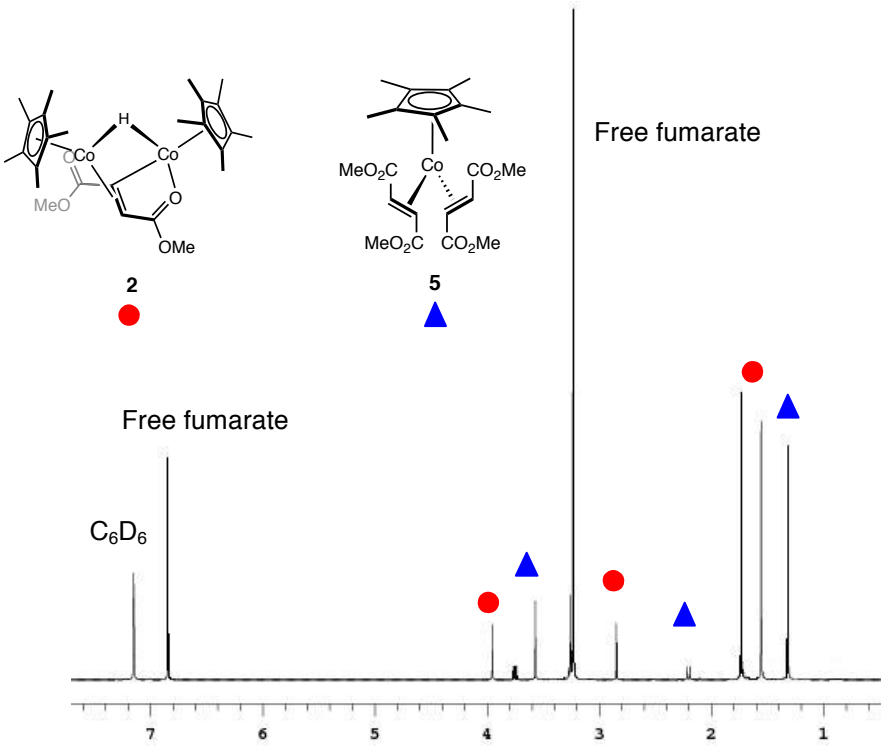


Figure S9. ^{1}H NMR spectrum of addition of excess dimethyl fumarate to **2** in benzene-d_6 at 25 ºC.

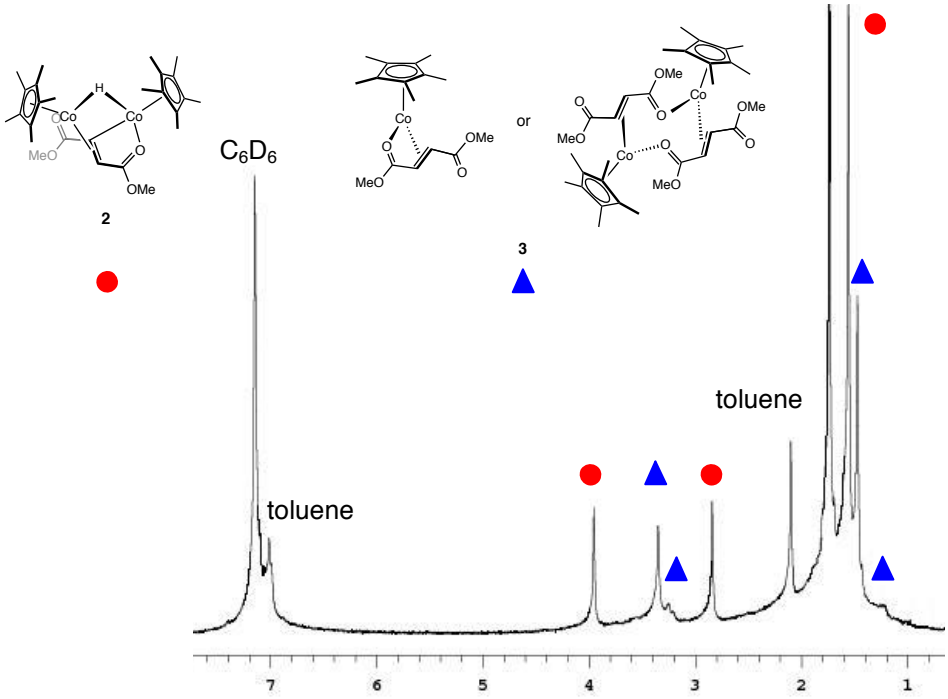


Figure S10. ^{1}H NMR spectrum of addition of **1** to **5** after 16 hours in benzene-d_6 at 25 ºC.

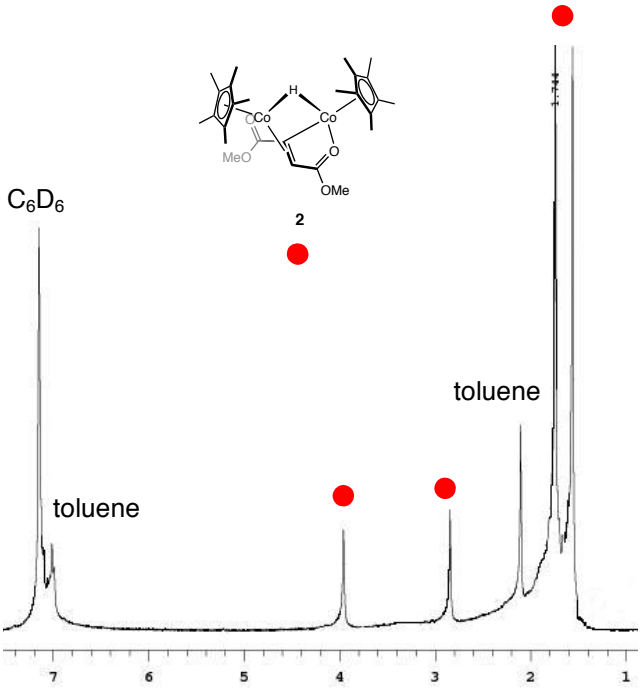


Figure S11. ^{1}H NMR spectrum of addition of **1** to **3** after 16 hours in benzene-d_6 at 25 ºC.

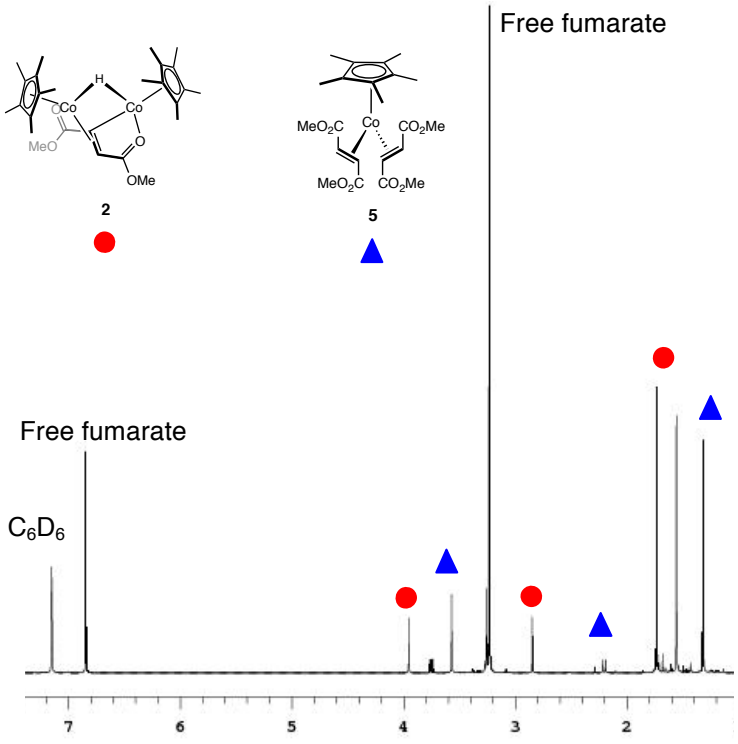


Figure S12. ^{1}H NMR spectrum of addition of excess dimethyl fumarate to a mixture of **3** and **2** after 15 minutes in benzene-d_6 at 25 ºC.

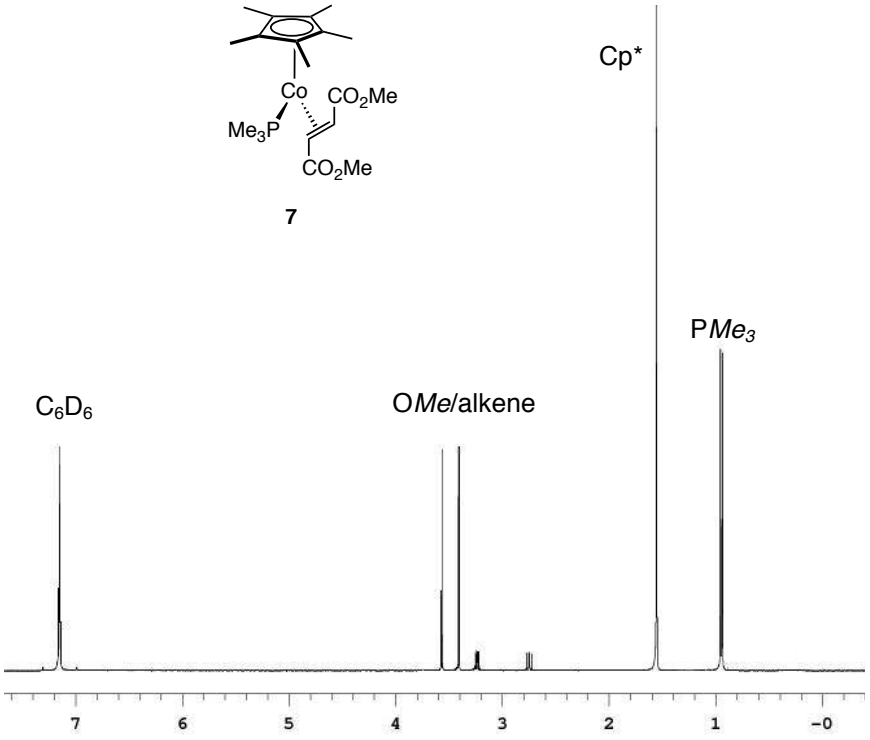


Figure S13. ^{1}H NMR spectrum of **7** in benzene-d_6 at 25 ºC.

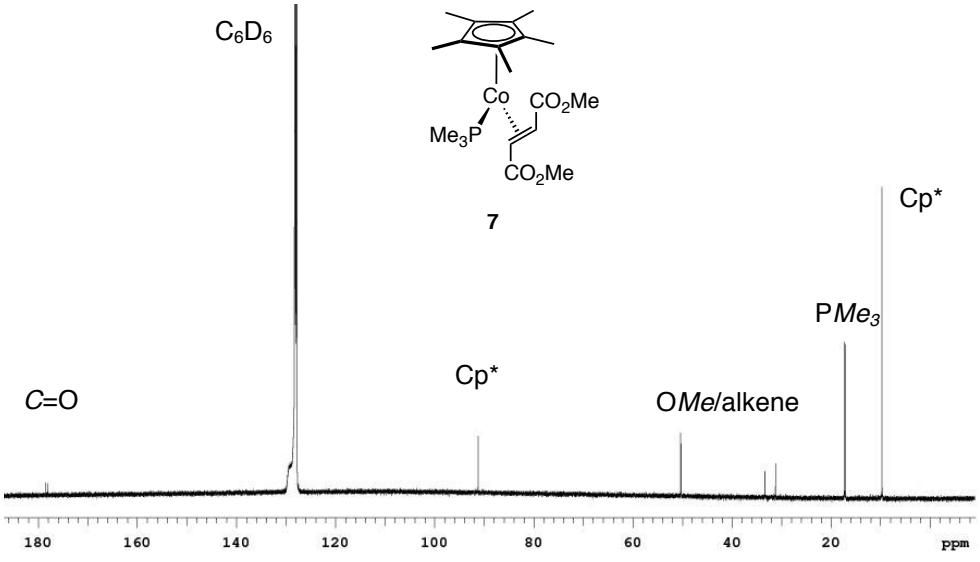


Figure S14. ^{13}C NMR spectrum of **7** in benzene-d_6 at 25 ºC.

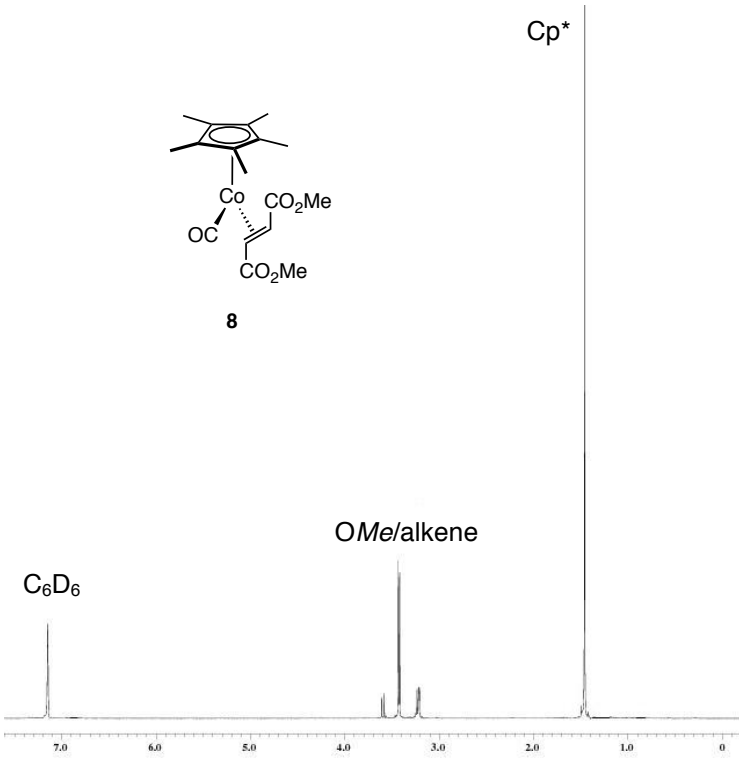


Figure S15. ^{1}H NMR spectrum of **8** in benzene-d_6 at 25 ºC.

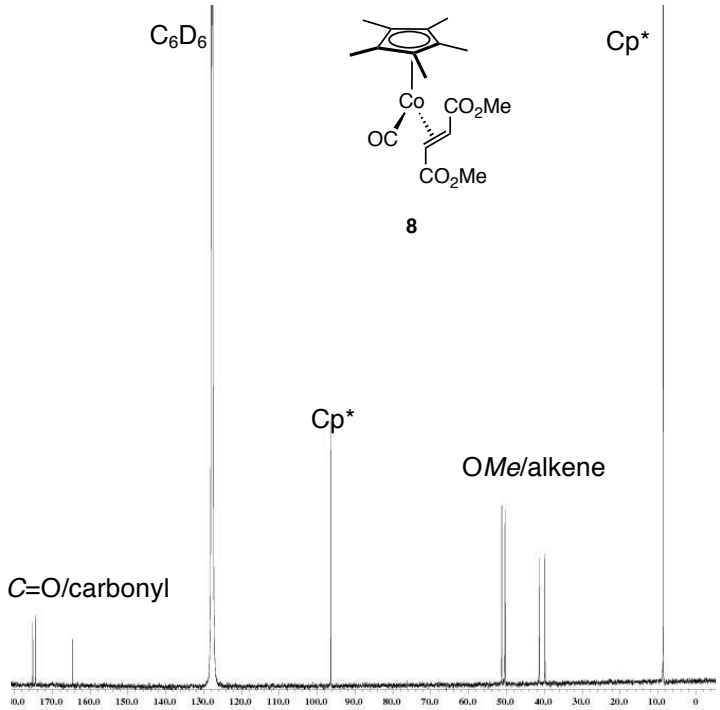


Figure S16. ^{13}C NMR spectrum of **8** in benzene-d_6 at 25 ºC.

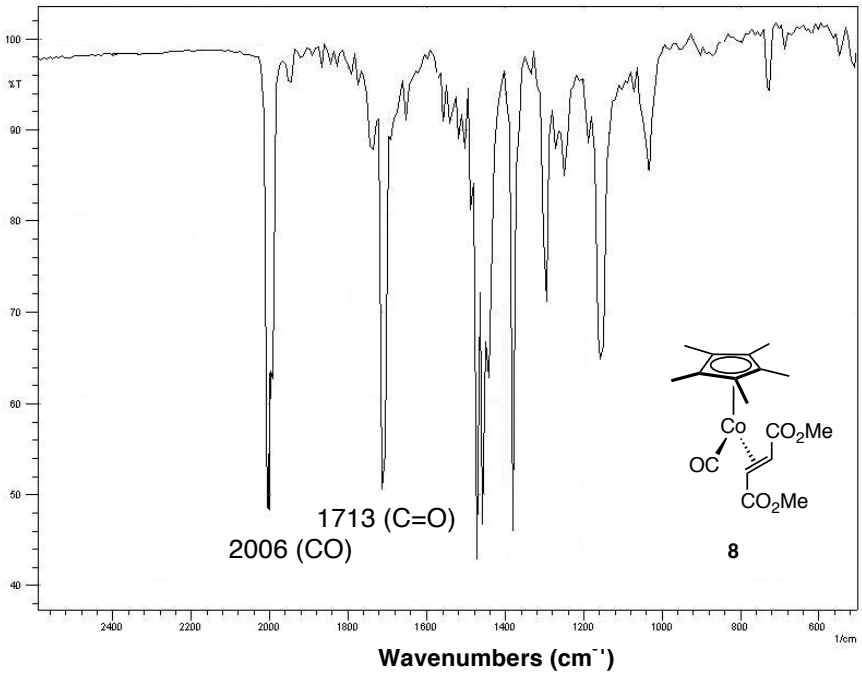


Figure S17. Solution IR spectrum of **8** recorded in pentane.

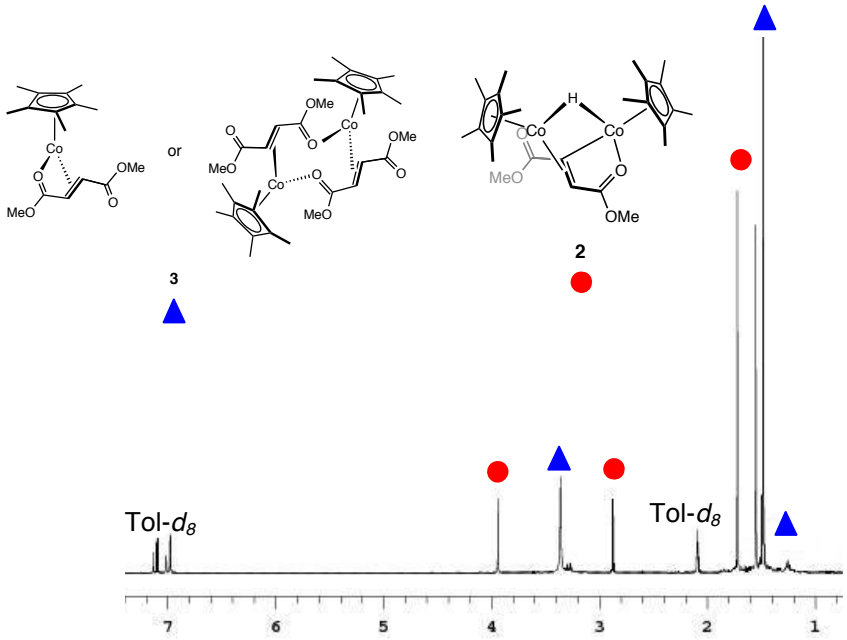


Figure S18. ^{1}H NMR spectrum of 1:1 reaction of **1** with dimethyl maleate in toluene-d_8 at 25 ºC.

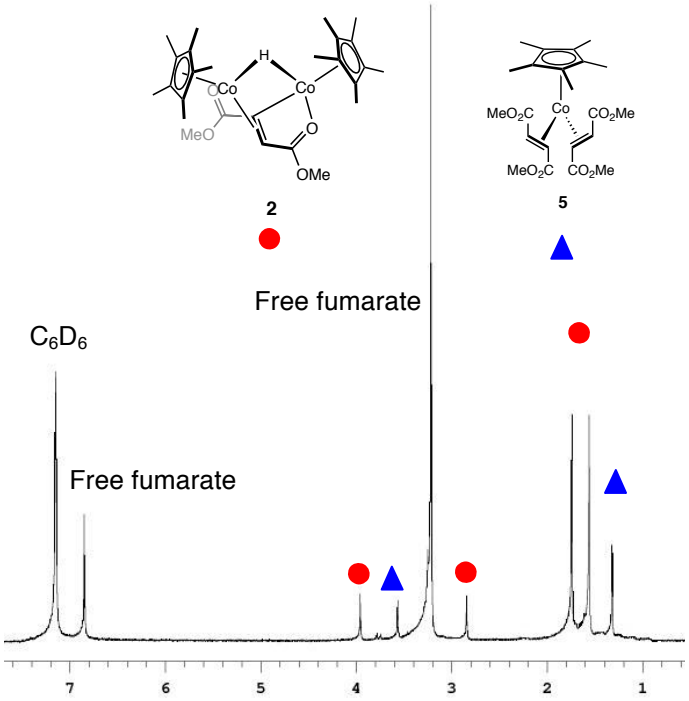


Figure S19. ^{1}H NMR spectrum of catalytic reaction of **1** with dimethyl maleate after heating for 3 hours in benzene-d_6 at 70 ºC.

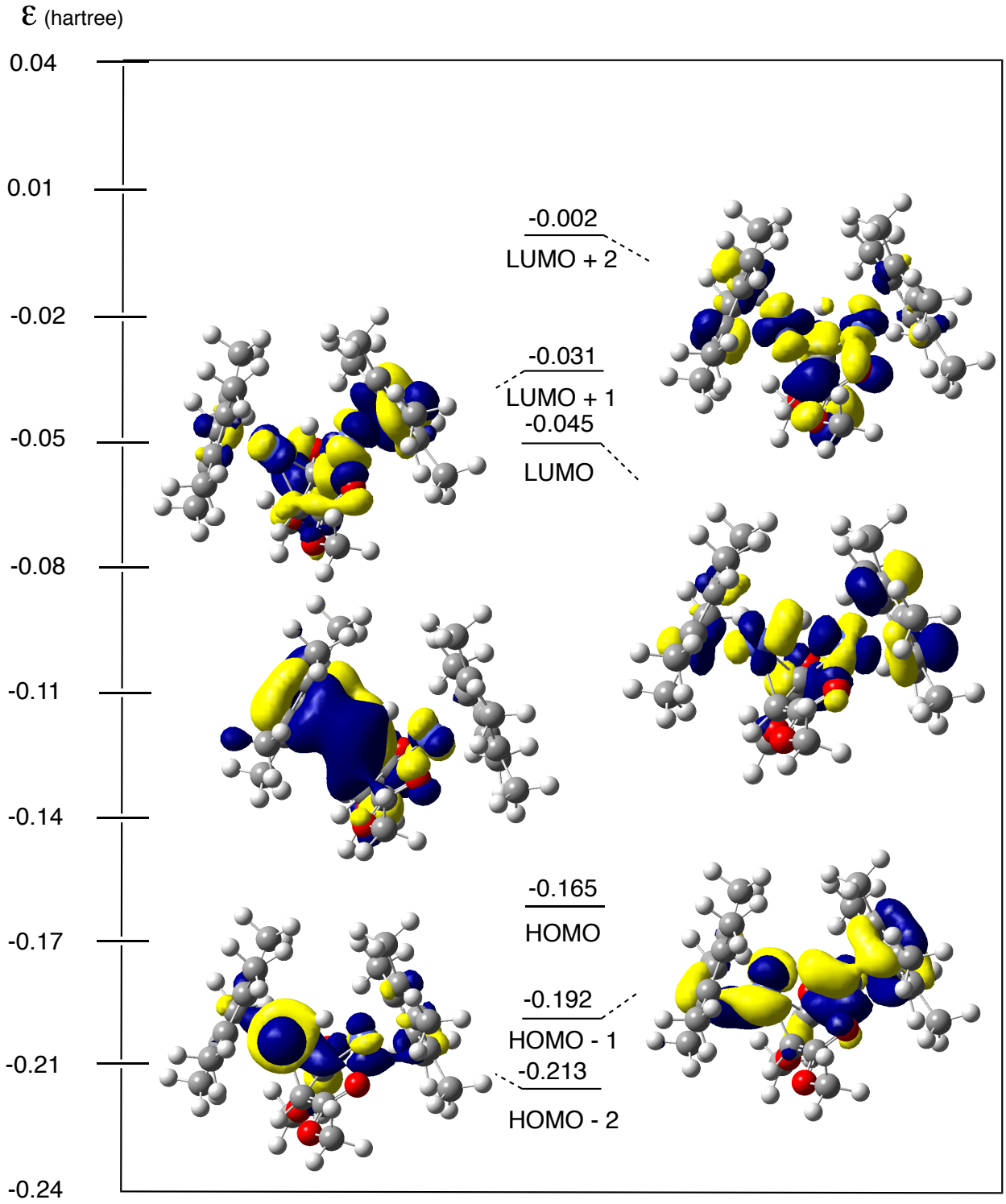


Figure S20. Frontier Kohn-Sham molecular orbital diagram of **2** as calculated using the Gaussian 09 program suite. Rendered at an isovalue of 0.03 e/ Å^3 (e/Å^3 = electrons per Angstrom cubed). Functional: B3LYP, Basis set: 6-31g(d',p') (C/O/H); LANL2DZ + F polarization (Co).

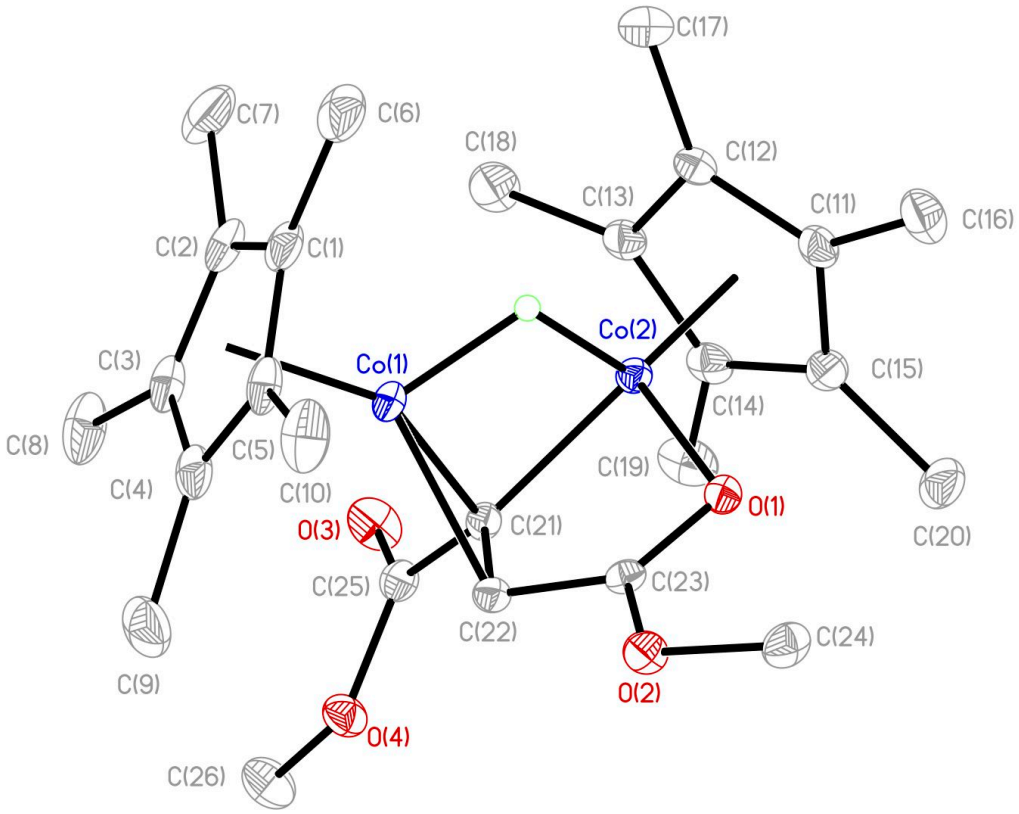


Figure S21. Molecular structure of **2** with 30 % probability ellipsoids and full atom labeling schemes. Hydrogen atoms omitted for clarity.

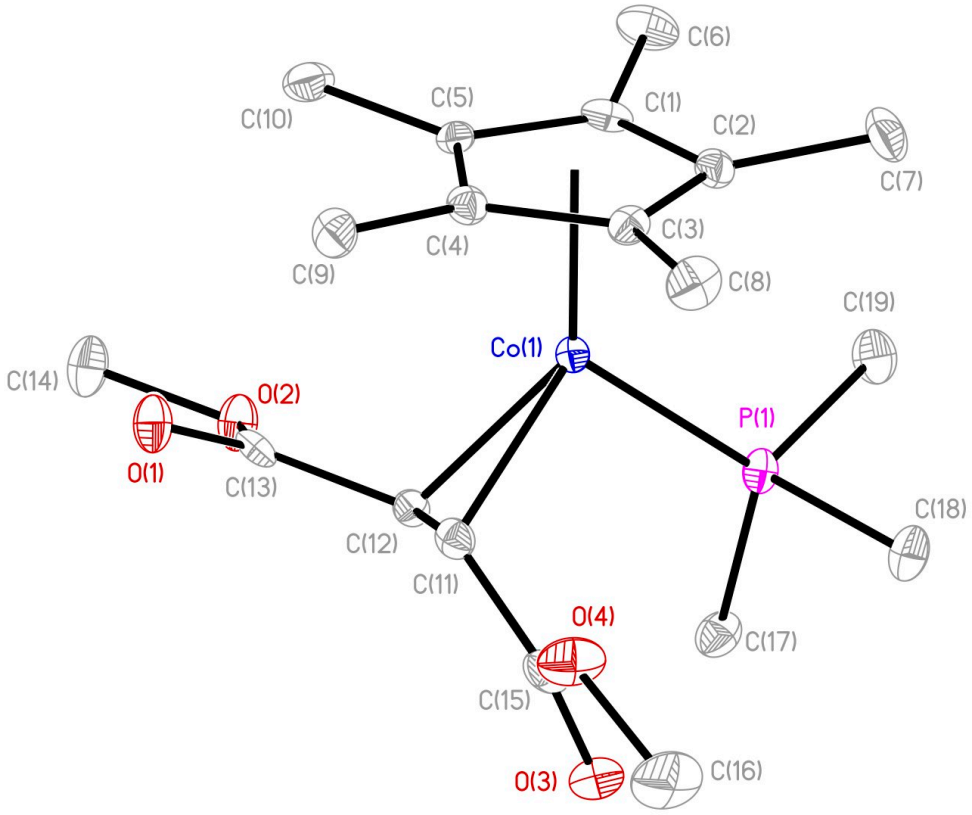


Figure S22. Molecular structure of **7** with 30 % probability ellipsoids and full atom labeling schemes. Hydrogen atoms omitted for clarity.

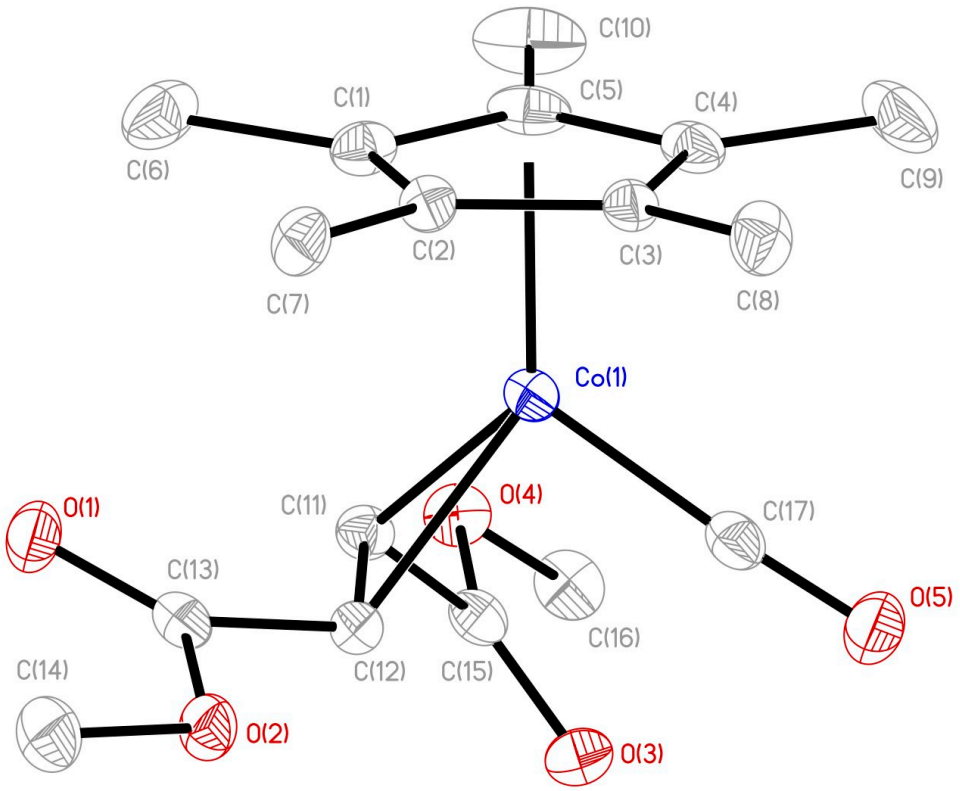


Figure S23. Molecular structure of **8** with 30 % probability ellipsoids and full atom labeling schemes. Hydrogen atoms omitted for clarity.

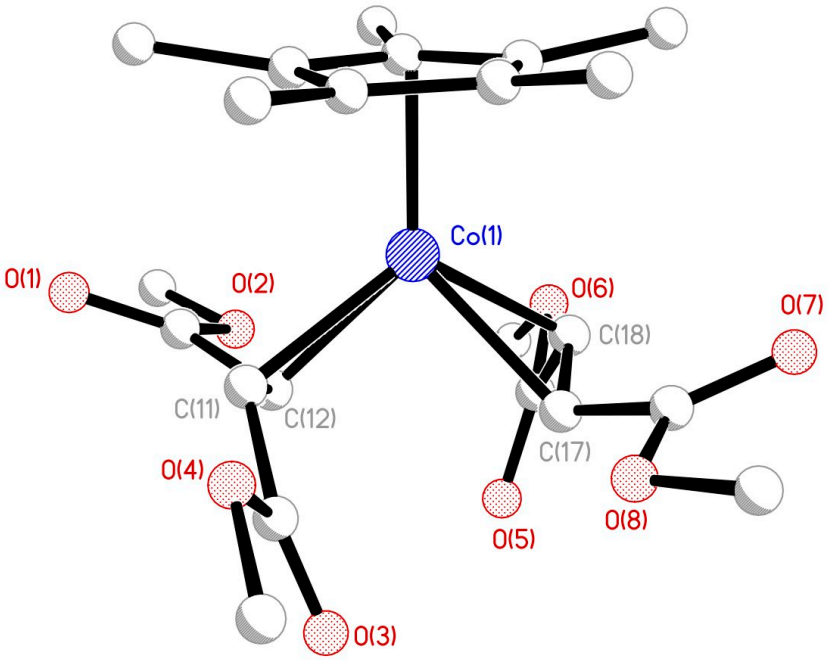


Figure S24. Ball and stick representation of the X-ray structure of **5**, establishing molecular connectivity.

Table 1. Crystallographic data for complexes **2**, **7**, and **8.**

Compound	**2**	**7**	**8**
Empirical formula	$C_{26}H_{38}Co_2O_4$	$C_{19}H_{32}CoO_4P$	$C_{17}H_{23}CoO_5$
Formula mass	532.42	414.35	366.28
a [Å]	9.2061(7)	14.986(4)	8.331(4)
b [Å]	10.7316(8)	14.019(4)	9.448(4)
c [Å]	13.5466(10)	9.855(3)	11.207(5)
α [°]	90.0490(10)	90	86.917(4)
β [°]	108.9940(10)	90	83.484(4)
γ [°]	95.4980(10)	90	78.249(4)
V [Å^3]	1258.93(16)	2070.3(10)	857.5(6)
Z	2	4	2
Crystal system	Triclinic	Orthorhombic	Triclinic
Space group	P-1	Pna2(1)	P-1
T [K]	150(2)	150(2)	150(2)
$D_{calcd.}$ [g cm^{-3}]	1.405	1.329	1.419
μ [mm^{-1}]	1.346	0.925	1.022
$2\theta_{max.}$ [°]	25.68	25.70	25.68
Reflections measured	12056	18967	6823
Reflections used (R_{int})	4749(0.0204)	3929(0.0546)	3218(0.0339)
Restraints/parameters	0/309	1/245	0/223
R_1 [$I > 2\sigma(I)$]	0.0266	0.0296	0.0405
wR_2 [$I > 2\sigma(I)$]	0.0671	0.0563	0.1064
$R(F_o^2)$ (all data)	0.0329	0.0379	0.0519
$R_w(F_o^2)$ (all data)	0.0712	0.0597	0.1137
GOF on F^2	1.035	1.029	1.042

Further crystallographic information can be found on the Cambridge Structural Database (CSD) for **2** (CCDC #: 865144), **7** (CCDC #: 865145), and **8** (CCDC #: 865146).

Table 2. Bond lengths [Å] and angles [°] for **2**.

Co(1)-C(21)	1.9055(19)
Co(1)-C(22)	2.0212(19)
Co(1)-C(4)	2.043(2)
Co(1)-C(5)	2.064(2)
Co(1)-C(1)	2.083(2)
Co(1)-C(2)	2.100(2)
Co(1)-C(3)	2.104(2)
Co(1)-Co(2)	2.5795(4)
Co(1)-H(1H)	1.54(2)
Co(2)-C(21)	1.9347(19)
Co(2)-O(1)	2.0058(13)
Co(2)-C(13)	2.045(2)
Co(2)-C(15)	2.065(2)
Co(2)-C(14)	2.076(2)
Co(2)-C(12)	2.0812(19)
Co(2)-C(11)	2.084(2)
Co(2)-H(1H)	1.66(2)
O(1)-C(23)	1.256(2)
O(2)-C(23)	1.343(2)
O(2)-C(24)	1.442(2)
O(3)-C(25)	1.210(2)
O(4)-C(25)	1.373(2)
O(4)-C(26)	1.436(2)
C(1)-C(5)	1.408(3)
C(1)-C(2)	1.443(3)
C(1)-C(6)	1.506(3)
C(2)-C(3)	1.410(3)
C(2)-C(7)	1.504(3)
C(3)-C(4)	1.419(3)
C(3)-C(8)	1.502(3)
C(4)-C(5)	1.440(3)
C(4)-C(9)	1.502(3)
C(5)-C(10)	1.503(3)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.408(3)
C(11)-C(15)	1.442(3)
C(11)-C(16)	1.495(3)
C(12)-C(13)	1.443(3)

C(12)-C(17)	1.496(3)
C(13)-C(14)	1.427(3)
C(13)-C(18)	1.497(3)
C(14)-C(15)	1.412(3)
C(14)-C(19)	1.499(3)
C(15)-C(20)	1.493(3)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.456(3)
C(21)-C(25)	1.461(3)
C(22)-C(23)	1.418(3)
C(22)-H(22)	0.96(2)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800

C(21)-Co(1)-C(22)	43.41(8)
C(21)-Co(1)-C(4)	116.72(9)
C(22)-Co(1)-C(4)	97.54(9)
C(21)-Co(1)-C(5)	148.57(9)
C(22)-Co(1)-C(5)	108.86(9)
C(4)-Co(1)-C(5)	41.04(9)
C(21)-Co(1)-C(1)	170.94(9)
C(22)-Co(1)-C(1)	145.57(9)
C(4)-Co(1)-C(1)	67.46(9)
C(5)-Co(1)-C(1)	39.69(9)
C(21)-Co(1)-C(2)	132.30(9)
C(22)-Co(1)-C(2)	160.85(9)
C(4)-Co(1)-C(2)	66.96(9)
C(5)-Co(1)-C(2)	67.42(9)
C(1)-Co(1)-C(2)	40.36(9)
C(21)-Co(1)-C(3)	110.59(8)
C(22)-Co(1)-C(3)	121.66(9)
C(4)-Co(1)-C(3)	39.97(9)
C(5)-Co(1)-C(3)	67.69(8)
C(1)-Co(1)-C(3)	66.91(9)
C(2)-Co(1)-C(3)	39.19(9)
C(21)-Co(1)-Co(2)	48.28(6)

C(22)-Co(1)-Co(2)	70.83(6)
C(4)-Co(1)-Co(2)	164.98(7)
C(5)-Co(1)-Co(2)	150.87(6)
C(1)-Co(1)-Co(2)	127.46(6)
C(2)-Co(1)-Co(2)	122.09(7)
C(3)-Co(1)-Co(2)	138.61(6)
C(21)-Co(1)-H(1H)	85.9(9)
C(22)-Co(1)-H(1H)	96.1(9)
C(4)-Co(1)-H(1H)	156.9(9)
C(5)-Co(1)-H(1H)	116.4(9)
C(1)-Co(1)-H(1H)	90.9(9)
C(2)-Co(1)-H(1H)	102.3(9)
C(3)-Co(1)-H(1H)	139.4(9)
Co(2)-Co(1)-H(1H)	37.8(9)
C(21)-Co(2)-O(1)	86.46(7)
C(21)-Co(2)-C(13)	111.69(8)
O(1)-Co(2)-C(13)	158.17(7)
C(21)-Co(2)-C(15)	128.28(8)
O(1)-Co(2)-C(15)	91.56(7)
C(13)-Co(2)-C(15)	67.87(8)
C(21)-Co(2)-C(14)	104.43(8)
O(1)-Co(2)-C(14)	125.18(7)
C(13)-Co(2)-C(14)	40.52(8)
C(15)-Co(2)-C(14)	39.88(8)
C(21)-Co(2)-C(12)	146.42(8)
O(1)-Co(2)-C(12)	125.41(7)
C(13)-Co(2)-C(12)	40.95(8)
C(15)-Co(2)-C(12)	67.45(8)
C(14)-Co(2)-C(12)	67.84(8)
C(21)-Co(2)-C(11)	168.84(8)
O(1)-Co(2)-C(11)	91.86(7)
C(13)-Co(2)-C(11)	67.94(8)
C(15)-Co(2)-C(11)	40.67(8)
C(14)-Co(2)-C(11)	67.68(8)
C(12)-Co(2)-C(11)	39.52(8)
C(21)-Co(2)-Co(1)	47.32(6)
O(1)-Co(2)-Co(1)	87.98(4)
C(13)-Co(2)-Co(1)	113.10(6)
C(15)-Co(2)-Co(1)	175.60(6)
C(14)-Co(2)-Co(1)	138.18(6)
C(12)-Co(2)-Co(1)	116.26(6)
C(11)-Co(2)-Co(1)	143.71(6)
C(21)-Co(2)-H(1H)	81.9(8)
O(1)-Co(2)-H(1H)	86.1(8)
C(13)-Co(2)-H(1H)	107.7(8)
C(15)-Co(2)-H(1H)	149.6(8)
C(14)-Co(2)-H(1H)	148.0(8)
C(12)-Co(2)-H(1H)	89.4(8)
C(11)-Co(2)-H(1H)	109.0(8)
Co(1)-Co(2)-H(1H)	34.7(8)
C(23)-O(1)-Co(2)	106.75(12)
C(23)-O(2)-C(24)	117.49(16)
C(25)-O(4)-C(26)	114.60(16)
C(5)-C(1)-C(2)	108.3(2)

C(5)-C(1)-C(6)	127.7(2)
C(2)-C(1)-C(6)	123.7(2)
C(5)-C(1)-Co(1)	69.43(12)
C(2)-C(1)-Co(1)	70.43(12)
C(6)-C(1)-Co(1)	130.72(16)
C(3)-C(2)-C(1)	108.0(2)
C(3)-C(2)-C(7)	125.8(2)
C(1)-C(2)-C(7)	125.6(2)
C(3)-C(2)-Co(1)	70.59(12)
C(1)-C(2)-Co(1)	69.21(12)
C(7)-C(2)-Co(1)	132.33(16)
C(2)-C(3)-C(4)	107.8(2)
C(2)-C(3)-C(8)	126.2(2)
C(4)-C(3)-C(8)	125.9(2)
C(2)-C(3)-Co(1)	70.23(12)
C(4)-C(3)-Co(1)	67.67(12)
C(8)-C(3)-Co(1)	130.04(16)
C(3)-C(4)-C(5)	108.6(2)
C(3)-C(4)-C(9)	125.4(2)
C(5)-C(4)-C(9)	125.8(2)
C(3)-C(4)-Co(1)	72.35(12)
C(5)-C(4)-Co(1)	70.28(12)
C(9)-C(4)-Co(1)	126.71(16)
C(1)-C(5)-C(4)	107.14(19)
C(1)-C(5)-C(10)	127.3(2)
C(4)-C(5)-C(10)	125.6(2)
C(1)-C(5)-Co(1)	70.88(12)
C(4)-C(5)-Co(1)	68.68(12)
C(10)-C(5)-Co(1)	126.52(15)
C(1)-C(6)-H(6A)	109.5
C(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(3)-C(8)-H(8A)	109.5
C(3)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(3)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(4)-C(9)-H(9A)	109.5
C(4)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(4)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-H(10A)	109.5

C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(15)	107.74(18)
C(12)-C(11)-C(16)	127.8(2)
C(15)-C(11)-C(16)	124.4(2)
C(12)-C(11)-Co(2)	70.12(11)
C(15)-C(11)-Co(2)	68.96(11)
C(16)-C(11)-Co(2)	125.61(15)
C(11)-C(12)-C(13)	108.03(18)
C(11)-C(12)-C(17)	126.6(2)
C(13)-C(12)-C(17)	125.3(2)
C(11)-C(12)-Co(2)	70.36(11)
C(13)-C(12)-Co(2)	68.16(11)
C(17)-C(12)-Co(2)	127.91(15)
C(14)-C(13)-C(12)	107.83(18)
C(14)-C(13)-C(18)	125.9(2)
C(12)-C(13)-C(18)	125.96(19)
C(14)-C(13)-Co(2)	70.93(11)
C(12)-C(13)-Co(2)	70.89(11)
C(18)-C(13)-Co(2)	128.86(15)
C(15)-C(14)-C(13)	107.81(18)
C(15)-C(14)-C(19)	125.6(2)
C(13)-C(14)-C(19)	126.4(2)
C(15)-C(14)-Co(2)	69.65(12)
C(13)-C(14)-Co(2)	68.55(11)
C(19)-C(14)-Co(2)	131.17(14)
C(14)-C(15)-C(11)	108.51(18)
C(14)-C(15)-C(20)	126.6(2)
C(11)-C(15)-C(20)	124.9(2)
C(14)-C(15)-Co(2)	70.47(12)
C(11)-C(15)-Co(2)	70.38(11)
C(20)-C(15)-Co(2)	125.61(14)
C(11)-C(16)-H(16A)	109.5
C(11)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(11)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(12)-C(17)-H(17A)	109.5
C(12)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(12)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(13)-C(18)-H(18A)	109.5
C(13)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(14)-C(19)-H(19A)	109.5

C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(15)-C(20)-H(20A)	109.5
C(15)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(15)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(22)-C(21)-C(25)	121.42(17)
C(22)-C(21)-Co(1)	72.53(11)
C(25)-C(21)-Co(1)	118.86(13)
C(22)-C(21)-Co(2)	104.94(13)
C(25)-C(21)-Co(2)	132.07(14)
Co(1)-C(21)-Co(2)	84.39(8)
C(23)-C(22)-C(21)	114.25(17)
C(23)-C(22)-Co(1)	107.73(13)
C(21)-C(22)-Co(1)	64.06(10)
C(23)-C(22)-H(22)	120.0(13)
C(21)-C(22)-H(22)	121.7(13)
Co(1)-C(22)-H(22)	114.5(13)
O(1)-C(23)-O(2)	120.47(17)
O(1)-C(23)-C(22)	122.14(17)
O(2)-C(23)-C(22)	117.38(17)
O(2)-C(24)-H(24A)	109.5
O(2)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
O(2)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
O(3)-C(25)-O(4)	120.40(18)
O(3)-C(25)-C(21)	127.32(19)
O(4)-C(25)-C(21)	112.28(17)
O(4)-C(26)-H(26A)	109.5
O(4)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
O(4)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

Table 3. Bond lengths [Å] and angles [°] for **7**.

Co(1)-C(11)	2.008(2)
Co(1)-C(12)	2.029(3)
Co(1)-C(3)	2.097(3)
Co(1)-C(4)	2.103(3)
Co(1)-C(2)	2.104(3)
Co(1)-C(1)	2.119(3)
Co(1)-C(5)	2.127(3)
Co(1)-P(1)	2.1969(10)
O(1)-C(13)	1.210(3)
O(2)-C(13)	1.353(3)
O(2)-C(14)	1.442(3)
O(3)-C(15)	1.217(3)
O(4)-C(15)	1.359(3)
O(4)-C(16)	1.439(4)
P(1)-C(18)	1.822(3)
P(1)-C(19)	1.832(3)
P(1)-C(17)	1.835(3)
C(1)-C(5)	1.414(4)
C(1)-C(2)	1.445(4)
C(1)-C(6)	1.504(4)
C(2)-C(3)	1.416(4)
C(2)-C(7)	1.511(4)
C(3)-C(4)	1.441(4)
C(3)-C(8)	1.500(4)
C(4)-C(5)	1.420(4)
C(4)-C(9)	1.500(4)
C(5)-C(10)	1.507(4)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.437(4)
C(11)-C(15)	1.458(4)
C(11)-H(11)	0.89(3)
C(12)-C(13)	1.464(4)
C(12)-H(12)	0.97(2)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800

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C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800

C(11)-Co(1)-C(12)	41.69(12)
C(11)-Co(1)-C(3)	104.59(13)
C(12)-Co(1)-C(3)	140.37(12)
C(11)-Co(1)-C(4)	91.96(13)
C(12)-Co(1)-C(4)	108.57(10)
C(3)-Co(1)-C(4)	40.12(11)
C(11)-Co(1)-C(2)	142.62(13)
C(12)-Co(1)-C(2)	171.03(11)
C(3)-Co(1)-C(2)	39.39(11)
C(4)-Co(1)-C(2)	66.10(11)
C(11)-Co(1)-C(1)	154.78(13)
C(12)-Co(1)-C(1)	131.77(11)
C(3)-Co(1)-C(1)	66.96(11)
C(4)-Co(1)-C(1)	66.00(11)
C(2)-Co(1)-C(1)	40.01(10)
C(11)-Co(1)-C(5)	115.97(12)
C(12)-Co(1)-C(5)	105.25(11)
C(3)-Co(1)-C(5)	66.71(10)
C(4)-Co(1)-C(5)	39.23(10)
C(2)-Co(1)-C(5)	65.97(10)
C(1)-Co(1)-C(5)	38.91(10)
C(11)-Co(1)-P(1)	100.69(10)
C(12)-Co(1)-P(1)	92.52(8)
C(3)-Co(1)-P(1)	118.65(8)
C(4)-Co(1)-P(1)	158.21(7)
C(2)-Co(1)-P(1)	93.64(8)
C(1)-Co(1)-P(1)	104.13(8)
C(5)-Co(1)-P(1)	140.73(8)
C(13)-O(2)-C(14)	116.5(2)
C(15)-O(4)-C(16)	117.0(2)
C(18)-P(1)-C(19)	102.72(14)
C(18)-P(1)-C(17)	101.94(14)
C(19)-P(1)-C(17)	96.79(14)
C(18)-P(1)-Co(1)	113.32(10)
C(19)-P(1)-Co(1)	118.34(10)
C(17)-P(1)-Co(1)	120.72(10)
C(5)-C(1)-C(2)	107.3(2)
C(5)-C(1)-C(6)	125.5(3)
C(2)-C(1)-C(6)	126.4(2)
C(5)-C(1)-Co(1)	70.84(15)
C(2)-C(1)-Co(1)	69.44(15)

C(6)-C(1)-Co(1)	132.9(2)
C(3)-C(2)-C(1)	108.8(2)
C(3)-C(2)-C(7)	123.5(3)
C(1)-C(2)-C(7)	126.2(3)
C(3)-C(2)-Co(1)	70.02(15)
C(1)-C(2)-Co(1)	70.55(14)
C(7)-C(2)-Co(1)	136.5(2)
C(2)-C(3)-C(4)	106.9(2)
C(2)-C(3)-C(8)	126.7(3)
C(4)-C(3)-C(8)	126.2(3)
C(2)-C(3)-Co(1)	70.60(16)
C(4)-C(3)-Co(1)	70.17(15)
C(8)-C(3)-Co(1)	128.0(2)
C(5)-C(4)-C(3)	108.5(2)
C(5)-C(4)-C(9)	125.8(2)
C(3)-C(4)-C(9)	125.3(3)
C(5)-C(4)-Co(1)	71.29(15)
C(3)-C(4)-Co(1)	69.70(15)
C(9)-C(4)-Co(1)	130.30(19)
C(1)-C(5)-C(4)	108.4(2)
C(1)-C(5)-C(10)	125.2(3)
C(4)-C(5)-C(10)	126.1(3)
C(1)-C(5)-Co(1)	70.26(16)
C(4)-C(5)-Co(1)	69.48(15)
C(10)-C(5)-Co(1)	131.02(19)
C(1)-C(6)-H(6A)	109.5
C(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(3)-C(8)-H(8A)	109.5
C(3)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(3)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(4)-C(9)-H(9A)	109.5
C(4)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(4)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5

H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(15)	125.0(3)
C(12)-C(11)-Co(1)	69.96(15)
C(15)-C(11)-Co(1)	116.97(18)
C(12)-C(11)-H(11)	115.3(17)
C(15)-C(11)-H(11)	113.1(16)
Co(1)-C(11)-H(11)	108.0(16)
C(11)-C(12)-C(13)	119.8(2)
C(11)-C(12)-Co(1)	68.35(14)
C(13)-C(12)-Co(1)	117.54(19)
C(11)-C(12)-H(12)	118.0(14)
C(13)-C(12)-H(12)	113.8(14)
Co(1)-C(12)-H(12)	111.4(14)
O(1)-C(13)-O(2)	121.8(3)
O(1)-C(13)-C(12)	126.9(3)
O(2)-C(13)-C(12)	111.3(2)
O(2)-C(14)-H(14A)	109.5
O(2)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
O(2)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(3)-C(15)-O(4)	122.1(3)
O(3)-C(15)-C(11)	128.3(3)
O(4)-C(15)-C(11)	109.6(3)
O(4)-C(16)-H(16A)	109.5
O(4)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
O(4)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
P(1)-C(17)-H(17A)	109.5
P(1)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
P(1)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
P(1)-C(18)-H(18A)	109.5
P(1)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
P(1)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
P(1)-C(19)-H(19A)	109.5
P(1)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
P(1)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

Table 4. Bond lengths [Å] and angles [°] for **8**.

Co(1)-C(17)	1.748(3)
Co(1)-C(11)	2.011(3)
Co(1)-C(12)	2.030(3)
Co(1)-C(4)	2.070(3)
Co(1)-C(5)	2.088(3)
Co(1)-C(1)	2.090(3)
Co(1)-C(3)	2.092(3)
Co(1)-C(2)	2.121(3)
O(1)-C(13)	1.212(4)
O(2)-C(13)	1.350(4)
O(2)-C(14)	1.445(3)
O(3)-C(15)	1.205(4)
O(4)-C(15)	1.355(3)
O(4)-C(16)	1.447(4)
O(5)-C(17)	1.145(4)
C(1)-C(2)	1.431(4)
C(1)-C(5)	1.438(4)
C(1)-C(6)	1.493(4)
C(2)-C(3)	1.414(4)
C(2)-C(7)	1.504(4)
C(3)-C(4)	1.440(4)
C(3)-C(8)	1.497(4)
C(4)-C(5)	1.410(5)
C(4)-C(9)	1.513(4)
C(5)-C(10)	1.504(4)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.427(4)
C(11)-C(15)	1.471(4)
C(11)-H(11)	0.98(3)
C(12)-C(13)	1.474(4)
C(12)-H(12)	1.00(3)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800

C(17)-Co(1)-C(11)	99.43(13)
C(17)-Co(1)-C(12)	91.39(13)
C(11)-Co(1)-C(12)	41.33(11)
C(17)-Co(1)-C(4)	92.64(13)
C(11)-Co(1)-C(4)	139.57(12)
C(12)-Co(1)-C(4)	175.48(11)
C(17)-Co(1)-C(5)	123.10(14)
C(11)-Co(1)-C(5)	104.39(13)
C(12)-Co(1)-C(5)	138.17(13)
C(4)-Co(1)-C(5)	39.65(13)
C(17)-Co(1)-C(1)	159.66(13)
C(11)-Co(1)-C(1)	97.23(12)
C(12)-Co(1)-C(1)	108.86(12)
C(4)-Co(1)-C(1)	67.06(12)
C(5)-Co(1)-C(1)	40.27(12)
C(17)-Co(1)-C(3)	97.41(13)
C(11)-Co(1)-C(3)	163.08(12)
C(12)-Co(1)-C(3)	136.79(11)
C(4)-Co(1)-C(3)	40.47(11)
C(5)-Co(1)-C(3)	67.15(12)
C(1)-Co(1)-C(3)	66.67(11)
C(17)-Co(1)-C(2)	132.27(13)
C(11)-Co(1)-C(2)	124.53(12)
C(12)-Co(1)-C(2)	108.82(11)
C(4)-Co(1)-C(2)	66.87(11)
C(5)-Co(1)-C(2)	67.00(12)
C(1)-Co(1)-C(2)	39.71(11)
C(3)-Co(1)-C(2)	39.21(10)
C(13)-O(2)-C(14)	116.3(2)
C(15)-O(4)-C(16)	114.6(2)
C(2)-C(1)-C(5)	108.2(3)
C(2)-C(1)-C(6)	125.8(3)
C(5)-C(1)-C(6)	125.7(3)
C(2)-C(1)-Co(1)	71.31(17)
C(5)-C(1)-Co(1)	69.79(18)
C(6)-C(1)-Co(1)	129.8(2)
C(3)-C(2)-C(1)	107.8(2)
C(3)-C(2)-C(7)	126.6(3)
C(1)-C(2)-C(7)	125.5(3)
C(3)-C(2)-Co(1)	69.29(16)
C(1)-C(2)-Co(1)	68.98(16)
C(7)-C(2)-Co(1)	130.0(2)
C(2)-C(3)-C(4)	108.1(3)
C(2)-C(3)-C(8)	126.7(3)
C(4)-C(3)-C(8)	124.8(3)
C(2)-C(3)-Co(1)	71.50(16)
C(4)-C(3)-Co(1)	68.92(16)
C(8)-C(3)-Co(1)	130.5(2)
C(5)-C(4)-C(3)	108.4(3)
C(5)-C(4)-C(9)	127.0(3)
C(3)-C(4)-C(9)	124.4(3)
C(5)-C(4)-Co(1)	70.88(18)
C(3)-C(4)-Co(1)	70.61(16)
C(9)-C(4)-Co(1)	128.1(2)

C(4)-C(5)-C(1)	107.5(3)
C(4)-C(5)-C(10)	125.9(3)
C(1)-C(5)-C(10)	126.6(3)
C(4)-C(5)-Co(1)	69.47(18)
C(1)-C(5)-Co(1)	69.94(18)
C(10)-C(5)-Co(1)	126.4(2)
C(1)-C(6)-H(6A)	109.5
C(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(3)-C(8)-H(8A)	109.5
C(3)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(3)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(4)-C(9)-H(9A)	109.5
C(4)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(4)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(15)	119.6(3)
C(12)-C(11)-Co(1)	70.06(16)
C(15)-C(11)-Co(1)	112.0(2)
C(12)-C(11)-H(11)	119.0(17)
C(15)-C(11)-H(11)	115.7(17)
Co(1)-C(11)-H(11)	110.6(17)
C(11)-C(12)-C(13)	121.2(3)
C(11)-C(12)-Co(1)	68.61(16)
C(13)-C(12)-Co(1)	116.7(2)
C(11)-C(12)-H(12)	117.8(17)
C(13)-C(12)-H(12)	113.9(17)
Co(1)-C(12)-H(12)	110.2(17)
O(1)-C(13)-O(2)	122.8(3)
O(1)-C(13)-C(12)	127.6(3)
O(2)-C(13)-C(12)	109.5(3)
O(2)-C(14)-H(14A)	109.5
O(2)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5

O(2)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(3)-C(15)-O(4)	122.6(3)
O(3)-C(15)-C(11)	126.3(3)
O(4)-C(15)-C(11)	111.1(3)
O(4)-C(16)-H(16A)	109.5
O(4)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
O(4)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
O(5)-C(17)-Co(1)	175.8(3)