Supplementary Material (ESI) for Dalton Transactions

An NMR Study of cobalt-catalyzed hydroformylation using *Para*-Hydrogen Induced Polarisation

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Supplementary Information

Synthesis of $Co(\eta^3\text{-}C_3H_5)(CO)_2(PPhMe_2)$ 2. A THF solution of $Co(\eta^3\text{-}C_3H_5)(CO)_3$ (3.4 mmol) was prepared as described above for **1.** A THF solution (20 ml) containing a slight excess of $PPhMe_2$ (270 µl, 1.88 mmol, 1.1 eq) was then slowly added via cannula transfer and the reaction mixture stirred at room temperature for 15-20 minutes. The orange solution was then filtered, and the solvent removed under vacuum at 0°C. **2** was isolated as a red oil in 40 % yield. ν_{CO} in CH_2Cl_2 (cm^{-1}) 1980, 1916.

Synthesis of $Co(\eta^3\text{-}C_3H_5)(CO)_2(PBz_3)$ 3. A THF solution of $Co(\eta^3\text{-}C_3H_5)(CO)_3$ (3.4 mmol) was prepared as described above for **1.** A THF solution (20 ml) containing a slight excess of PBz_3 (1.1 g, 3.75 mmol, 1.1 eq) was then slowly added via cannula transfer and the reaction mixture stirred at room temperature for 15-20 minutes. The yellow orange solution was then filtered, and the solvent removed under vacuum. The product was then extracted from hexane and dried under vacuum. **3** was isolated as a yellow solid in 52 % yield. ν_{CO} in CH_2Cl_2 (cm^{-1}) 1980, 1920.

Synthesis of $Co(\eta^3\text{-}C_3H_5)(CO)_2(PCy_3)$ 4. A THF solution of $Co(\eta^3\text{-}C_3H_5)(CO)_3$ (3.4 mmol) was prepared as described above for **1.** A THF solution (20 ml) containing a slight excess of PCy_3 (1 g, 3.75 mmol, 1.1 eq) was then slowly added via cannula transfer and the reaction mixture stirred at room temperature for 15-20 minutes (note that when the reaction mixture was left stirring for several hours, decomposition of the product was observed). The yellow-orange solution was then filtered, and the solvent removed under vacuum. **4** was extracted from pentane and was isolated as a yellow-orange solid in 55 % yield. ν_{CO} in CH_2Cl_2 (cm^{-1}) 1971, 1910.

Synthesis of $Co(\eta^3\text{-}C_3H_5)(CO)_2(PPh_3)$ 5. A THF solution of $Co(\eta^3\text{-}C_3H_5)(CO)_3$ (3.4 mmol) was prepared as described above for **1.** A THF solution (20 ml) containing a slight excess of PPh_3 (1 g, 3.75 mmol, 1.1 eq) was then slowly added via cannula transfer and the reaction mixture stirred at room temperature for 15-20 minutes. The orange solution was then filtered, and the solvent removed under vacuum.

p-H_2 based NMR signal intensities for species **4a, 4b** and the corresponding aldehydes as a function of temperature for samples of **1** reacting in toluene with 3 atm. of a 2 : 1 mixture of CO and H_2 normalised relative to free branched aldehyde.

Raw data collected as integrals of the parahydrogen enhanced peak for each site.
With simulated correction factors to take into account internal cancellation within the antiphase multipletes prior to magnitude calculation and site degeneracy.

Temp	lin al	lin be	bra a	lin bet	bran bet
363	59	27	12	12	15
368	65	75	16	12	16
373	38	58	11	12	12
378	53	62	14	26	28
383	65	85	16	42	46
388	48	70	19	71	65
Correction factor					
	1.14	1.71	1	1.71	6.85

Actual data used in the generation of Figure 6.

Normalised

	lin al	lin be	bra a	lin bet	bran bet
368.0	23.6	7.2	5.5	3.2	1.0
373.0	24.4	18.8	6.9	3.0	1.0
378.0	19.0	19.4	6.3	4.0	1.0
383.0	11.4	8.9	3.4	3.7	1.0
388.0	8.5	7.4	2.4	3.7	1.0
392.0	4.4	4.3	2.0	4.4	1.0

Data used for Figure 7, 8, 9 and 10.

Data for	Temp	Fig 9	Temp	Fig 7	Fig 8	Fig 10	373 K
dppe	368.0	1.2	376.4	2.7			
	373.0	1.3	382.8	2.7	0.8	CO/H2	lin/bra
	378.0	1.3	389.2	2.6	0.8	04:01	4.0
	383.0	1.2	395.8	2.3	0.8	01:01	2.7
	388.0	1.2	402.4	2.0	0.8	01:02	2.6
	392.0	1.1	409.1	1.8	0.9	01:04	1.8
dppm	368.0	1.8	376.4	1.6			
	373.0	1.8	382.8	1.6	0.6	CO/H2	lin/bra
	378.0	1.7	389.2	1.7	0.6	04:01	2.0
	383.0	1.7	395.8	1.6	0.6	01:01	1.2
	388.0	1.5	402.4	1.5	0.7	01:02	1.7
	392.0	1.4	409.1	1.2	0.7	01:04	1.7

PPh3	368.0	1.1	376.4			CO/H2	lin/bra
	373.0	1.3	382.8	3.1	0.9	04:01	2.3
	378.0	1.3	389.2	2.9	0.8	01:01	2.9
	383.0	1.4	395.8	2.9	0.7	01:02	2.9
	388.0	1.3	402.4	2.9	0.7	01:04	2.8
			409.1	2.6	0.8		
PPh2Me	368.0	1.0	376.4	2.5	0.4	CO/H2	lin/bra
	373.0	1.2	382.8	2.6	0.4	04:01	3.8
	378.0	1.3	389.2	3.2	0.4	01:01	3.4
	383.0	1.3	395.8	3.4	0.4	01:02	3.4
	388.0	1.4	402.4	3.4	0.3	01:04	3.6
	392.0	1.3	409.1	3.4	0.3		
PMe2Ph	368.0	1.2	376.4	2.9	0.6		
	373.0	1.0	382.8	3.1	0.5	CO/H2	lin/bra
	378.0	1.2	389.2	3.2	0.5	4	3.7
	383.0	1.3	395.8	3.6	0.4	1	3.2
	388.0	1.3	402.4	3.7	0.4	0.5	3.2
	392.0	1.2	409.1	3.3	0.5	0.25	3.4
PCy3	368.0	0.3	376.4	2.0	3.3		
	373.0	0.8	382.8	2.1	1.3	CO/H2	lin/bra
	378.0	1.0	389.2	2.1	1.0	4	1.6
	383.0	0.8	395.8	2.5	1.3	1	1.8
	388.0	0.9	402.4	2.7	1.1	0.5	2.1
	392.0	1.0	409.1	3.2	1.0	0.25	1.3

X-ray crystallography

Table 1. Crystal data and structure refinement for $Co(\eta^3\text{-}C_3H_5)(CO)_2PPh_2Me$ (1).

Identification code	sbd0419	
Empirical formula	C18 H18 Co O2 P	
Formula weight	356.22	
Temperature	388(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 15.2928(17) Å	α= 90°.
	b = 13.6440(16) Å	β= 90°.
	c = 15.9287(18) Å	γ = 90°.

Volume	3323.6(7) $Å^3$
Z	8
Density (calculated)	1.424 Mg/m^3
Absorption coefficient	1.132 mm^{-1}
F(000)	1472
Crystal size	0.3 x 0.2 x 0.1 mm^3
Theta range for data collection	2.37 to 30.98°.
Index ranges	-22<=h<=21, -19<=k<=18, -22<=l<=22
Reflections collected	35594
Independent reflections	5049 [R(int) = 0.0696]
Completeness to theta = 30.98°	95.5 %
Absorption correction	Multi_scan
Max. and min. transmission	1.000 and 0.824
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5049 / 0 / 200
Goodness-of-fit on F^2	1.061
Final R indices [I>2sigma(I)]	R1 = 0.0511, wR2 = 0.1133
R indices (all data)	R1 = 0.0736, wR2 = 0.1227
Largest diff. peak and hole	1.234 and -0.384 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $Co(\eta^3\text{-}C_3H_5)(CO)_2PPh_2Me$ (1).. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2132(2)	2149(2)	1526(2)	29(1)
C(2)	3265(2)	3871(2)	1965(2)	25(1)
C(3)	1754(2)	4167(2)	1020(2)	32(1)
C(4)	1432(2)	4465(2)	1814(2)	34(1)
C(5)	936(2)	3800(3)	2240(2)	42(1)
C(6)	1392(2)	2168(2)	3720(2)	18(1)
C(7)	1279(2)	1200(2)	3451(2)	22(1)
C(8)	574(2)	654(2)	3724(2)	27(1)
C(9)	-32(2)	1057(2)	4268(2)	30(1)
C(10)	73(2)	2012(2)	4540(2)	37(1)
C(11)	786(2)	2570(2)	4269(2)	30(1)
C(12)	3229(2)	2048(2)	3608(2)	17(1)
C(13)	3234(2)	1621(2)	4401(2)	22(1)
C(14)	3912(2)	1002(2)	4637(2)	26(1)
C(15)	4593(2)	823(2)	4089(2)	28(1)
C(16)	4600(2)	1248(2)	3305(2)	28(1)
C(17)	3912(2)	1859(2)	3063(2)	23(1)
C(18)	2454(2)	3860(2)	4059(2)	26(1)
Co(1)	2231(1)	3313(1)	2011(1)	17(1)
O(1)	2099(2)	1392(2)	1216(2)	51(1)
O(2)	3936(1)	4240(2)	1915(1)	39(1)
P(2)	2323(1)	2859(1)	3315(1)	16(1)

Table 3. Bond lengths [Å] and angles [°] for $Co(\eta^3\text{-}C_3H_5)(CO)_2PPh_2Me$ (1)..

C(1)-O(1)	1.146(3)
C(1)-Co(1)	1.772(3)
C(2)-O(2)	1.146(3)
C(2)-Co(1)	1.757(3)
C(3)-C(4)	1.416(4)
C(3)-Co(1)	2.093(3)
C(3)-H(3A)	0.9300
C(3)-H(3B)	0.9300
C(4)-C(5)	1.364(4)
C(4)-Co(1)	2.016(3)
C(4)-H(4)	0.9300
C(5)-Co(1)	2.119(3)
C(5)-H(5A)	0.9300
C(5)-H(5B)	0.9300
C(6)-C(11)	1.387(3)
C(6)-C(7)	1.398(3)
C(6)-P(2)	1.825(2)
C(7)-C(8)	1.381(4)
C(7)-H(7)	0.9300
C(8)-C(9)	1.384(4)
C(8)-H(8)	0.9300
C(9)-C(10)	1.382(4)
C(9)-H(9)	0.9300
C(10)-C(11)	1.397(4)
C(10)-H(10)	0.9300
C(11)-H(11)	0.9300
C(12)-C(17)	1.382(3)
C(12)-C(13)	1.390(3)
C(12)-P(2)	1.835(2)
C(13)-C(14)	1.390(3)
C(13)-H(13)	0.9300
C(14)-C(15)	1.380(4)
C(14)-H(14)	0.9300
C(15)-C(16)	1.378(4)
C(15)-H(15)	0.9300
C(16)-C(17)	1.396(4)

C(16)-H(16)	0.9300
C(17)-H(17)	0.9300
C(18)-P(2)	1.818(3)
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
Co(1)-P(2)	2.1715(7)

O(1)-C(1)-Co(1)	177.6(3)
O(2)-C(2)-Co(1)	178.4(2)
C(4)-C(3)-Co(1)	66.91(16)
C(4)-C(3)-H(3A)	120.0
Co(1)-C(3)-H(3A)	80.3
C(4)-C(3)-H(3B)	120.0
Co(1)-C(3)-H(3B)	124.1
H(3A)-C(3)-H(3B)	120.0
C(5)-C(4)-C(3)	116.5(3)
C(5)-C(4)-Co(1)	74.92(18)
C(3)-C(4)-Co(1)	72.82(16)
C(5)-C(4)-H(4)	121.8
C(3)-C(4)-H(4)	121.8
Co(1)-C(4)-H(4)	121.8
C(4)-C(5)-Co(1)	66.67(17)
C(4)-C(5)-H(5A)	120.0
Co(1)-C(5)-H(5A)	79.6
C(4)-C(5)-H(5B)	120.0
Co(1)-C(5)-H(5B)	125.2
H(5A)-C(5)-H(5B)	120.0
C(11)-C(6)-C(7)	118.9(2)
C(11)-C(6)-P(2)	122.66(19)
C(7)-C(6)-P(2)	118.43(18)
C(8)-C(7)-C(6)	120.7(2)
C(8)-C(7)-H(7)	119.7
C(6)-C(7)-H(7)	119.7
C(7)-C(8)-C(9)	120.3(3)
C(7)-C(8)-H(8)	119.8
C(9)-C(8)-H(8)	119.8
C(10)-C(9)-C(8)	119.6(2)

C(10)-C(9)-H(9)	120.2
C(8)-C(9)-H(9)	120.2
C(9)-C(10)-C(11)	120.4(3)
C(9)-C(10)-H(10)	119.8
C(11)-C(10)-H(10)	119.8
C(6)-C(11)-C(10)	120.1(3)
C(6)-C(11)-H(11)	120.0
C(10)-C(11)-H(11)	120.0
C(17)-C(12)-C(13)	119.2(2)
C(17)-C(12)-P(2)	121.57(19)
C(13)-C(12)-P(2)	119.18(18)
C(14)-C(13)-C(12)	120.3(2)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8
C(15)-C(14)-C(13)	119.9(2)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0
C(16)-C(15)-C(14)	120.3(2)
C(16)-C(15)-H(15)	119.8
C(14)-C(15)-H(15)	119.8
C(15)-C(16)-C(17)	119.7(2)
C(15)-C(16)-H(16)	120.2
C(17)-C(16)-H(16)	120.2
C(12)-C(17)-C(16)	120.5(2)
C(12)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
P(2)-C(18)-H(18A)	109.5
P(2)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
P(2)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(2)-Co(1)-C(1)	116.52(13)
C(2)-Co(1)-C(4)	101.56(13)
C(1)-Co(1)-C(4)	125.41(13)
C(2)-Co(1)-C(3)	92.32(12)
C(1)-Co(1)-C(3)	98.06(12)
C(4)-Co(1)-C(3)	40.27(12)

C(2)-Co(1)-C(5)	135.39(14)
C(1)-Co(1)-C(5)	106.05(15)
C(4)-Co(1)-C(5)	38.41(12)
C(3)-Co(1)-C(5)	68.26(12)
C(2)-Co(1)-P(2)	96.05(9)
C(1)-Co(1)-P(2)	99.65(9)
C(4)-Co(1)-P(2)	114.23(9)
C(3)-Co(1)-P(2)	154.46(8)
C(5)-Co(1)-P(2)	89.16(10)
C(18)-P(2)-C(6)	104.12(12)
C(18)-P(2)-C(12)	101.78(12)
C(6)-P(2)-C(12)	100.79(10)
C(18)-P(2)-Co(1)	114.61(9)
C(6)-P(2)-Co(1)	115.76(8)
C(12)-P(2)-Co(1)	117.65(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Co(\eta^3\text{-}C_3H_5)(CO)_2PPh_2Me$ (1).. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	43(2)	24(1)	20(1)	2(1)	4(1)	3(1)
C(2)	22(1)	33(1)	20(1)	4(1)	0(1)	0(1)
C(3)	38(2)	32(1)	27(1)	7(1)	-1(1)	14(1)
C(4)	31(2)	31(1)	39(2)	3(1)	-1(1)	11(1)
C(5)	27(2)	43(2)	56(2)	14(2)	7(1)	17(1)
C(6)	15(1)	19(1)	20(1)	3(1)	0(1)	0(1)
C(7)	23(1)	21(1)	20(1)	-1(1)	-3(1)	-1(1)
C(8)	25(1)	24(1)	31(2)	1(1)	-5(1)	-7(1)
C(9)	19(1)	33(1)	39(2)	10(1)	1(1)	-7(1)
C(10)	25(1)	33(1)	55(2)	3(1)	19(1)	4(1)
C(11)	26(1)	21(1)	43(2)	0(1)	14(1)	2(1)
C(12)	15(1)	17(1)	20(1)	-2(1)	-1(1)	-1(1)
C(13)	18(1)	27(1)	20(1)	0(1)	0(1)	0(1)
C(14)	26(1)	30(1)	23(1)	5(1)	-5(1)	3(1)

C(15)	24(1)	29(1)	30(1)	-2(1)	-6(1)	11(1)
C(16)	22(1)	33(1)	30(1)	-2(1)	4(1)	10(1)
C(17)	25(1)	25(1)	20(1)	2(1)	1(1)	6(1)
C(18)	37(1)	19(1)	24(1)	-5(1)	4(1)	-4(1)
Co(1)	16(1)	17(1)	19(1)	2(1)	1(1)	2(1)
O(1)	93(2)	27(1)	32(1)	-7(1)	7(1)	2(1)
O(2)	28(1)	53(1)	36(1)	7(1)	0(1)	-11(1)
P(2)	16(1)	14(1)	19(1)	0(1)	2(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Co(η^3-C_3H_5)$(CO)_2PPh_2Me$ (1).

	x	y	z	U(eq)
H(3A)	1623	3545	816	39
H(3B)	2095	4592	703	39
H(4)	1553	5082	2033	40
H(5A)	826	3188	2006	51
H(5B)	709	3958	2764	51
H(7)	1683	922	3085	26
H(8)	507	11	3541	32
H(9)	-507	689	4450	36
H(10)	-334	2286	4905	45
H(11)	854	3210	4457	36
H(13)	2781	1751	4774	26
H(14)	3907	708	5164	32
H(15)	5049	413	4251	33
H(16)	5061	1129	2938	34
H(17)	3913	2141	2531	28
H(18A)	1983	4319	3991	40
H(18B)	3000	4185	3957	40
H(18C)	2447	3605	4620	40

Table 6. Torsion angles [°] for $Co(\eta^3\text{-}C_3H_5)(CO)_2PPh_2Me$ (1).

Co(1)-C(3)-C(4)-C(5)	-62.7(2)
C(3)-C(4)-C(5)-Co(1)	61.6(2)
C(11)-C(6)-C(7)-C(8)	0.3(4)
P(2)-C(6)-C(7)-C(8)	-178.5(2)
C(6)-C(7)-C(8)-C(9)	0.0(4)
C(7)-C(8)-C(9)-C(10)	-0.1(4)
C(8)-C(9)-C(10)-C(11)	-0.1(5)
C(7)-C(6)-C(11)-C(10)	-0.5(4)
P(2)-C(6)-C(11)-C(10)	178.2(2)
C(9)-C(10)-C(11)-C(6)	0.4(5)
C(17)-C(12)-C(13)-C(14)	-0.9(4)
P(2)-C(12)-C(13)-C(14)	179.9(2)
C(12)-C(13)-C(14)-C(15)	1.3(4)
C(13)-C(14)-C(15)-C(16)	-0.6(4)
C(14)-C(15)-C(16)-C(17)	-0.3(4)
C(13)-C(12)-C(17)-C(16)	0.0(4)
P(2)-C(12)-C(17)-C(16)	179.2(2)
C(15)-C(16)-C(17)-C(12)	0.7(4)
O(2)-C(2)-Co(1)-C(1)	74(10)
O(2)-C(2)-Co(1)-C(4)	-66(10)
O(2)-C(2)-Co(1)-C(3)	-26(10)
O(2)-C(2)-Co(1)-C(5)	-87(10)
O(2)-C(2)-Co(1)-P(2)	178(100)
O(1)-C(1)-Co(1)-C(2)	25(6)
O(1)-C(1)-Co(1)-C(4)	154(6)
O(1)-C(1)-Co(1)-C(3)	122(6)
O(1)-C(1)-Co(1)-C(5)	-169(6)
O(1)-C(1)-Co(1)-P(2)	-77(6)
C(5)-C(4)-Co(1)-C(2)	-155.7(2)
C(3)-C(4)-Co(1)-C(2)	79.8(2)
C(5)-C(4)-Co(1)-C(1)	69.5(3)
C(3)-C(4)-Co(1)-C(1)	-55.0(2)
C(5)-C(4)-Co(1)-C(3)	124.5(3)
C(3)-C(4)-Co(1)-C(5)	-124.5(3)
C(5)-C(4)-Co(1)-P(2)	-53.6(2)
C(3)-C(4)-Co(1)-P(2)	-178.10(16)

C(4)-C(3)-Co(1)-C(2)	-105.2(2)
C(4)-C(3)-Co(1)-C(1)	137.6(2)
C(4)-C(3)-Co(1)-C(5)	33.4(2)
C(4)-C(3)-Co(1)-P(2)	4.0(3)
C(4)-C(5)-Co(1)-C(2)	35.0(3)
C(4)-C(5)-Co(1)-C(1)	-127.4(2)
C(4)-C(5)-Co(1)-C(3)	-35.0(2)
C(4)-C(5)-Co(1)-P(2)	132.8(2)
C(11)-C(6)-P(2)-C(18)	20.4(3)
C(7)-C(6)-P(2)-C(18)	-160.8(2)
C(11)-C(6)-P(2)-C(12)	125.6(2)
C(7)-C(6)-P(2)-C(12)	-55.6(2)
C(11)-C(6)-P(2)-Co(1)	-106.3(2)
C(7)-C(6)-P(2)-Co(1)	72.5(2)
C(17)-C(12)-P(2)-C(18)	-115.4(2)
C(13)-C(12)-P(2)-C(18)	63.8(2)
C(17)-C(12)-P(2)-C(6)	137.5(2)
C(13)-C(12)-P(2)-C(6)	-43.3(2)
C(17)-C(12)-P(2)-Co(1)	10.7(2)
C(13)-C(12)-P(2)-Co(1)	-170.12(16)
C(2)-Co(1)-P(2)-C(18)	60.78(14)
C(1)-Co(1)-P(2)-C(18)	179.04(14)
C(4)-Co(1)-P(2)-C(18)	-44.81(15)
C(3)-Co(1)-P(2)-C(18)	-47.7(2)
C(5)-Co(1)-P(2)-C(18)	-74.81(15)
C(2)-Co(1)-P(2)-C(6)	-177.95(12)
C(1)-Co(1)-P(2)-C(6)	-59.69(13)
C(4)-Co(1)-P(2)-C(6)	76.46(13)
C(3)-Co(1)-P(2)-C(6)	73.6(2)
C(5)-Co(1)-P(2)-C(6)	46.45(13)
C(2)-Co(1)-P(2)-C(12)	-58.79(12)
C(1)-Co(1)-P(2)-C(12)	59.48(13)
C(4)-Co(1)-P(2)-C(12)	-164.38(13)
C(3)-Co(1)-P(2)-C(12)	-167.2(2)
C(5)-Co(1)-P(2)-C(12)	165.62(13)

Symmetry transformations used to generate equivalent atoms:

Table 7. Crystal data and structure refinement for $Co(\eta^3\text{-}C_3H_5)(CO)_2PCy_3$ 4

Empirical formula	$C_{23}H_{38}CoO_2P$	Identification code
Formula weight	436.43	SBD0402
Temperature	115(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.4726(8) Å	α= 90°.
	b = 15.4811(12) Å	β= 92.511(2)°.
	c = 13.8229(11) Å	γ = 90°.
Volume	2238.9(3) $Å^3$	
Z	4	
Density (calculated)	1.295 Mg/m^3	
Absorption coefficient	0.853 mm^{-1}	
F(000)	936	
Crystal size	0.32 x 0.24 x 0.14 mm^3	
Theta range for data collection	1.98 to 30.00°.	
Index ranges	-14<=h<=13, -21<=k<=21, -8<=l<=19	
Reflections collected	17426	
Independent reflections	6425 [R(int) = 0.0247]	
Completeness to theta = 30.00°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.890 and 0.730	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6425 / 0 / 244	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0321, wR2 = 0.0851	
R indices (all data)	R1 = 0.0402, wR2 = 0.0905	

Largest diff. peak and hole	0.920 and -0.565 e.Å^{-3}	

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for Co(η^3-C_3H_5)$(CO)_2PCy_3$ 4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Co(1)	9602(1)	1451(1)	8240(1)	15(1)
P(1)	8527(1)	1978(1)	6953(1)	14(1)
C(1)	8621(1)	597(1)	8650(1)	20(1)
O(1)	7988(1)	88(1)	9002(1)	30(1)
C(18)	9286(1)	2923(1)	6362(1)	17(1)
C(2)	9354(1)	2356(1)	8978(1)	21(1)
C(19)	9483(1)	3672(1)	7079(1)	22(1)
C(12)	8288(1)	1192(1)	5936(1)	18(1)
C(6)	6943(1)	2422(1)	7275(1)	17(1)
C(5)	10938(1)	830(1)	7365(1)	23(1)
O(2)	9185(1)	2914(1)	9509(1)	33(1)
C(22)	11147(2)	3497(1)	5436(1)	27(1)
C(11)	6011(1)	1715(1)	7584(1)	23(1)
C(23)	10570(1)	2701(1)	5917(1)	23(1)
C(7)	6265(1)	3033(1)	6550(1)	22(1)
C(8)	5068(1)	3429(1)	6972(1)	25(1)
C(17)	7420(2)	1478(1)	5074(1)	25(1)
C(4)	11495(1)	1336(1)	8106(1)	24(1)
C(20)	10078(2)	4466(1)	6605(1)	26(1)
C(10)	4822(1)	2116(1)	8011(1)	27(1)
C(21)	11329(1)	4242(1)	6147(1)	26(1)
C(9)	4147(1)	2731(1)	7293(1)	26(1)
C(16)	7445(2)	822(1)	4244(1)	31(1)
C(14)	7933(2)	-368(1)	5435(1)	29(1)
C(15)	7061(2)	-76(1)	4585(1)	32(1)
C(13)	7912(2)	280(1)	6272(1)	24(1)
C(3)	11233(2)	1088(1)	9058(1)	29(1)

Table 9. Bond lengths [Å] and angles [°] for $Co(\eta^3\text{-}C_3H_5)(CO)_2PCy_3$ 4

Co(1) C(2)	1.7592(14)	C(7) H(7B)	0.9900
Co(1) C(1)	1.7812(14)	C(8) C(9)	1.527(2)
Co(1) C(4)	2.0074(14)	C(8) H(8A)	0.9900
Co(1) C(3)	2.0841(15)	C(8) H(8B)	0.9900
Co(1) C(5)	2.1197(14)	C(17) C(16)	1.534(2)
Co(1) P(1)	2.2190(4)	C(17) H(17A)	0.9900
P(1) C(6)	1.8672(13)	C(17) H(17B)	0.9900
P(1) C(12)	1.8685(14)	C(4) C(3)	1.410(2)
P(1) C(18)	1.8692(13)	C(4) H(4)	0.9500
C(1) O(1)	1.1513(18)	C(20) C(21)	1.519(2)
C(18) C(19)	1.5341(19)	C(20) H(20A)	0.9900
C(18) C(23)	1.5416(18)	C(20) H(20B)	0.9900
C(18) H(18)	1.0000	C(10) C(9)	1.526(2)
C(2) O(2)	1.1522(18)	C(10) H(10A)	0.9900
C(19) C(20)	1.5371(19)	C(10) H(10B)	0.9900
C(19) H(19A)	0.9900	C(21) H(21A)	0.9900
C(19) H(19B)	0.9900	C(21) H(21B)	0.9900
C(12) C(17)	1.532(2)	C(9) H(9A)	0.9900
C(12) C(13)	1.5424(19)	C(9) H(9B)	0.9900
C(12) H(12)	1.0000	C(16) C(15)	1.527(2)
C(6) C(7)	1.5306(19)	C(16) H(16A)	0.9900
C(6) C(11)	1.5395(18)	C(16) H(16B)	0.9900
C(6) H(6)	1.0000	C(14) C(15)	1.525(3)
C(5) C(4)	1.397(2)	C(14) C(13)	1.532(2)
C(5) H(5A)	0.9500	C(14) H(14A)	0.9900
C(5) H(5B)	0.9500	C(14) H(14B)	0.9900
C(22) C(21)	1.522(2)	C(15) H(15A)	0.9900
C(22) C(23)	1.5360(19)	C(15) H(15B)	0.9900
C(22) H(22A)	0.9900	C(13) H(13A)	0.9900
C(22) H(22B)	0.9900	C(13) H(13B)	0.9900
C(11) C(10)	1.533(2)	C(3) H(3A)	0.9500
C(11) H(11A)	0.9900	C(3) H(3B)	0.9500
C(11) H(11B)	0.9900		
C(23) H(23A)	0.9900		
C(23) H(23B)	0.9900		

C(7) C(8)	1.533(2)		
C(7) H(7A)	0.9900		

C(2)-Co(1)-C(1)	107.73(7)	C(17)-C(12)-H(12)	105.0
C(2)-Co(1)-C(4)	107.20(6)	C(13)-C(12)-H(12)	105.0
C(1)-Co(1)-C(4)	123.33(6)	P(1)-C(12)-H(12)	105.0
C(2)-Co(1)-C(3)	92.21(6)	C(7)-C(6)-C(11)	109.84(11)
C(1)-Co(1)-C(3)	95.62(7)	C(7)-C(6)-P(1)	117.59(9)
C(4)-Co(1)-C(3)	40.25(6)	C(11)-C(6)-P(1)	112.69(9)
C(2)-Co(1)-C(5)	144.11(6)	C(7)-C(6)-H(6)	105.2
C(1)-Co(1)-C(5)	104.44(6)	C(11)-C(6)-H(6)	105.2
C(4)-Co(1)-C(5)	39.46(6)	P(1)-C(6)-H(6)	105.2
C(3)-Co(1)-C(5)	69.01(6)	C(4)-C(5)-Co(1)	65.93(8)
C(2)-Co(1)-P(1)	95.12(5)	C(4)-C(5)-H(5A)	120.0
C(1)-Co(1)-P(1)	104.39(5)	Co(1)-C(5)-H(5A)	80.1
C(4)-Co(1)-P(1)	115.27(5)	C(4)-C(5)-H(5B)	120.0
C(3)-Co(1)-P(1)	155.40(5)	Co(1)-C(5)-H(5B)	125.5
C(5)-Co(1)-P(1)	91.91(4)	H(5A)-C(5)-H(5B)	120.0
C(6)-P(1)-C(12)	109.14(6)	C(21)-C(22)-C(23)	111.67(13)
C(6)-P(1)-C(18)	102.45(6)	C(21)-C(22)-H(22A)	109.3
C(12)-P(1)-C(18)	103.07(6)	C(23)-C(22)-H(22A)	109.3
C(6)-P(1)-Co(1)	111.66(5)	C(21)-C(22)-H(22B)	109.3
C(12)-P(1)-Co(1)	114.21(4)	C(23)-C(22)-H(22B)	109.3
C(18)-P(1)-Co(1)	115.35(4)	H(22A)-C(22)-H(22B)	107.9
O(1)-C(1)-Co(1)	173.20(13)	C(10)-C(11)-C(6)	110.80(12)
C(19)-C(18)-C(23)	109.32(11)	C(10)-C(11)-H(11A)	109.5
C(19)-C(18)-P(1)	110.90(9)	C(6)-C(11)-H(11A)	109.5
C(23)-C(18)-P(1)	113.30(9)	C(10)-C(11)-H(11B)	109.5
C(19)-C(18)-H(18)	107.7	C(6)-C(11)-H(11B)	109.5
C(23)-C(18)-H(18)	107.7	H(11A)-C(11)-H(11B)	108.1
P(1)-C(18)-H(18)	107.7	C(22)-C(23)-C(18)	111.13(12)
O(2)-C(2)-Co(1)	175.71(13)	C(22)-C(23)-H(23A)	109.4
C(18)-C(19)-C(20)	112.00(12)	C(18)-C(23)-H(23A)	109.4
C(18)-C(19)-H(19A)	109.2	C(22)-C(23)-H(23B)	109.4
C(20)-C(19)-H(19A)	109.2	C(18)-C(23)-H(23B)	109.4
C(18)-C(19)-H(19B)	109.2	H(23A)-C(23)-H(23B)	108.0
C(20)-C(19)-H(19B)	109.2	C(6)-C(7)-C(8)	111.17(12)

H(19A)-C(19)-H(19B)	107.9	C(6)-C(7)-H(7A)	109.4
C(17)-C(12)-C(13)	110.39(12)	C(8)-C(7)-H(7A)	109.4
C(17)-C(12)-P(1)	116.85(9)	C(6)-C(7)-H(7B)	109.4
C(13)-C(12)-P(1)	113.40(9)	C(8)-C(7)-H(7B)	109.4
C(9)-C(8)-C(7)	111.43(12)	C(10)-C(9)-H(9B)	109.6
C(9)-C(8)-H(8A)	109.3	C(8)-C(9)-H(9B)	109.6
C(7)-C(8)-H(8A)	109.3	H(9A)-C(9)-H(9B)	108.1
C(9)-C(8)-H(8B)	109.3	C(15)-C(16)-C(17)	111.01(13)
C(7)-C(8)-H(8B)	109.3	C(15)-C(16)-H(16A)	109.4
H(8A)-C(8)-H(8B)	108.0	C(17)-C(16)-H(16A)	109.4
C(12)-C(17)-C(16)	111.16(12)	C(15)-C(16)-H(16B)	109.4
C(12)-C(17)-H(17A)	109.4	C(17)-C(16)-H(16B)	109.4
C(16)-C(17)-H(17A)	109.4	H(16A)-C(16)-H(16B)	108.0
C(12)-C(17)-H(17B)	109.4	C(15)-C(14)-C(13)	111.10(13)
C(16)-C(17)-H(17B)	109.4	C(15)-C(14)-H(14A)	109.4
H(17A)-C(17)-H(17B)	108.0	C(13)-C(14)-H(14A)	109.4
C(5)-C(4)-C(3)	116.08(14)	C(15)-C(14)-H(14B)	109.4
C(5)-C(4)-Co(1)	74.61(8)	C(13)-C(14)-H(14B)	109.4
C(3)-C(4)-Co(1)	72.80(9)	H(14A)-C(14)-H(14B)	108.0
C(5)-C(4)-H(4)	122.0	C(14)-C(15)-C(16)	110.58(13)
C(3)-C(4)-H(4)	122.0	C(14)-C(15)-H(15A)	109.5
Co(1)-C(4)-H(4)	122.0	C(16)-C(15)-H(15A)	109.5
C(21)-C(20)-C(19)	111.64(12)	C(14)-C(15)-H(15B)	109.5
C(21)-C(20)-H(20A)	109.3	C(16)-C(15)-H(15B)	109.5
C(19)-C(20)-H(20A)	109.3	H(15A)-C(15)-H(15B)	108.1
C(21)-C(20)-H(20B)	109.3	C(14)-C(13)-C(12)	111.07(12)
C(19)-C(20)-H(20B)	109.3	C(14)-C(13)-H(13A)	109.4
H(20A)-C(20)-H(20B)	108.0	C(12)-C(13)-H(13A)	109.4
C(9)-C(10)-C(11)	111.26(13)	C(14)-C(13)-H(13B)	109.4
C(9)-C(10)-H(10A)	109.4	C(12)-C(13)-H(13B)	109.4
C(11)-C(10)-H(10A)	109.4	H(13A)-C(13)-H(13B)	108.0
C(9)-C(10)-H(10B)	109.4	C(4)-C(3)-Co(1)	66.95(8)
C(11)-C(10)-H(10B)	109.4	C(4)-C(3)-H(3A)	120.0
H(10A)-C(10)-H(10B)	108.0	Co(1)-C(3)-H(3A)	80.1
C(20)-C(21)-C(22)	110.79(12)	C(4)-C(3)-H(3B)	120.0
C(20)-C(21)-H(21A)	109.5	Co(1)-C(3)-H(3B)	124.3
C(22)-C(21)-H(21A)	109.5	H(3A)-C(3)-H(3B)	120.0

C(20)-C(21)-H(21B)	109.5	H(7A)-C(7)-H(7B)	108.0
C(22)-C(21)-H(21B)	109.5		
H(21A)-C(21)-H(21B)	108.1		
C(10)-C(9)-C(8)	110.49(13)		
C(10)-C(9)-H(9A)	109.6		
C(8)-C(9)-H(9A)	109.6		

Table 10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Co(\eta^3-C_3H_5)(CO)_2PCy_3$ 4. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	16(1)	14(1)	16(1)	1(1)	1(1)	2(1)
P(1)	14(1)	12(1)	16(1)	1(1)	1(1)	0(1)
C(1)	22(1)	19(1)	21(1)	1(1)	2(1)	4(1)
O(1)	32(1)	22(1)	35(1)	8(1)	7(1)	-1(1)
C(18)	16(1)	14(1)	19(1)	2(1)	2(1)	-3(1)
C(2)	20(1)	23(1)	21(1)	1(1)	-2(1)	4(1)
C(19)	24(1)	15(1)	26(1)	-2(1)	5(1)	-4(1)
C(12)	19(1)	16(1)	18(1)	-2(1)	1(1)	-1(1)
C(6)	15(1)	15(1)	22(1)	1(1)	2(1)	1(1)
C(5)	21(1)	24(1)	25(1)	0(1)	6(1)	4(1)
O(2)	38(1)	30(1)	29(1)	-10(1)	-5(1)	10(1)
C(22)	29(1)	24(1)	30(1)	2(1)	11(1)	-7(1)
C(11)	17(1)	19(1)	32(1)	8(1)	4(1)	2(1)
C(23)	23(1)	18(1)	27(1)	0(1)	9(1)	-2(1)
C(7)	20(1)	18(1)	27(1)	6(1)	2(1)	2(1)
C(8)	22(1)	18(1)	35(1)	4(1)	1(1)	4(1)
C(17)	29(1)	26(1)	21(1)	-4(1)	-4(1)	4(1)
C(4)	17(1)	23(1)	32(1)	0(1)	0(1)	3(1)
C(20)	28(1)	14(1)	37(1)	1(1)	5(1)	-4(1)
C(10)	19(1)	30(1)	34(1)	10(1)	7(1)	4(1)
C(21)	24(1)	21(1)	33(1)	3(1)	3(1)	-7(1)
C(9)	17(1)	26(1)	36(1)	5(1)	2(1)	3(1)
C(16)	34(1)	37(1)	23(1)	-9(1)	-4(1)	3(1)
C(14)	32(1)	20(1)	37(1)	-9(1)	7(1)	-5(1)
C(15)	25(1)	35(1)	36(1)	-19(1)	3(1)	-4(1)

C(13)	29(1)	16(1)	27(1)	-3(1)	3(1)	-4(1)
C(3)	25(1)	35(1)	26(1)	-2(1)	-6(1)	10(1)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for Co(η^3-C_3H_5)$(CO)_2PCy_3$ 4.

	x	y	z	U(eq)
H(18)	8687	3125	5825	20
H(19A)	10047	3480	7630	26
H(19B)	8649	3836	7335	26
H(12)	9153	1120	5666	21
H(6)	7122	2778	7869	21
H(5A)	10417	350	7518	28
H(5B)	11079	965	6708	28
H(22A)	11983	3341	5178	33
H(22B)	10576	3683	4886	33
H(11A)	5751	1357	7016	27
H(11B)	6444	1336	8072	27
H(23A)	11175	2483	6430	27
H(23B)	10436	2239	5428	27
H(7A)	6019	2711	5951	26
H(7B)	6858	3501	6376	26
H(8A)	5324	3796	7534	30
H(8B)	4630	3800	6478	30
H(17A)	7707	2048	4841	30
H(17B)	6534	1541	5285	30
H(4)	12020	1819	7976	29
H(20A)	9470	4699	6101	32
H(20B)	10234	4920	7100	32
H(10A)	4224	1651	8185	33
H(10B)	5075	2435	8610	33
H(21A)	11975	4081	6660	31
H(21B)	11650	4755	5805	31
H(9A)	3412	3005	7600	31
H(9B)	3817	2403	6721	31
H(16A)	6849	1010	3709	37
H(16B)	8315	797	3993	37

H(14A)	8818	-428	5220	35
H(14B)	7650	-940	5663	35
H(15A)	6165	-64	4784	38
H(15B)	7118	-492	4045	38
H(13A)	8515	89	6801	29
H(13B)	7045	298	6529	29
H(3A)	10704	601	9165	35
H(3B)	11585	1407	9593	35

Table 12. Torsion angles [°] for Co(η^3-C_3H_5)$(CO)_2PCy_3$ 4.

C(2)-Co(1)-P(1)-C(6)	-48.01(7)	C(3)-Co(1)-C(5)-C(4)	-34.90(10)
C(1)-Co(1)-P(1)-C(6)	61.78(6)	P(1)-Co(1)-C(5)-C(4)	129.16(9)
C(4)-Co(1)-P(1)-C(6)	-159.76(7)	C(7)-C(6)-C(11)-C(10)	-56.91(16)
C(3)-Co(1)-P(1)-C(6)	-154.78(12)	P(1)-C(6)-C(11)-C(10)	169.89(10)
C(5)-Co(1)-P(1)-C(6)	-167.22(6)	C(21)-C(22)-C(23)-C(18)	56.99(18)
C(2)-Co(1)-P(1)-C(12)	-172.43(7)	C(19)-C(18)-C(23)-C(22)	-56.10(16)
C(1)-Co(1)-P(1)-C(12)	-62.63(7)	P(1)-C(18)-C(23)-C(22)	179.67(10)
C(4)-Co(1)-P(1)-C(12)	75.82(7)	C(11)-C(6)-C(7)-C(8)	56.56(16)
C(3)-Co(1)-P(1)-C(12)	80.80(13)	P(1)-C(6)-C(7)-C(8)	-172.80(10)
C(5)-Co(1)-P(1)-C(12)	42.80(6)	C(6)-C(7)-C(8)-C(9)	-56.53(17)
C(2)-Co(1)-P(1)-C(18)	68.40(7)	C(13)-C(12)-C(17)-C(16)	-55.61(16)
C(1)-Co(1)-P(1)-C(18)	178.20(6)	P(1)-C(12)-C(17)-C(16)	172.85(11)
C(4)-Co(1)-P(1)-C(18)	-43.35(7)	Co(1)-C(5)-C(4)-C(3)	61.56(11)
C(3)-Co(1)-P(1)-C(18)	-38.37(13)	C(2)-Co(1)-C(4)-C(5)	-163.42(9)
C(5)-Co(1)-P(1)-C(18)	-76.37(6)	C(1)-Co(1)-C(4)-C(5)	70.77(11)
C(6)-P(1)-C(18)-C(19)	63.06(11)	C(3)-Co(1)-C(4)-C(5)	124.23(13)
C(12)-P(1)-C(18)-C(19)	176.38(10)	P(1)-Co(1)-C(4)-C(5)	-58.97(9)
Co(1)-P(1)-C(18)-C(19)	-58.47(10)	C(2)-Co(1)-C(4)-C(3)	72.35(11)
C(6)-P(1)-C(18)-C(23)	-173.57(10)	C(1)-Co(1)-C(4)-C(3)	-53.46(12)
C(12)-P(1)-C(18)-C(23)	-60.25(11)	C(5)-Co(1)-C(4)-C(3)	-124.23(13)
Co(1)-P(1)-C(18)-C(23)	64.90(11)	P(1)-Co(1)-C(4)-C(3)	176.79(8)
C(23)-C(18)-C(19)-C(20)	55.67(16)	C(18)-C(19)-C(20)-C(21)	-55.76(17)
P(1)-C(18)-C(19)-C(20)	-178.70(10)	C(6)-C(11)-C(10)-C(9)	57.23(18)
C(6)-P(1)-C(12)-C(17)	47.21(12)	C(19)-C(20)-C(21)-C(22)	54.63(18)
C(18)-P(1)-C(12)-C(17)	-61.14(12)	C(23)-C(22)-C(21)-C(20)	-55.59(18)
Co(1)-P(1)-C(12)-C(17)	172.97(9)	C(11)-C(10)-C(9)-C(8)	-56.11(18)
C(6)-P(1)-C(12)-C(13)	-82.92(11)	C(7)-C(8)-C(9)-C(10)	55.65(18)

C(18)-P(1)-C(12)-C(13)	168.73(10)	C(12)-C(17)-C(16)-C(15)	56.70(18)
Co(1)-P(1)-C(12)-C(13)	42.83(11)	C(13)-C(14)-C(15)-C(16)	56.94(17)
C(12)-P(1)-C(6)-C(7)	-70.12(12)	C(17)-C(16)-C(15)-C(14)	-56.93(18)
C(18)-P(1)-C(6)-C(7)	38.65(12)	C(15)-C(14)-C(13)-C(12)	-56.48(17)
Co(1)-P(1)-C(6)-C(7)	162.67(9)	C(17)-C(12)-C(13)-C(14)	55.52(16)
C(12)-P(1)-C(6)-C(11)	59.19(12)	P(1)-C(12)-C(13)-C(14)	-171.17(11)
C(18)-P(1)-C(6)-C(11)	167.96(10)	C(5)-C(4)-C(3)-Co(1)	-62.56(11)
Co(1)-P(1)-C(6)-C(11)	-68.02(11)	C(2)-Co(1)-C(3)-C(4)	-114.35(10)
C(2)-Co(1)-C(5)-C(4)	27.72(15)	C(1)-Co(1)-C(3)-C(4)	137.58(10)
C(1)-Co(1)-C(5)-C(4)	-125.45(10)	C(5)-Co(1)-C(3)-C(4)	34.25(9)

Table 13. Crystal data and structure refinement for Co(η^3-C_3H_5)(CO)dppe 7

Empirical formula	$C_{30}H_{29}CoOP_2$	Identification code
Formula weight	526.40	SBD0401M
Temperature	115(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.4425(7) Å	α= 93.077(2)°.
	b = 9.4559(6) Å	β= 104.880(2)°.
	c = 14.7071(10) Å	γ = 101.761(2)°
Volume	1234.65(15) $Å^3$	
Z	2	
Density (calculated)	1.416 Mg/m^3	
Absorption coefficient	0.846 mm^{-1}	
F(000)	548	
Crystal size	0.21 x 0.11 x 0.05 mm^3	
Theta range for data collection	1.44 to 25.03°.	
Index ranges	-11<=h<=5, -11<=k<=11, -16<=l<=17	
Reflections collected	7070	
Independent reflections	4325 [R(int) = 0.0211]	
Completeness to theta = 25.03°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.960 and 0.822	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	4325 / 0 / 307	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0343, wR2 = 0.0827	
R indices (all data)	R1 = 0.0461, wR2 = 0.0874	
Largest diff. peak and hole	0.587 and -0.607 e.Å^{-3}	

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for Co(η3-C_3H_5)(CO)dppe. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(5)	-668(3)	4369(3)	7445(2)	18(1)
Co(1)	2212(1)	3133(1)	7102(1)	16(1)
P(2)	1935(1)	5343(1)	6967(1)	15(1)
P(1)	379(1)	2906(1)	7754(1)	15(1)
O(1)	1012(2)	1771(2)	5150(1)	36(1)
C(30)	3274(3)	5781(3)	5486(2)	21(1)
C(25)	2542(3)	6377(3)	6065(2)	18(1)
C(10)	2026(3)	3276(3)	11033(2)	21(1)
C(12)	1530(3)	4413(3)	9597(2)	20(1)
C(24)	1824(3)	7555(3)	8341(2)	21(1)
C(20)	4107(3)	6724(3)	8593(2)	20(1)
C(18)	-2388(3)	1174(3)	7833(2)	19(1)
C(17)	-3552(3)	-51(3)	7606(2)	21(1)
C(13)	-1137(3)	1248(2)	7477(2)	17(1)
C(14)	-1076(3)	62(3)	6902(2)	20(1)
C(3)	4070(3)	2967(3)	8058(2)	22(1)
C(26)	2319(3)	7785(3)	5957(2)	24(1)
C(16)	-3485(3)	-1217(3)	7022(2)	23(1)
C(11)	2067(3)	4521(3)	10577(2)	22(1)
C(22)	3791(3)	8364(3)	9789(2)	25(1)
C(15)	-2251(3)	-1169(3)	6672(2)	24(1)
C(21)	4681(3)	7568(3)	9466(2)	24(1)
C(7)	923(3)	3068(3)	9059(2)	17(1)
C(28)	3577(3)	7964(3)	4725(2)	27(1)
C(8)	901(3)	1823(3)	9530(2)	22(1)
C(23)	2373(3)	8372(3)	9224(2)	24(1)

C(4)	4521(3)	3511(3)	7273(2)	22(1)
C(29)	3795(3)	6579(3)	4823(2)	25(1)
C(6)	-106(3)	5189(3)	6691(2)	18(1)
C(1)	1475(3)	2293(3)	5923(2)	22(1)
C(9)	1457(3)	1926(3)	10507(2)	22(1)
C(2)	3100(3)	1570(3)	7864(2)	24(1)
C(27)	2829(3)	8573(3)	5293(2)	29(1)
C(19)	2669(3)	6687(2)	8021(2)	17(1)

Table 15. Bond lengths [Å] and angles [°] for Co(η^3-C_3H_5)(CO)dppe 7.

C(5)-C(6)	1.529(3)	C(13)-C(14)	1.388(3)
C(5)-P(1)	1.869(2)	C(14)-C(15)	1.393(4)
C(5)-H(5A)	0.9900	C(14)-H(14)	0.9500
C(5)-H(5B)	0.9900	C(3)-C(2)	1.413(4)
Co(1)-C(1)	1.770(3)	C(3)-C(4)	1.417(4)
Co(1)-C(3)	1.987(3)	C(3)-H(3)	0.9500
Co(1)-C(4)	2.082(3)	C(26)-C(27)	1.384(4)
Co(1)-C(2)	2.084(3)	C(26)-H(26)	0.9500
Co(1)-P(1)	2.1640(7)	C(16)-C(15)	1.383(4)
Co(1)-P(2)	2.1709(7)	C(16)-H(16)	0.9500
P(2)-C(25)	1.830(2)	C(11)-H(11)	0.9500
P(2)-C(19)	1.838(2)	C(22)-C(23)	1.385(4)
P(2)-C(6)	1.838(2)	C(22)-C(21)	1.387(4)
P(1)-C(13)	1.841(2)	C(22)-H(22)	0.9500
P(1)-C(7)	1.844(2)	C(15)-H(15)	0.9500
O(1)-C(1)	1.150(3)	C(21)-H(21)	0.9500
C(30)-C(25)	1.389(4)	C(7)-C(8)	1.396(3)
C(30)-C(29)	1.392(3)	C(28)-C(29)	1.376(4)
C(30)-H(30)	0.9500	C(28)-C(27)	1.395(4)
C(25)-C(26)	1.401(3)	C(28)-H(28)	0.9500
C(10)-C(11)	1.384(4)	C(8)-C(9)	1.388(4)
C(10)-C(9)	1.385(4)	C(8)-H(8)	0.9500
C(10)-H(10)	0.9500	C(23)-H(23)	0.9500
C(12)-C(11)	1.390(3)	C(4)-H(4A)	0.9500
C(12)-C(7)	1.391(3)	C(4)-H(4B)	0.9500
C(12)-H(12)	0.9500	C(29)-H(29)	0.9500

C(24)-C(23)	1.391(4)	C(6)-H(6A)	0.9900
C(24)-C(19)	1.396(3)	C(6)-H(6B)	0.9900
C(24)-H(24)	0.9500	C(9)-H(9)	0.9500
C(20)-C(21)	1.390(4)	C(2)-H(2A)	0.9500
C(20)-C(19)	1.395(4)	C(2)-H(2B)	0.9500
C(20)-H(20)	0.9500	C(27)-H(27)	0.9500
C(18)-C(17)	1.382(4)	C(17)-H(17)	0.9500
C(18)-C(13)	1.401(3)	C(17)-C(16)	1.383(4)
C(18)-H(18)	0.9500		

P(1)-C(5)-H(5B)	109.8	C(25)-P(2)-Co(1)	121.32(8)
H(5A)-C(5)-H(5B)	108.3	C(19)-P(2)-Co(1)	118.73(8)
C(6)-C(5)-P(1)	109.25(16)	C(6)-P(2)-Co(1)	104.71(8)
C(6)-C(5)-H(5A)	109.8	C(13)-P(1)-C(7)	100.58(11)
P(1)-C(5)-H(5A)	109.8	C(13)-P(1)-C(5)	102.73(11)
C(6)-C(5)-H(5B)	109.8	C(7)-P(1)-C(5)	104.69(11)
P(1)-C(5)-H(5B)	109.8	C(13)-P(1)-Co(1)	121.08(8)
H(5A)-C(5)-H(5B)	108.3	C(7)-P(1)-Co(1)	115.78(8)
C(6)-C(5)-P(1)	109.25(16)	C(5)-P(1)-Co(1)	110.06(8)
C(6)-C(5)-H(5A)	109.8	C(25)-C(30)-C(29)	120.5(2)
P(1)-C(5)-H(5A)	109.8	C(25)-C(30)-H(30)	119.7
C(6)-C(5)-H(5B)	109.8	C(29)-C(30)-H(30)	119.7
C(1)-Co(1)-C(3)	128.64(11)	C(30)-C(25)-C(26)	118.7(2)
C(1)-Co(1)-C(4)	102.12(11)	C(30)-C(25)-P(2)	119.92(19)
C(3)-Co(1)-C(4)	40.66(10)	C(26)-C(25)-P(2)	121.34(19)
C(1)-Co(1)-C(2)	104.84(11)	C(11)-C(10)-C(9)	119.6(2)
C(3)-Co(1)-C(2)	40.53(10)	C(11)-C(10)-H(10)	120.2
C(4)-Co(1)-C(2)	69.86(10)	C(9)-C(10)-H(10)	120.2
C(1)-Co(1)-P(1)	107.89(9)	C(11)-C(12)-C(7)	121.1(2)
C(3)-Co(1)-P(1)	109.22(8)	C(11)-C(12)-H(12)	119.4
C(4)-Co(1)-P(1)	148.17(7)	C(7)-C(12)-H(12)	119.4
C(2)-Co(1)-P(1)	92.05(8)	C(23)-C(24)-C(19)	120.9(2)
C(1)-Co(1)-P(2)	102.69(8)	C(23)-C(24)-H(24)	119.6
C(3)-Co(1)-P(2)	114.63(8)	C(19)-C(24)-H(24)	119.6
C(4)-Co(1)-P(2)	98.66(7)	C(21)-C(20)-C(19)	121.6(2)
C(2)-Co(1)-P(2)	151.84(8)	C(21)-C(20)-H(20)	119.2
P(1)-Co(1)-P(2)	85.06(3)	C(19)-C(20)-H(20)	119.2

C(25)-P(2)-C(19)	101.80(11)	C(17)-C(18)-C(13)	120.7(2)
C(25)-P(2)-C(6)	105.39(11)	C(17)-C(18)-H(18)	119.7
C(19)-P(2)-C(6)	102.81(11)	C(13)-C(18)-H(18)	119.7
C(18)-C(17)-C(16)	119.9(2)	C(8)-C(7)-P(1)	120.24(18)
C(18)-C(17)-H(17)	120.1	C(29)-C(28)-C(27)	119.9(2)
C(16)-C(17)-H(17)	120.1	C(29)-C(28)-H(28)	120.1
C(14)-C(13)-C(18)	118.8(2)	C(27)-C(28)-H(28)	120.1
C(14)-C(13)-P(1)	120.85(19)	C(9)-C(8)-C(7)	121.0(2)
C(18)-C(13)-P(1)	120.32(18)	C(9)-C(8)-H(8)	119.5
C(13)-C(14)-C(15)	120.5(2)	C(7)-C(8)-H(8)	119.5
C(13)-C(14)-H(14)	119.8	C(22)-C(23)-C(24)	120.1(2)
C(15)-C(14)-H(14)	119.8	C(22)-C(23)-H(23)	119.9
C(2)-C(3)-C(4)	114.9(2)	C(24)-C(23)-H(23)	119.9
C(2)-C(3)-Co(1)	73.41(15)	C(3)-C(4)-Co(1)	66.07(14)
C(4)-C(3)-Co(1)	73.27(15)	C(3)-C(4)-H(4A)	120.0
C(2)-C(3)-H(3)	122.5	Co(1)-C(4)-H(4A)	80.3
C(4)-C(3)-H(3)	122.5	C(3)-C(4)-H(4B)	120.0
Co(1)-C(3)-H(3)	122.2	Co(1)-C(4)-H(4B)	125.0
C(27)-C(26)-C(25)	120.7(2)	H(4A)-C(4)-H(4B)	120.0
C(27)-C(26)-H(26)	119.7	C(28)-C(29)-C(30)	120.4(2)
C(25)-C(26)-H(26)	119.7	C(28)-C(29)-H(29)	119.8
C(15)-C(16)-C(17)	120.2(2)	C(30)-C(29)-H(29)	119.8
C(15)-C(16)-H(16)	119.9	C(5)-C(6)-P(2)	107.59(16)
C(17)-C(16)-H(16)	119.9	C(5)-C(6)-H(6A)	110.2
C(10)-C(11)-C(12)	120.1(2)	P(2)-C(6)-H(6A)	110.2
C(10)-C(11)-H(11)	120.0	C(5)-C(6)-H(6B)	110.2
C(12)-C(11)-H(11)	120.0	P(2)-C(6)-H(6B)	110.2
C(23)-C(22)-C(21)	120.0(2)	H(6A)-C(6)-H(6B)	108.5
C(23)-C(22)-H(22)	120.0	O(1)-C(1)-Co(1)	178.6(2)
C(21)-C(22)-H(22)	120.0	C(10)-C(9)-C(8)	120.1(2)
C(16)-C(15)-C(14)	119.9(2)	C(10)-C(9)-H(9)	119.9
C(16)-C(15)-H(15)	120.0	C(8)-C(9)-H(9)	119.9
C(14)-C(15)-H(15)	120.0	C(3)-C(2)-Co(1)	66.06(14)
C(22)-C(21)-C(20)	119.4(3)	C(3)-C(2)-H(2A)	120.0
C(22)-C(21)-H(21)	120.3	Co(1)-C(2)-H(2A)	80.3
C(20)-C(21)-H(21)	120.3	C(3)-C(2)-H(2B)	120.0
C(12)-C(7)-C(8)	118.0(2)	Co(1)-C(2)-H(2B)	125.1

C(12)-C(7)-P(1)	121.30(18)	H(2A)-C(2)-H(2B)	120.0
C(26)-C(27)-C(28)	119.8(3)	C(20)-C(19)-C(24)	117.9(2)
C(26)-C(27)-H(27)	120.1	C(20)-C(19)-P(2)	117.49(18)
C(28)-C(27)-H(27)	120.1	C(24)-C(19)-P(2)	124.26(19)

Table 16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Co(\eta^3\text{-}C_3H_5)(CO)dppe$ 7. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(5)	17(1)	18(1)	19(1)	1(1)	5(1)	5(1)
Co(1)	17(1)	17(1)	15(1)	2(1)	6(1)	5(1)
P(2)	16(1)	17(1)	13(1)	3(1)	5(1)	4(1)
P(1)	16(1)	15(1)	15(1)	2(1)	5(1)	4(1)
O(1)	38(1)	45(1)	22(1)	-9(1)	7(1)	6(1)
C(30)	19(1)	26(1)	17(1)	4(1)	3(1)	4(1)
C(25)	14(1)	22(1)	14(1)	5(1)	1(1)	1(1)
C(10)	18(1)	31(1)	14(1)	6(1)	5(1)	7(1)
C(12)	24(1)	17(1)	19(1)	4(1)	8(1)	5(1)
C(24)	23(1)	16(1)	25(1)	6(1)	8(1)	4(1)
C(20)	21(1)	22(1)	18(1)	2(1)	9(1)	3(1)
C(18)	22(1)	20(1)	18(1)	4(1)	7(1)	6(1)
C(17)	18(1)	26(1)	21(1)	7(1)	5(1)	5(1)
C(13)	19(1)	16(1)	14(1)	4(1)	4(1)	2(1)
C(14)	24(1)	19(1)	19(1)	2(1)	8(1)	4(1)
C(3)	20(1)	28(1)	21(1)	6(1)	4(1)	11(1)
C(26)	26(2)	26(1)	21(1)	5(1)	7(1)	8(1)
C(16)	21(1)	21(1)	21(1)	5(1)	0(1)	-2(1)
C(11)	24(1)	23(1)	20(1)	-2(1)	8(1)	6(1)
C(22)	33(2)	19(1)	20(1)	-3(1)	10(1)	-3(1)
C(15)	31(2)	20(1)	18(1)	0(1)	5(1)	4(1)
C(21)	21(1)	27(1)	20(1)	1(1)	4(1)	-2(1)
C(7)	15(1)	20(1)	17(1)	3(1)	6(1)	6(1)
C(28)	25(2)	36(2)	18(1)	12(1)	6(1)	1(1)
C(8)	19(1)	20(1)	26(1)	4(1)	6(1)	5(1)
C(23)	30(2)	15(1)	29(1)	0(1)	14(1)	6(1)
C(4)	17(1)	28(1)	22(1)	2(1)	5(1)	6(1)
C(29)	23(1)	37(2)	16(1)	4(1)	8(1)	4(1)

C(6)	15(1)	20(1)	17(1)	3(1)	2(1)	5(1)
C(1)	21(1)	23(1)	25(2)	2(1)	11(1)	8(1)
C(9)	19(1)	25(1)	25(1)	13(1)	7(1)	5(1)
C(2)	26(2)	28(1)	25(1)	12(1)	9(1)	13(1)
C(27)	33(2)	27(1)	28(2)	12(1)	9(1)	8(1)
C(19)	21(1)	14(1)	15(1)	5(1)	7(1)	3(1)

Table 17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for Co(η3-C_3H_5)(CO)dppe 7.

	x	y	z	U(eq)
H(5A)	-1759	3935	7201	21
H(5B)	-506	5049	8017	21
H(30)	3420	4821	5543	26
H(10)	2387	3348	11703	25
H(12)	1580	5273	9290	23
H(24)	862	7589	7950	25
H(20)	4710	6160	8382	24
H(18)	-2437	1973	8235	23
H(17)	-4396	-91	7850	25
H(14)	-227	91	6664	24
H(3)	4396	3500	8669	27
H(26)	1813	8204	6344	28
H(16)	-4290	-2055	6860	27
H(11)	2461	5450	10934	27
H(22)	4154	8904	10398	30
H(15)	-2205	-1975	6274	28
H(21)	5674	7600	9837	29
H(28)	3935	8504	4271	32
H(8)	500	893	9176	26
H(23)	1774	8937	9439	28
H(4A)	4171	2944	6673	27
H(4B)	5174	4443	7346	27
H(29)	4304	6164	4436	30
H(6A)	-329	6168	6698	21
H(6B)	-611	4655	6055	21
H(9)	1447	1068	10815	27

H(2A)	2799	1071	7244	29
H(2B)	2747	1131	8355	29
H(27)	2670	9526	5224	34

Table 18. Torsion angles [°] for Co(η3-C_3H_5)(CO)dppe 7.

C(1)-Co(1)-P(2)-C(25)	-48.70(13)	C(2)-Co(1)-P(1)-C(5)	170.51(11)
C(3)-Co(1)-P(2)-C(25)	95.14(12)	P(2)-Co(1)-P(1)-C(5)	18.58(9)
C(4)-Co(1)-P(2)-C(25)	55.89(12)	C(29)-C(30)-C(25)-C(26)	1.0(4)
C(2)-Co(1)-P(2)-C(25)	118.93(18)	C(29)-C(30)-C(25)-P(2)	-177.38(19)
P(1)-Co(1)-P(2)-C(25)	-155.96(9)	C(19)-P(2)-C(25)-C(30)	130.8(2)
C(1)-Co(1)-P(2)-C(19)	-176.04(12)	C(6)-P(2)-C(25)-C(30)	-122.2(2)
C(3)-Co(1)-P(2)-C(19)	-32.20(13)	Co(1)-P(2)-C(25)-C(30)	-3.8(2)
C(4)-Co(1)-P(2)-C(19)	-71.45(12)	C(19)-P(2)-C(25)-C(26)	-47.5(2)
C(2)-Co(1)-P(2)-C(19)	-8.41(19)	C(6)-P(2)-C(25)-C(26)	59.5(2)
P(1)-Co(1)-P(2)-C(19)	76.70(9)	Co(1)-P(2)-C(25)-C(26)	177.91(17)
C(1)-Co(1)-P(2)-C(6)	70.05(12)	C(13)-C(18)-C(17)-C(16)	0.0(4)
C(3)-Co(1)-P(2)-C(6)	-146.11(11)	C(17)-C(18)-C(13)-C(14)	-0.9(4)
C(4)-Co(1)-P(2)-C(6)	174.64(11)	C(17)-C(18)-C(13)-P(1)	178.08(18)
C(2)-Co(1)-P(2)-C(6)	-122.32(18)	C(7)-P(1)-C(13)-C(14)	-123.9(2)
P(1)-Co(1)-P(2)-C(6)	-37.21(8)	C(5)-P(1)-C(13)-C(14)	128.3(2)
C(6)-C(5)-P(1)-C(13)	-121.44(17)	Co(1)-P(1)-C(13)-C(14)	5.1(2)
C(6)-C(5)-P(1)-C(7)	133.85(17)	C(7)-P(1)-C(13)-C(18)	57.2(2)
C(6)-C(5)-P(1)-Co(1)	8.80(18)	C(5)-P(1)-C(13)-C(18)	-50.7(2)
C(1)-Co(1)-P(1)-C(13)	36.43(12)	Co(1)-P(1)-C(13)-C(18)	-173.80(16)
C(3)-Co(1)-P(1)-C(13)	-107.42(12)	C(18)-C(13)-C(14)-C(15)	1.0(4)
C(4)-Co(1)-P(1)-C(13)	-123.34(16)	P(1)-C(13)-C(14)-C(15)	-177.90(18)
C(2)-Co(1)-P(1)-C(13)	-69.88(12)	C(1)-Co(1)-C(3)-C(2)	-64.5(2)
P(2)-Co(1)-P(1)-C(13)	138.19(9)	C(4)-Co(1)-C(3)-C(2)	-123.3(2)
C(1)-Co(1)-P(1)-C(7)	158.38(12)	P(1)-Co(1)-C(3)-C(2)	69.55(15)
C(3)-Co(1)-P(1)-C(7)	14.54(12)	P(2)-Co(1)-C(3)-C(2)	162.96(13)
C(4)-Co(1)-P(1)-C(7)	-1.39(17)	C(1)-Co(1)-C(3)-C(4)	58.8(2)
C(2)-Co(1)-P(1)-C(7)	52.07(12)	C(2)-Co(1)-C(3)-C(4)	123.3(2)
P(2)-Co(1)-P(1)-C(7)	-99.86(9)	P(1)-Co(1)-C(3)-C(4)	-167.17(13)
C(1)-Co(1)-P(1)-C(5)	-83.18(12)	P(2)-Co(1)-C(3)-C(4)	-73.75(16)
C(3)-Co(1)-P(1)-C(5)	132.97(12)	C(30)-C(25)-C(26)-C(27)	-0.5(4)

C(4)-Co(1)-P(1)-C(5)	117.05(16)	P(2)-C(25)-C(26)-C(27)	177.8(2)
C(18)-C(17)-C(16)-C(15)	0.6(4)	C(1)-Co(1)-C(2)-C(3)	133.17(16)
C(9)-C(10)-C(11)-C(12)	0.4(4)	C(4)-Co(1)-C(2)-C(3)	35.46(16)
C(7)-C(12)-C(11)-C(10)	1.1(4)	P(1)-Co(1)-C(2)-C(3)	-117.71(14)
C(17)-C(16)-C(15)-C(14)	-0.5(4)	P(2)-Co(1)-C(2)-C(3)	-34.3(2)
C(13)-C(14)-C(15)-C(16)	-0.4(4)	C(25)-C(26)-C(27)-C(28)	-0.2(4)
C(23)-C(22)-C(21)-C(20)	-3.3(4)	C(29)-C(28)-C(27)-C(26)	0.5(4)
C(19)-C(20)-C(21)-C(22)	1.7(4)	C(21)-C(20)-C(19)-C(24)	1.5(3)
C(11)-C(12)-C(7)-C(8)	-1.6(4)	C(21)-C(20)-C(19)-P(2)	-171.62(19)
C(11)-C(12)-C(7)-P(1)	-174.0(2)	C(23)-C(24)-C(19)-C(20)	-3.3(3)
C(13)-P(1)-C(7)-C(12)	-151.6(2)	C(23)-C(24)-C(19)-P(2)	169.35(18)
C(5)-P(1)-C(7)-C(12)	-45.3(2)	C(25)-P(2)-C(19)-C(20)	-91.0(2)
Co(1)-P(1)-C(7)-C(12)	76.0(2)	C(6)-P(2)-C(19)-C(20)	159.96(18)
C(13)-P(1)-C(7)-C(8)	36.1(2)	Co(1)-P(2)-C(19)-C(20)	45.0(2)
C(5)-P(1)-C(7)-C(8)	142.4(2)	C(25)-P(2)-C(19)-C(24)	96.3(2)
Co(1)-P(1)-C(7)-C(8)	-96.3(2)	C(6)-P(2)-C(19)-C(24)	-12.7(2)
C(12)-C(7)-C(8)-C(9)	0.5(4)	Co(1)-P(2)-C(19)-C(24)	-127.64(18)
P(1)-C(7)-C(8)-C(9)	173.1(2)	C(27)-C(28)-C(29)-C(30)	0.0(4)
C(21)-C(22)-C(23)-C(24)	1.6(4)	C(25)-C(30)-C(29)-C(28)	-0.7(4)
C(19)-C(24)-C(23)-C(22)	1.8(4)	P(1)-C(5)-C(6)-P(2)	-37.7(2)
C(2)-C(3)-C(4)-Co(1)	62.07(19)	C(25)-P(2)-C(6)-C(5)	-178.36(16)
C(1)-Co(1)-C(4)-C(3)	-136.90(16)	C(19)-P(2)-C(6)-C(5)	-72.09(18)
C(2)-Co(1)-C(4)-C(3)	-35.35(16)	Co(1)-P(2)-C(6)-C(5)	52.61(17)
P(1)-Co(1)-C(4)-C(3)	23.4(2)	C(11)-C(10)-C(9)-C(8)	-1.4(4)
P(2)-Co(1)-C(4)-C(3)	118.03(14)	C(7)-C(8)-C(9)-C(10)	0.9(4)
C(4)-C(3)-C(2)-Co(1)	-61.99(19)		

Table 20. Crystal data and structure refinement for $[Co(CO)_3PPh_3]_2$.

Identification code	sbd0420m	
Empirical formula	C21 H15 Co O3 P	
Formula weight	405.23	
Temperature	393(2) K	
Wavelength	0.71073 Å	
Crystal system	Rhombohedral	
Space group	R-3	
Unit cell dimensions	a = 15.2724(19) Å	α= 90°.
	b = 15.2724(19) Å	β= 90°.
	c = 13.854(4) Å	γ = 120°.
Volume	2798.5(9) $Å^3$	
Z	6	
Density (calculated)	1.443 Mg/m^3	
Absorption coefficient	1.022 mm^{-1}	
F(000)	1242	
Crystal size	0.19 x 0.18 x 0.02 mm^3	
Theta range for data collection	2.13 to 25.01°.	
Index ranges	-18<=h<=18, -18<=k<=17, -16<=l<=16	
Reflections collected	6523	
Independent reflections	1091 [R(int) = 0.0342]	
Completeness to theta = 25.01°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.785	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1091 / 0 / 79	
Goodness-of-fit on F^2	1.110	
Final R indices [I>2sigma(I)]	R1 = 0.0242, wR2 = 0.0671	
R indices (all data)	R1 = 0.0261, wR2 = 0.0679	
Largest diff. peak and hole	0.339 and -0.293 $e.Å^{-3}$	

Table 21. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[Co(CO)_3PPh_3]_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7145(1)	2483(1)	4195(1)	22(1)
C(2)	7688(1)	3205(1)	6410(1)	23(1)
C(3)	8657(1)	3763(1)	6031(1)	34(1)
C(4)	9451(1)	3695(2)	6438(1)	45(1)
C(5)	9281(2)	3062(2)	7218(1)	46(1)
C(6)	8325(2)	2503(2)	7591(1)	42(1)
C(7)	7526(1)	2572(1)	7193(1)	30(1)
Co(1)	6667	3333	4290(1)	17(1)
O(1)	7454(1)	1938(1)	4150(1)	32(1)
P(1)	6667	3333	5870(1)	18(1)

Table 22. Bond lengths [Å] and angles [°] for $[Co(CO)_3PPh_3]_2$

C(1)-O(1)	1.1467(19)
C(1)-Co(1)	1.7845(16)
C(2)-C(7)	1.390(2)
C(2)-C(3)	1.390(2)
C(2)-P(1)	1.8265(15)
C(3)-C(4)	1.387(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.384(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.372(3)
C(5)-H(5)	0.9300
C(6)-C(7)	1.391(2)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
Co(1)-C(1)#1	1.7845(16)
Co(1)-C(1)#2	1.7845(16)
Co(1)-P(1)	2.1895(9)
Co(1)-Co(1)#3	2.6506(9)

P(1)-C(2)#2	1.8265(15)
P(1)-C(2)#1	1.8265(15)

O(1)-C(1)-Co(1)	178.83(13)
C(7)-C(2)-C(3)	119.08(15)
C(7)-C(2)-P(1)	121.99(12)
C(3)-C(2)-P(1)	118.93(12)
C(4)-C(3)-C(2)	120.19(17)
C(4)-C(3)-H(3)	119.9
C(2)-C(3)-H(3)	119.9
C(5)-C(4)-C(3)	120.26(18)
C(5)-C(4)-H(4)	119.9
C(3)-C(4)-H(4)	119.9
C(6)-C(5)-C(4)	119.86(17)
C(6)-C(5)-H(5)	120.1
C(4)-C(5)-H(5)	120.1
C(5)-C(6)-C(7)	120.31(18)
C(5)-C(6)-H(6)	119.8
C(7)-C(6)-H(6)	119.8
C(2)-C(7)-C(6)	120.29(17)
C(2)-C(7)-H(7)	119.9
C(6)-C(7)-H(7)	119.9
C(1)-Co(1)-C(1)#1	119.457(12)
C(1)-Co(1)-C(1)#2	119.457(12)
C(1)#1-Co(1)-C(1)#2	119.457(12)
C(1)-Co(1)-P(1)	94.25(5)
C(1)#1-Co(1)-P(1)	94.25(5)
C(1)#2-Co(1)-P(1)	94.25(5)
C(1)-Co(1)-Co(1)#3	85.75(5)
C(1)#1-Co(1)-Co(1)#3	85.75(5)
C(1)#2-Co(1)-Co(1)#3	85.75(5)
P(1)-Co(1)-Co(1)#3	180.0
C(2)-P(1)-C(2)#2	104.37(6)
C(2)-P(1)-C(2)#1	104.37(6)
C(2)#2-P(1)-C(2)#1	104.37(6)
C(2)-P(1)-Co(1)	114.18(5)
C(2)#2-P(1)-Co(1)	114.18(5)
C(2)#1-P(1)-Co(1)	114.18(5)

Symmetry transformations used to generate equivalent atoms:

#1 -y+1,x-y,z #2 -x+y+1,-x+1,z #3 -x+4/3,-y+2/3,-z+2/3

Table 23. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Co(CO)_3PPh_3]_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	24(1)	24(1)	17(1)	-1(1)	-3(1)	10(1)
C(2)	26(1)	28(1)	18(1)	-7(1)	-5(1)	16(1)
C(3)	28(1)	46(1)	26(1)	-3(1)	-5(1)	16(1)
C(4)	27(1)	66(1)	41(1)	-15(1)	-8(1)	23(1)
C(5)	48(1)	71(1)	40(1)	-20(1)	-21(1)	44(1)
C(6)	58(1)	55(1)	31(1)	-5(1)	-12(1)	42(1)
C(7)	39(1)	37(1)	22(1)	-1(1)	-4(1)	25(1)
Co(1)	19(1)	19(1)	14(1)	0	0	9(1)
O(1)	40(1)	33(1)	34(1)	-3(1)	-5(1)	25(1)
P(1)	20(1)	20(1)	14(1)	0	0	10(1)

Table 24. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for $[Co(CO)_3PPh_3]_2$.

	x	y	z	U(eq)
H(3)	8773	4182	5502	41
H(4)	10099	4077	6187	54
H(5)	9814	3016	7487	55
H(6)	8211	2076	8113	50
H(7)	6880	2193	7452	36

Table 25. Torsion angles [°] for $[Co(CO)_3PPh_3]_2$.

C(7)-C(2)-C(3)-C(4)	-0.8(2)
P(1)-C(2)-C(3)-C(4)	178.74(14)
C(2)-C(3)-C(4)-C(5)	0.8(3)
C(3)-C(4)-C(5)-C(6)	-0.3(3)
C(4)-C(5)-C(6)-C(7)	-0.2(3)
C(3)-C(2)-C(7)-C(6)	0.2(2)
P(1)-C(2)-C(7)-C(6)	-179.27(13)
C(5)-C(6)-C(7)-C(2)	0.3(3)
C(7)-C(2)-P(1)-C(2)#2	-11.36(15)
C(3)-C(2)-P(1)-C(2)#2	169.15(12)
C(7)-C(2)-P(1)-C(2)#1	97.92(10)
C(3)-C(2)-P(1)-C(2)#1	-81.57(17)
C(7)-C(2)-P(1)-Co(1)	-136.72(12)
C(3)-C(2)-P(1)-Co(1)	43.79(14)
C(1)-Co(1)-P(1)-C(2)	33.32(7)
C(1)#1-Co(1)-P(1)-C(2)	-86.68(7)
C(1)#2-Co(1)-P(1)-C(2)	153.32(7)
C(1)-Co(1)-P(1)-C(2)#2	-86.68(7)
C(1)#1-Co(1)-P(1)-C(2)#2	153.32(7)
C(1)#2-Co(1)-P(1)-C(2)#2	33.32(7)
C(1)-Co(1)-P(1)-C(2)#1	153.32(7)
C(1)#1-Co(1)-P(1)-C(2)#1	33.32(7)
C(1)#2-Co(1)-P(1)-C(2)#1	-86.68(7)

Symmetry transformations used to generate equivalent atoms:

#1 -y+1,x-y,z #2 -x+y+1,-x+1,z #3 -x+4/3,-y+2/3,-z+2/3