

## Hydridotetrakis(triphenylphosphito)cobalt(I)

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## Key indicators

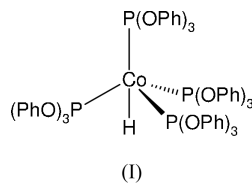
Single-crystal X-ray study  
 $T = 150$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
Disorder in main residue  
 $R$  factor = 0.036  
 $wR$  factor = 0.069  
Data-to-parameter ratio = 17.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.At 150 K, the coordination geometry of the Co atom in the  
title compound,  $[\text{CoH}(\text{C}_{18}\text{H}_{15}\text{O}_3\text{P})_4]$ , is monocapped tetra-  
hedral, with the hydride as the face-capping ligand.

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## Comment

In the title compound, (I), the P atoms of the four triphenyl-  
phosphite ligands are disposed in a distorted tetrahedral  
geometry around the cobalt(I) ion. The location of the face-  
capping hydride ligand *trans* to P1 was strongly indicated by  
the long Co1–P1 bond distance of 2.1191 (7) Å caused by the  
*trans* influence of the hydride, and the pattern of bond angles  
subtended at the cobalt centre (Table 1). The location was  
confirmed by the high residual electron density observed at  
this position in the difference Fourier map and the subsequent  
successful free refinement of the positional parameters for the  
hydride ligand, with a Co1–H1 distance of 1.36 (2) Å. This  
apparent bond shortening relative to the typical value of  
1.55 Å for first row transition metal hydrides is characteristic  
of X-ray crystallography (Teller & Bau, 1981).

## Experimental

The title compound, (I), was prepared by the method of Levison &  
Robinson (1970). Crystals were grown by the slow diffusion of  
methanol into a dichloromethane solution of (I) at room tempera-  
ture. Two crystal morphologies were observed: the majority were thin  
hexagonal plates which were found to be intractably twinned, and the  
minority were oblong blocks which were found to be suitable.

## Crystal data

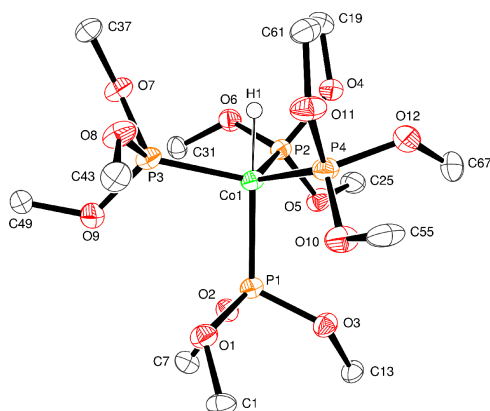
$[\text{CoH}(\text{C}_{18}\text{H}_{15}\text{O}_3\text{P})_4]$   
 $M_r = 1301.02$   
Monoclinic,  $Cc$   
 $a = 20.2331$  (14) Å  
 $b = 17.2635$  (10) Å  
 $c = 18.3682$  (11) Å  
 $\beta = 100.117$  (5)°  
 $V = 6316.1$  (7) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.368$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 17065  
reflections  
 $\theta = 2.0$ – $28.0^\circ$   
 $\mu = 0.44$  mm<sup>-1</sup>  
 $T = 150$  (2) K  
Block, pale yellow  
 $0.60 \times 0.20 \times 0.20$  mm

## Data collection

Stoe IPDS-II area-detector  
diffractometer  
 $\varphi$  and  $\omega$  scans  
Absorption correction: numerical  
(*X-SHAPE*; Stoe & Cie, 2001)  
 $T_{\min} = 0.803$ ,  $T_{\max} = 0.930$   
35963 measured reflections

14644 independent reflections  
10146 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.052$   
 $\theta_{\text{max}} = 28.0^\circ$   
 $h = -26 \rightarrow 26$   
 $k = -22 \rightarrow 22$   
 $l = -24 \rightarrow 24$


**Figure 1**

View of the molecule of (I), showing the atom-labelling scheme. For clarity, only the *ipso*-C atoms of the phenyl rings are shown; these rings are numbered sequentially round the ring starting from the *ipso*-C atom. Displacement ellipsoids are drawn at the 50% probability level.

### Refinement

Refinement on  $F^2$

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.069$

$S = 0.80$

14644 reflections

821 parameters

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.31 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$$

Absolute structure: Flack (1983),

7006 Friedel pairs

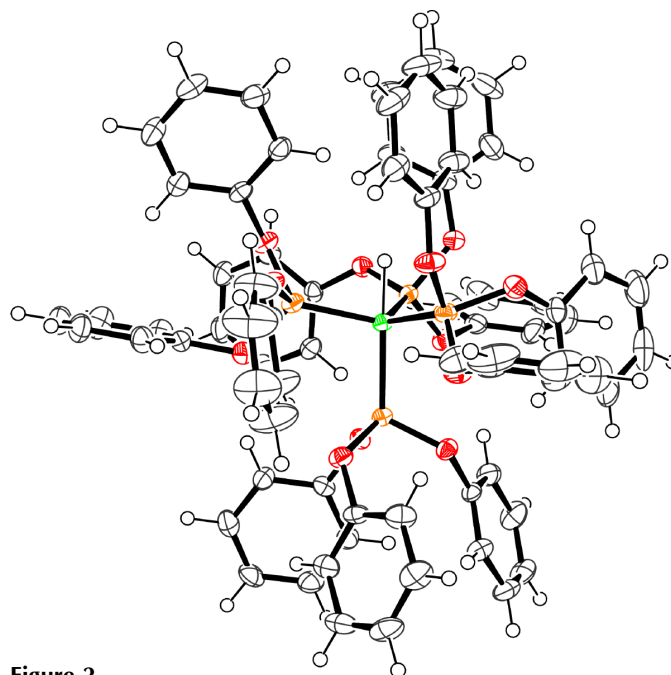
Flack parameter =  $-0.022(9)$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Co1—H1	1.36 (2)	Co1—P3	2.0903 (8)
Co1—P1	2.1191 (7)	Co1—P4	2.0816 (7)
Co1—P2	2.0860 (8)		
P1—Co1—H1	177.6 (11)	P3—Co1—P1	102.89 (3)
P2—Co1—H1	76.4 (11)	P4—Co1—P1	101.41 (3)
P3—Co1—H1	78.6 (11)	P3—Co1—P2	114.86 (3)
P4—Co1—H1	79.5 (11)	P4—Co1—P2	118.38 (3)
P2—Co1—P1	101.19 (3)	P4—Co1—P3	114.50 (3)

The C25–C30 phenyl ring was modelled as disordered over two orientations with a common *ipso*-C atom C25, giving occupancies of 0.725 (17) and 0.275 (17). The displacement parameters for corresponding atoms in the two components were constrained to be the same. All H atoms were initially located in a difference Fourier map. They were then constrained to an ideal geometry, with a C–H distance of 0.95  $\text{\AA}$  and  $U_{\text{iso}}(\text{H})$  values set at  $1.2U_{\text{eq}}(\text{C})$ . The positional


**Figure 2**

View of the molecule of (I), in the same orientation as Fig. 1, but showing all the atoms. Only the major component of the disordered phenyl ring C25–C30 is shown.

parameters for the hydride ligand were freely refined, but  $U_{\text{iso}}(\text{H})$  was set to  $1.2U_{\text{eq}}(\text{Co})$ .

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2001); program(s) used to solve structure: *X-STEP32* (Stoe & Cie, 2001) and *WinGX* (Farrugia, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2001).

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