

Chloridotris[tris(4-fluorophenyl)-phosphine]rhodium(I) methanol solvate

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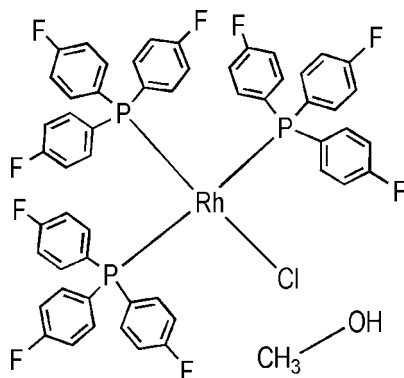
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 Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; disorder in main residue; R factor = 0.034; wR factor = 0.075; data-to-parameter ratio = 8.9.

In the title compound, $[\text{RhCl}\{\text{P}(p\text{-FC}_6\text{H}_4)_3\}_3]\cdot\text{CH}_3\text{OH}$, the Rh atom adopts a distorted square-planar geometry. Rh, Cl and one P atom lie on a mirror plane, as does the solvent molecule. There are two intermolecular hydrogen bonds, one between the methanol O atom and an aryl H atom (2.51 Å), and one between the Cl atom and the hydroxy H atom of methanol [2.34 (3) Å]. The complex precipitates in trace amounts from a reaction between $\text{RhCl}(\text{cod})(\text{thp})$ [cod is 1,5-cyclooctadiene and thp is tris(hydroxymethyl)phosphine] and $\text{P}(p\text{-FC}_6\text{H}_4)_3$ under argon in CD_3OD . Two $\text{C}_6\text{H}_4\text{-F}$ units are disordered over two positions; for one the site occupancy factors are *ca.* 0.53 and 0.47, for the other the values are *ca.* 0.64 and 0.36. The methyl H atoms of the solvent molecule are disordered across the mirror plane.

Related literature

For related literature, see: Beck *et al.* (1999) and references therein; Bennett & Donaldson (1977); Bennett *et al.* (1971); Evans *et al.* (1999); Higham *et al.* (2004); Hoye *et al.* (1993); Jones *et al.* (1980); Lorenzini *et al.* (2007*a,b,c*, 2008*a,b*); Montelatici *et al.* (1968); Young *et al.* (1965).



Experimental

Crystal data

$[\text{RhCl}(\text{C}_{18}\text{H}_{12}\text{F}_3\text{P}_3)]\cdot\text{CH}_4\text{O}$
 $M_r = 1119.14$
 Monoclinic, C_m
 $a = 10.831$ (3) Å
 $b = 23.724$ (7) Å
 $c = 9.845$ (3) Å
 $\beta = 108.213$ (8)°

$V = 2403.0$ (12) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.59$ mm⁻¹
 $T = 173.0$ (1) K
 $0.30 \times 0.15 \times 0.03$ mm

Data collection

Bruker X8 APEXII diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2003)
 $T_{\text{min}} = 0.544$, $T_{\text{max}} = 0.983$

10921 measured reflections
 3312 independent reflections
 3094 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.048$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.075$
 $S = 1.03$
 3312 reflections
 372 parameters
 15 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.67$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.47$ e Å⁻³
 Absolute structure: Flack (1983), 812 Friedel pairs
 Flack parameter: -0.03 (3)

Table 1

Hydrogen-bond geometry (Å, °).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
$\text{C3---H3}\cdots\text{O1}^i$	0.95	2.51	3.458 (9)	172
$\text{O1---H1O}\cdots\text{Cl1}^{ii}$	1.03 (5)	2.34 (5)	3.369 (9)	174 (11)

 Symmetry codes: (i) $x, y, z + 1$; (ii) $x + 1, y, z - 1$.

Data collection: *SAINT* (Bruker, 2003); cell refinement: *SAINT*; data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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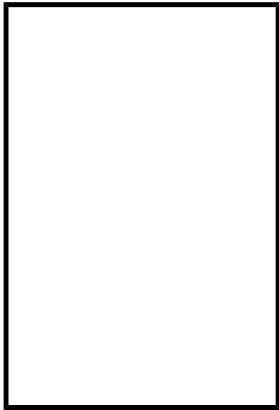
Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2075).

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