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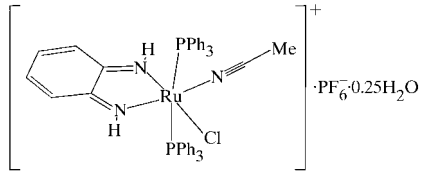
The Ru atom in the title compound, $[RuCl(CH_3CN)\{P(C_6H_5)_3\}_2\{C_6H_4(NH)_2\}]PF_6\cdot0.25H_2O$, has a six-coordinate octahedral geometry, with a *trans* arrangement of the triphenylphosphine groups. The asymmetric unit contains two complex molecules and a partially occupied water site. Principal dimensions include Ru—N 1.958 (4)–2.044 (5), Ru—P 2.3897 (16)–2.4092 (15), and Ru—Cl 2.4280 (15) and 2.4295 (16) Å

Comment

In order to understand the mixing between ruthenium and redox-active (non-innocent) ligands and its implication on the electrochemical parameter (Lever, 1990; Masui *et al.*, 2000; Venegas-Yazigi *et al.*, 2000, and references therein), we synthesized a family of ruthenium complexes containing *o*-benzoquinone diimine (BQDI), two triphenylphosphine ligands in a *trans* arrangement and two other non-redox-active ligands such as chlorine, acetonitrile, diethyldithiocarbamate *etc*. The unit cell of the title compound, (I), contains two molecules of complex, two hexafluorophosphate anions and a half molecule of water. The Ru atom shows a six-coordinate octahedral geometry, with a *trans* arrangement of the triphenylphosphine groups. C—C distances in the quinone ligand have been very important in confirming the quinoid form of BQDI.



(I)

Experimental

Crystal data

$[RuCl(C_2H_3N)(C_6H_6N_2)(C_{18}H_{15}P)_2]PF_6\cdot0.25H_2O$
M_r = 957.72
Monoclinic, $P2_1/c$
a = 24.2211 (8) Å
b = 10.6752 (4) Å
c = 35.1913 (12) Å
β = 107.747 (2)°
V = 8666.2 (5) Å^3
Z = 8
D_x = 1.468 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 36022 reflections
θ = 3.41–25.02°
μ = 0.596 mm^{-1}
T = 150 (2) K
Very fine needle, purple
0.17 × 0.09 × 0.04 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans with κ offsets
Absorption correction: multi-scan (*DENZOSMN*; Otwinowski & Minor, 1997)
T_{min} = 0.906, T_{max} = 0.977
36 022 measured reflections
15 108 independent reflections
6785 reflections with $I > 2\sigma(I)$
R_{int} = 0.108
θ_{max} = 25.02°
$h = -29 \rightarrow 28$
$k = -13 \rightarrow 12$
$l = -41 \rightarrow 39$

Refinement

Refinement on F^2
$R(F)$ = 0.056
$wR(F^2)$ = 0.118
S = 0.875
15 108 reflections
1056 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.012
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ru1*A*—N3*A*	1.971 (4)	Ru1*B*—N1*B*	2.029 (5)
Ru1*A*—N2*A*	2.015 (4)	Ru1*B*—N2*B*	2.030 (4)
Ru1*A*—N1*A*	2.044 (5)	Ru1*B*—P2*B*	2.3897 (16)
Ru1*A*—P2*A*	2.3937 (15)	Ru1*B*—P1*B*	2.3899 (15)
Ru1*A*—P1*A*	2.4092 (15)	Ru1*B*—Cl1*B*	2.4295 (16)
Ru1*B*—N3*B*	1.958 (4)		
N3*A*—Ru1*A*—N2*A*	77.08 (18)	N3*B*—Ru1*B*—N1*B*	91.64 (19)
N3*A*—Ru1*A*—N1*A*	92.10 (18)	N3*B*—Ru1*B*—N2*B*	76.9 (2)
N2*A*—Ru1*A*—N1*A*	169.18 (18)	N1*B*—Ru1*B*—N2*B*	168.5 (2)
N3*A*—Ru1*A*—P2*A*	91.65 (12)	N3*B*—Ru1*B*—P2*B*	92.39 (12)
N2*A*—Ru1*A*—P2*A*	92.84 (12)	N1*B*—Ru1*B*—P2*B*	88.95 (14)
N1*A*—Ru1*A*—P2*A*	87.56 (12)	N2*B*—Ru1*B*—P2*B*	91.62 (12)
N3*A*—Ru1*A*—P1*A*	93.09 (12)	N3*B*—Ru1*B*—P1*B*	91.61 (12)
N2*A*—Ru1*A*—P1*A*	92.36 (12)	N1*B*—Ru1*B*—P1*B*	89.03 (13)
N1*A*—Ru1*A*—P1*A*	88.02 (13)	N2*B*—Ru1*B*—P1*B*	91.15 (12)
P2*A*—Ru1*A*—P1*A*	173.64 (6)	P2*B*—Ru1*B*—P1*B*	175.57 (6)

All H atoms were visible from difference Fourier maps (except for those bonded to the partial-occupancy water molecule) and were included in calculated positions and refined as riding atoms with C—H = 0.95–0.98 Å and N—H = 0.88 Å. The H atoms of the partial-occupancy water molecule were not included in the calculations, but are included in the molecular formula.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL/PC*; software used to prepare material for publication: *SHELXTL/PC*.

Data were collected at the University of Toronto (where all structural calculations were carried out) on a Nonius KappaCCD diffractometer purchased with funds from NSERC (Canada). We would like to acknowledge Proyectos FONDECYT 2980026 and 1970354.

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