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(2-Formyl-4-phenylcyclohexen-1-olato)-*cis*-dimethyl-*trans*-bis(trimethylphosphine)cobalt(III)

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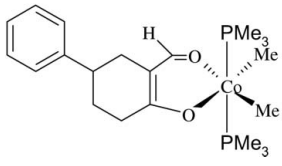
Key indicators: single-crystal X-ray study; T = 423 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.060; wR factor = 0.170; data-to-parameter ratio = 17.2.

In the title compound, $[Co(CH_3)_2(C_{13}H_{13}O_2)(C_3H_9P)_2]$, the Co is at the centre of a distorted octahedron, with two methyl groups *trans* to the chelating 2-formyl-4-phenylcyclohexen-1-olato ligand forming the equatorial plane and two trimethylphosphine groups in the axial positions. The cyclohexene is partially disordered equally over two positions.

Related literature

For related literature, see: Li *et al.* (2005).



Experimental

Crystal data

$[Co(CH_3)_2(C_{13}H_{13}O_2)(C_3H_9P)_2]$
M_r = 442.38
Monoclinic, $P2_1/c$
a = 14.109 (3) Å
b = 9.2740 (19) Å
c = 19.577 (4) Å
β = 106.94 (3)°
V = 2450.4 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.84 mm^{-1}
T = 423 (2) K
0.32 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.774, T_{max} = 0.906
15313 measured reflections
4287 independent reflections
3853 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.171
S = 1.05
4287 reflections
249 parameters
11 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 1997).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2225).

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supplementary materials

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(2-Formyl-4-phenylcyclohexen-1-olato)-*cis*-dimethyl-*trans*-bis(trimethylphosphine)cobalt(III)

J. Zhou, S. Fang, H. Sun and X. Li

Comment

Reaction of substituted enolated malonic dialdehydes (enol-form: b-keton-aldehyde) with $[CoMe_3(PMe_3)_3]$ was recently reported (Li *et al.*, 2005). 2-Hydroxy-5-phenyl-cyclohex-1-enecarbaldehyde reacts with $[CoMe_3(PMe_3)_3]$ (Scheme) by elimination of methane and trimethylphosphine utilizing both the phenolato and the keto-oxygen functions to afford the hexacoordinate title cobalt(III) complex as red solids that are soluble in pentane or diethyl ether. Single crystals suitable for X-ray diffraction analysis of title compound were obtained.

A view of the molecular structure is given in Figure 1. Cobalt atom displays an octahedral coordination with two equatorial *cis*-methyl groups (C20 and C21) and two axial trimethylphosphines as well as a bidentate ligand. The angle P1–Co–P2 of 174.59 (5) implies a slight distortion from an ideal octahedron. The substituted salicylaldehyde ligands have Co—O bond lengths of Co1—O1 1.987 (2), Co1—O2 1.980 (3). The chelate ring is planar with the largest deviation from the plane being 0.030 (3)Å at O2.

Experimental

Standard vacuum techniques were used in manipulations of volatile and air-sensitive material. 2-Hydroxy-5-phenyl-cyclohex-1-enecarbaldehyde (958 mg, 4.74 mmol) in diethyl ether (20 mL) was combined with $[CoMe_3(PMe_3)_3]$ (1,810 mg, 5.45 mmol) in diethyl ether(40 ml) at room temperature. The mixture was stirred for 20 h. During this period the solution turned red. The volatiles were removed *in vacuo* and the residue was extracted with pentane. Crystallization at −20 °C afforded red microcrystals.

Refinement

All H atoms were fixed geometrically and treated as riding on their parent atoms with C—H = 0.93Å (aromatic), 0.96Å (methyl), 0.97Å (methylene) and 0.98Å (methine) with $U_{iso}(H) = xU_{eq}(C)$, x having the value 1.2 or 1.5(methylene).

The cyclohexene is partially stastically distributed over two positions. This disordered moiety was treated using the restraints available in *SHELXL97* (SAME and PART instructions). The value of the occupancy factor, 1/2, was determined in the first stages of the refinement. The thermal displacement parameters for the disordered atoms were restrained using equal U^{ij} constraint.

Figures

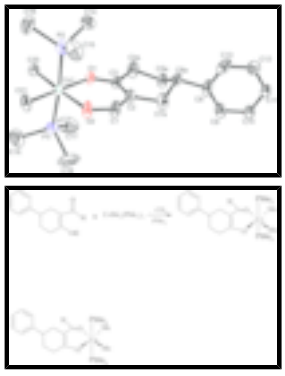

Fig. 1. Molecular structure of the title complex. Ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. Only one component of the disordered moiety is represented.

(2-Formyl-4-phenylcyclohexen-1-olato- *cis*-dimethyl-*trans*-bis(trimethylphosphine)cobalt(III)

Crystal data

$[Co(CH_3)_2(C_{13}H_{13}O_2)(C_3H_9P)_2]$	F_{000} = 944
M_r = 442.38	D_x = 1.199 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4681 reflections
a = 14.109 (3) Å	θ = 2.3–24.3º
b = 9.2740 (19) Å	μ = 0.84 mm^{-1}
c = 19.577 (4) Å	T = 423 (2) K
β = 106.94 (3)º	Block, red
V = 2450.4 (10) Å^3	0.32 × 0.20 × 0.12 mm
Z = 4	

Data collection

CCD area-detector diffractometer	4287 independent reflections
Radiation source: fine-focus sealed tube	3853 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.056
T = 423(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −16→16
T_{min} = 0.774, T_{max} = 0.906	k = −10→11
15313 measured reflections	l = −23→23

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.061$

$wR(F^2) = 0.171$

$S = 1.05$

4287 reflections

249 parameters

11 restraints

Primary atom site location: structure-invariant direct methods

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0921P)^2 + 3.5216P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.008$

$\Delta\rho_{max} = 1.68$ e Å^{-3}

$\Delta\rho_{min} = -0.85$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.3655 (3)	0.6037 (5)	0.2286 (2)	0.0656 (13)	
H1	0.4182	0.5404	0.2333	0.079*	
C2	0.3761 (3)	0.7006 (4)	0.2847 (2)	0.0507 (9)	
C3	0.3028 (3)	0.8021 (4)	0.28556 (19)	0.0443 (8)	
C4A	0.3159 (10)	0.8974 (17)	0.3510 (6)	0.0588 (14)	0.50
H4A1	0.2780	0.8565	0.3805	0.071*	0.50
H4A2	0.2884	0.9918	0.3354	0.071*	0.50
C5A	0.4261 (6)	0.9165 (10)	0.3979 (5)	0.0588 (14)	0.50
H5A1	0.4636	0.9709	0.3723	0.071*	0.50
H5A2	0.4291	0.9667	0.4419	0.071*	0.50
C6A	0.4676 (7)	0.7631 (11)	0.4136 (5)	0.050 (2)	0.50
H6A	0.4249	0.7052	0.4344	0.059*	0.50
C7A	0.4736 (15)	0.696 (3)	0.3447 (11)	0.0588 (14)	0.50
H7A1	0.4941	0.5962	0.3537	0.071*	0.50
H7A2	0.5240	0.7458	0.3290	0.071*	0.50
C4B	0.3213 (10)	0.9155 (16)	0.3432 (6)	0.0588 (14)	0.50
H4B1	0.2593	0.9388	0.3527	0.071*	0.50
H4B2	0.3457	1.0025	0.3265	0.071*	0.50
C5B	0.3982 (6)	0.8638 (11)	0.4139 (4)	0.0588 (14)	0.50
H5B1	0.4135	0.9414	0.4486	0.071*	0.50
H5B2	0.3718	0.7832	0.4342	0.071*	0.50
C6B	0.4903 (6)	0.8187 (12)	0.3946 (5)	0.051 (2)	0.50
H6B	0.5144	0.8987	0.3715	0.061*	0.50

C7B	0.4707 (15)	0.688 (3)	0.3465 (12)	0.0588 (14)	0.50
H7B1	0.4662	0.6038	0.3745	0.071*	0.50
H7B2	0.5263	0.6746	0.3274	0.071*	0.50
C8	0.5720 (3)	0.7739 (6)	0.4658 (3)	0.0711 (14)	
C9	0.6592 (3)	0.8420 (5)	0.4667 (2)	0.0612 (11)	
H9	0.6611	0.9020	0.4291	0.073*	
C10	0.7440 (3)	0.8217 (4)	0.5234 (2)	0.0528 (9)	
H10	0.8023	0.8685	0.5234	0.063*	
C11	0.7430 (3)	0.7336 (5)	0.5794 (2)	0.0538 (9)	
H11	0.8002	0.7205	0.6171	0.065*	
C12	0.6567 (3)	0.6648 (6)	0.5793 (3)	0.0705 (12)	
H12	0.6551	0.6043	0.6168	0.085*	
C13	0.5718 (3)	0.6866 (6)	0.5224 (3)	0.0806 (16)	
H13	0.5133	0.6408	0.5227	0.097*	
C14	0.1131 (4)	0.5802 (6)	0.2979 (2)	0.0703 (12)	
H14A	0.0843	0.6731	0.3006	0.106*	
H14B	0.1819	0.5817	0.3250	0.106*	
H14C	0.0791	0.5085	0.3172	0.106*	
C15	0.1576 (5)	0.3580 (6)	0.2137 (3)	0.0924 (18)	
H15A	0.2282	0.3659	0.2331	0.139*	
H15B	0.1419	0.3144	0.1673	0.139*	
H15C	0.1318	0.2995	0.2446	0.139*	
C16	−0.0301 (4)	0.4970 (8)	0.1689 (4)	0.108 (2)	
H16A	−0.0503	0.4318	0.2000	0.162*	
H16B	−0.0414	0.4533	0.1227	0.162*	
H16C	−0.0677	0.5845	0.1643	0.162*	
C17	0.2460 (7)	1.0381 (7)	0.1306 (4)	0.130 (3)	
H17A	0.2847	1.0260	0.1795	0.194*	
H17B	0.1848	1.0853	0.1289	0.194*	
H17C	0.2822	1.0957	0.1060	0.194*	
C18	0.1411 (6)	0.9086 (10)	−0.0004 (3)	0.131 (3)	
H18A	0.1655	0.9942	−0.0171	0.197*	
H18B	0.0747	0.9250	0.0016	0.197*	
H18C	0.1412	0.8303	−0.0324	0.197*	
C19	0.3384 (6)	0.8276 (11)	0.0729 (5)	0.145 (3)	
H19A	0.3328	0.7439	0.0432	0.218*	
H19B	0.3875	0.8107	0.1178	0.218*	
H19C	0.3576	0.9091	0.0498	0.218*	
C20	0.0439 (3)	0.8123 (5)	0.1320 (2)	0.0554 (10)	
H20A	0.0173	0.8009	0.1716	0.083*	
H20B	−0.0034	0.7780	0.0892	0.083*	
H20C	0.0574	0.9124	0.1265	0.083*	
C21	0.1195 (4)	0.5831 (5)	0.0613 (2)	0.0681 (12)	
H21A	0.1637	0.5941	0.0325	0.102*	
H21B	0.0546	0.6156	0.0350	0.102*	
H21C	0.1166	0.4833	0.0737	0.102*	
Co1	0.16868 (3)	0.69957 (5)	0.14988 (2)	0.0409 (2)	
O1	0.22006 (17)	0.8152 (3)	0.23848 (13)	0.0436 (6)	
O2	0.2941 (2)	0.5894 (4)	0.17176 (15)	0.0665 (9)	

P2	0.10199 (9)	0.53792 (12)	0.20619 (6)	0.0583 (3)
P3	0.22019 (9)	0.86373 (15)	0.08824 (6)	0.0626 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.047 (2)	0.077 (3)	0.059 (2)	0.026 (2)	−0.0057 (18)	−0.028 (2)
C2	0.0403 (19)	0.056 (2)	0.046 (2)	0.0117 (16)	−0.0029 (16)	−0.0164 (17)
C3	0.0372 (18)	0.047 (2)	0.0448 (19)	0.0013 (14)	0.0054 (15)	−0.0117 (15)
C4A	0.0450 (16)	0.066 (3)	0.0544 (18)	0.0138 (15)	−0.0031 (14)	−0.0238 (17)
C5A	0.0450 (16)	0.066 (3)	0.0544 (18)	0.0138 (15)	−0.0031 (14)	−0.0238 (17)
C6A	0.032 (4)	0.068 (6)	0.045 (5)	−0.001 (4)	0.004 (3)	−0.015 (4)
C7A	0.0450 (16)	0.066 (3)	0.0544 (18)	0.0138 (15)	−0.0031 (14)	−0.0238 (17)
C4B	0.0450 (16)	0.066 (3)	0.0544 (18)	0.0138 (15)	−0.0031 (14)	−0.0238 (17)
C5B	0.0450 (16)	0.066 (3)	0.0544 (18)	0.0138 (15)	−0.0031 (14)	−0.0238 (17)
C6B	0.032 (4)	0.070 (7)	0.045 (5)	−0.003 (4)	0.002 (4)	−0.008 (4)
C7B	0.0450 (16)	0.066 (3)	0.0544 (18)	0.0138 (15)	−0.0031 (14)	−0.0238 (17)
C8	0.045 (2)	0.091 (4)	0.059 (3)	0.018 (2)	−0.013 (2)	−0.037 (3)
C9	0.068 (3)	0.060 (2)	0.044 (2)	0.017 (2)	−0.0030 (19)	−0.0113 (18)
C10	0.048 (2)	0.054 (2)	0.049 (2)	−0.0056 (17)	0.0014 (17)	−0.0088 (17)
C11	0.041 (2)	0.060 (2)	0.051 (2)	−0.0029 (17)	−0.0020 (16)	−0.0057 (18)
C12	0.056 (3)	0.083 (3)	0.068 (3)	−0.013 (2)	0.011 (2)	−0.005 (2)
C13	0.041 (2)	0.100 (4)	0.095 (4)	−0.016 (2)	0.011 (2)	−0.041 (3)
C14	0.081 (3)	0.071 (3)	0.060 (3)	−0.002 (2)	0.023 (2)	0.014 (2)
C15	0.137 (5)	0.049 (3)	0.082 (4)	0.013 (3)	0.018 (3)	0.006 (2)
C16	0.073 (3)	0.111 (5)	0.112 (5)	−0.039 (3)	−0.015 (3)	0.039 (4)
C17	0.200 (9)	0.068 (4)	0.147 (7)	−0.038 (5)	0.094 (7)	0.002 (4)
C18	0.131 (6)	0.165 (7)	0.083 (4)	−0.028 (5)	0.007 (4)	0.065 (5)
C19	0.104 (5)	0.196 (9)	0.174 (8)	−0.001 (6)	0.102 (6)	0.018 (7)
C20	0.039 (2)	0.071 (3)	0.051 (2)	0.0045 (18)	0.0064 (17)	0.0070 (19)
C21	0.074 (3)	0.072 (3)	0.042 (2)	0.006 (2)	−0.0099 (19)	−0.017 (2)
Co1	0.0373 (3)	0.0430 (3)	0.0352 (3)	0.00283 (18)	−0.0010 (2)	−0.00375 (18)
O1	0.0340 (12)	0.0474 (14)	0.0433 (13)	0.0069 (10)	0.0016 (10)	−0.0100 (10)
O2	0.0526 (16)	0.077 (2)	0.0533 (16)	0.0230 (14)	−0.0101 (13)	−0.0320 (15)
P2	0.0603 (6)	0.0510 (6)	0.0514 (6)	−0.0060 (5)	−0.0028 (5)	0.0062 (4)
P3	0.0606 (7)	0.0753 (8)	0.0574 (6)	−0.0078 (6)	0.0259 (5)	0.0036 (5)

Geometric parameters (Å, °)

C1—O2	1.271 (5)	C12—C13	1.393 (7)
C1—C2	1.394 (5)	C12—H12	0.9300
C1—H1	0.9300	C13—H13	0.9300
C2—C3	1.403 (5)	C14—P2	1.800 (5)
C2—C7B	1.521 (10)	C14—H14A	0.9600
C2—C7A	1.526 (10)	C14—H14B	0.9600
C3—O1	1.265 (4)	C14—H14C	0.9600
C3—C4A	1.523 (10)	C15—P2	1.831 (5)
C3—C4B	1.509 (10)	C15—H15A	0.9600
C4A—C5A	1.569 (12)	C15—H15B	0.9600

C4A—H4A1	0.9700	C15—H15C	0.9600
C4A—H4A2	0.9700	C16—P2	1.832 (5)
C5A—C6A	1.534 (11)	C16—H16A	0.9600
C5A—H5A1	0.9700	C16—H16B	0.9600
C5A—H5A2	0.9700	C16—H16C	0.9600
C6A—C7A	1.510 (16)	C17—P3	1.806 (7)
C6A—C8	1.533 (9)	C17—H17A	0.9600
C6A—H6A	0.9800	C17—H17B	0.9600
C7A—H7A1	0.9700	C17—H17C	0.9600
C7A—H7A2	0.9700	C18—P3	1.817 (6)
C4B—C5B	1.565 (12)	C18—H18A	0.9600
C4B—H4B1	0.9700	C18—H18B	0.9600
C4B—H4B2	0.9700	C18—H18C	0.9600
C5B—C6B	1.514 (10)	C19—P3	1.810 (6)
C5B—H5B1	0.9700	C19—H19A	0.9600
C5B—H5B2	0.9700	C19—H19B	0.9600
C6B—C7B	1.508 (16)	C19—H19C	0.9600
C6B—C8	1.584 (10)	C20—Co1	1.990 (4)
C6B—H6B	0.9800	C20—H20A	0.9600
C7B—H7B1	0.9700	C20—H20B	0.9600
C7B—H7B2	0.9700	C20—H20C	0.9600
C8—C13	1.372 (8)	C21—Co1	1.989 (4)
C8—C9	1.377 (7)	C21—H21A	0.9600
C9—C10	1.388 (6)	C21—H21B	0.9600
C9—H9	0.9300	C21—H21C	0.9600
C10—C11	1.370 (6)	Co1—O2	1.980 (3)
C10—H10	0.9300	Co1—O1	1.987 (2)
C11—C12	1.374 (6)	Co1—P3	2.1938 (13)
C11—H11	0.9300	Co1—P2	2.2254 (13)
O2—C1—C2	129.3 (4)	C8—C13—C12	121.8 (5)
O2—C1—H1	115.4	C8—C13—H13	119.1
C2—C1—H1	115.4	C12—C13—H13	119.1
C1—C2—C3	122.2 (3)	P2—C14—H14A	109.5
C1—C2—C7B	116.5 (5)	P2—C14—H14B	109.5
C3—C2—C7B	121.3 (5)	H14A—C14—H14B	109.5
C1—C2—C7A	117.0 (5)	P2—C14—H14C	109.5
C3—C2—C7A	120.8 (5)	H14A—C14—H14C	109.5
C7B—C2—C7A	3(3)	H14B—C14—H14C	109.5
O1—C3—C2	125.7 (3)	P2—C15—H15A	109.5
O1—C3—C4A	114.7 (5)	P2—C15—H15B	109.5
C2—C3—C4A	119.4 (5)	H15A—C15—H15B	109.5
O1—C3—C4B	113.6 (5)	P2—C15—H15C	109.5
C2—C3—C4B	120.6 (5)	H15A—C15—H15C	109.5
C4A—C3—C4B	9.6 (15)	H15B—C15—H15C	109.5
C3—C4A—C5A	114.4 (8)	P2—C16—H16A	109.5
C3—C4A—H4A1	108.6	P2—C16—H16B	109.5
C5A—C4A—H4A1	108.6	H16A—C16—H16B	109.5
C3—C4A—H4A2	108.7	P2—C16—H16C	109.5
C5A—C4A—H4A2	108.7	H16A—C16—H16C	109.5

H4A1—C4A—H4A2	107.6	H16B—C16—H16C	109.5
C6A—C5A—C4A	105.6 (8)	P3—C17—H17A	109.5
C6A—C5A—H5A1	110.6	P3—C17—H17B	109.5
C4A—C5A—H5A1	110.6	H17A—C17—H17B	109.5
C6A—C5A—H5A2	110.6	P3—C17—H17C	109.5
C4A—C5A—H5A2	110.6	H17A—C17—H17C	109.5
H5A1—C5A—H5A2	108.8	H17B—C17—H17C	109.5
C5A—C6A—C7A	108.7 (13)	P3—C18—H18A	109.5
C5A—C6A—C8	108.0 (7)	P3—C18—H18B	109.5
C7A—C6A—C8	109.3 (8)	H18A—C18—H18B	109.5
C5A—C6A—H6A	110.2	P3—C18—H18C	109.5
C7A—C6A—H6A	110.2	H18A—C18—H18C	109.5
C8—C6A—H6A	110.2	H18B—C18—H18C	109.5
C6A—C7A—C2	113.8 (11)	P3—C19—H19A	109.5
C6A—C7A—H7A1	108.8	P3—C19—H19B	109.5
C2—C7A—H7A1	108.8	H19A—C19—H19B	109.5
C6A—C7A—H7A2	108.8	P3—C19—H19C	109.5
C2—C7A—H7A2	108.8	H19A—C19—H19C	109.5
H7A1—C7A—H7A2	107.7	H19B—C19—H19C	109.5
C3—C4B—C5B	111.9 (8)	Co1—C20—H20A	109.5
C3—C4B—H4B1	109.2	Co1—C20—H20B	109.5
C5B—C4B—H4B1	109.2	H20A—C20—H20B	109.5
C3—C4B—H4B2	109.2	Co1—C20—H20C	109.5
C5B—C4B—H4B2	109.2	H20A—C20—H20C	109.5
H4B1—C4B—H4B2	107.9	H20B—C20—H20C	109.5
C6B—C5B—C4B	106.8 (9)	Co1—C21—H21A	109.5
C6B—C5B—H5B1	110.4	Co1—C21—H21B	109.5
C4B—C5B—H5B1	110.4	H21A—C21—H21B	109.5
C6B—C5B—H5B2	110.4	Co1—C21—H21C	109.5
C4B—C5B—H5B2	110.4	H21A—C21—H21C	109.5
H5B1—C5B—H5B2	108.6	H21B—C21—H21C	109.5
C5B—C6B—C7B	111.3 (13)	O2—Co1—O1	90.80 (10)
C5B—C6B—C8	108.1 (7)	O2—Co1—C21	88.33 (16)
C7B—C6B—C8	107.1 (10)	O1—Co1—C21	179.06 (16)
C5B—C6B—H6B	110.1	O2—Co1—C20	177.72 (14)
C7B—C6B—H6B	110.1	O1—Co1—C20	87.09 (15)
C8—C6B—H6B	110.1	C21—Co1—C20	93.79 (19)
C6B—C7B—C2	113.3 (11)	O2—Co1—P3	93.37 (12)
C6B—C7B—H7B1	108.9	O1—Co1—P3	90.61 (9)
C2—C7B—H7B1	108.9	C21—Co1—P3	89.12 (16)
C6B—C7B—H7B2	108.9	C20—Co1—P3	87.51 (13)
C2—C7B—H7B2	108.9	O2—Co1—P2	91.46 (12)
H7B1—C7B—H7B2	107.7	O1—Co1—P2	91.75 (9)
C13—C8—C9	118.2 (4)	C21—Co1—P2	88.60 (16)
C13—C8—C6A	105.8 (6)	C20—Co1—P2	87.76 (13)
C9—C8—C6A	136.0 (6)	P3—Co1—P2	174.60 (5)
C13—C8—C6B	133.8 (6)	C3—O1—Co1	127.5 (2)
C9—C8—C6B	108.0 (6)	C1—O2—Co1	124.5 (2)
C6A—C8—C6B	28.1 (4)	C14—P2—C15	102.0 (3)

C8—C9—C10	120.4 (5)	C14—P2—C16	103.1 (3)
C8—C9—H9	119.8	C15—P2—C16	101.9 (3)
C10—C9—H9	119.8	C14—P2—Co1	114.89 (17)
C11—C10—C9	120.8 (4)	C15—P2—Co1	114.9 (2)
C11—C10—H10	119.6	C16—P2—Co1	118.0 (2)
C9—C10—H10	119.6	C17—P3—C19	99.8 (5)
C10—C11—C12	119.5 (4)	C17—P3—C18	102.7 (4)
C10—C11—H11	120.3	C19—P3—C18	102.9 (4)
C12—C11—H11	120.3	C17—P3—Co1	115.1 (2)
C11—C12—C13	119.3 (5)	C19—P3—Co1	115.6 (3)
C11—C12—H12	120.4	C18—P3—Co1	118.3 (2)
C13—C12—H12	120.4		

Fig. 1

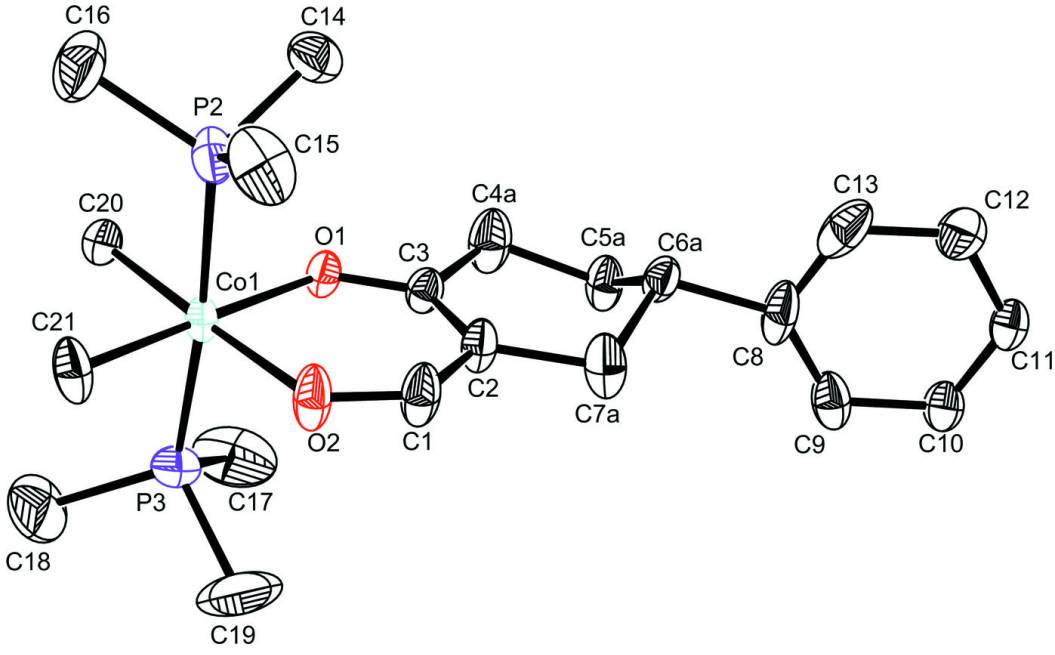
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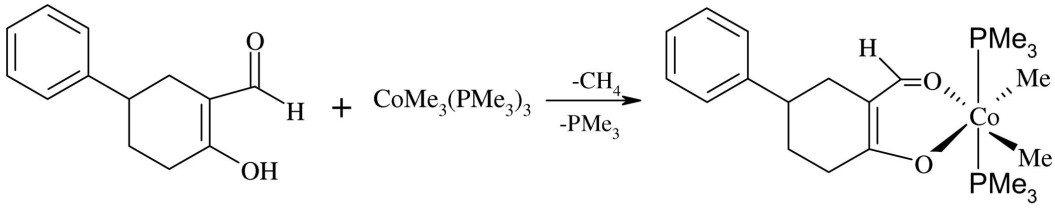
Fig. 2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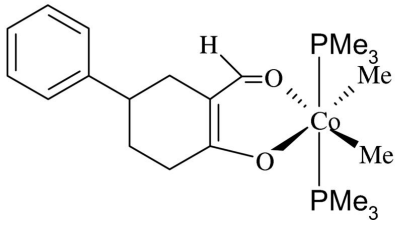
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