Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

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Electronic paper
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Bis(acetonitrile-*N*)(*o*-benzoquinone diimine-*N*,*N*′)-*trans*-bis(triphenylphosphine-*P*)ruthenium(II) bis(hexafluorophosphate) methanol solvate

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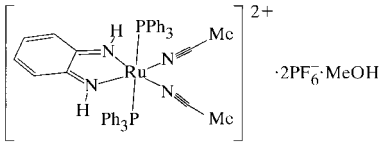
Received 3 May 2000
Accepted 23 May 2000

Data validation number: IUC0000145

The title complex, $[Ru(C_2H_3N)_2(C_6H_6N_2)(C_{18}H_{15}P)_2](PF_6)_2.CH_4O$, is the third of a series of ruthenium complexes containing two triphenylphosphine groups in a *trans* arrangement, *o*-benzoquinone diimine and two other non-redox active ligands to been characterized. The effect of electron donor–acceptor properties of the two non-redox active ligands does not change the quinone arrangement for the *o*-benzoquinone diimine ligand, as can be seen from the bond distances of the quinone ring. The asymmetric unit contains half a molecule of complex cation (on a twofold rotation axis), one hexafluorophosphate anion and half a molecule of methanol in a general position close to a twofold rotation axis.

Comment

In order to evaluate the effect of electron density on the quinone ligand and its effect on the possible quinone or semiquinone arrangement, we have synthesized a family of complexes which have different non-redox active ligands in



(I)

the same plane as the *o*-benzoquinone diimine (BQDI). The bond distances in the BQDI ring for a complex with two electron-donor ligands, such as chloride (Venegas-Yazigi *et al.*, 2000*b*), one electron donor (chloride) and one electron-acceptor ligand (acetonitrile) (Venegas-Yazigi *et al.*, 2000*a*), and the title compund, (I), with two electron-acceptor ligands (acetonitrile) show a quinone arrangement for the BQDI ring.

Experimental

Crystal data

$[Ru(C_2H_3N)_2(C_6H_6N_2)(C_{18}H_{15}P)_2](PF_6)_2.CH_4O$	D_x = 1.547 Mg m^{-3}
M_r = 1135.83	Mo $K\alpha$ radiation
Orthorhombic, *Aba*2	Cell parameters from 14495 reflections
a = 19.0603 (5) Å	θ = 4.19–23.67°
b = 16.5960 (4) Å	μ = 0.539 mm^{-1}
c = 15.4192 (3) Å	T = 100 (1) K
V = 4877.5 (2) Å^3	Block cut from needle, purple
Z = 4	0.39 × 0.38 × 0.31 mm

Data collection

Nonius KappaCCD diffractometer	4410 reflections with $I > 2\sigma(I)$
φ and ω scans with κ offsets	R_{int} = 0.049
Absorption correction: multi-scan (*DENZO–SMN*; Otwinowski & Minor, 1997)	θ_{max} = 26.37°
	$h = -23 \rightarrow 23$
	$k = -20 \rightarrow 20$
T_{min} = 0.817, T_{max} = 0.851	$l = -19 \rightarrow 19$
14 495 measured reflections	Intensity decay: none
4778 independent reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 4.8593P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R(F)$ = 0.027	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.073	$\Delta\rho_{max}$ = 0.43 e Å^{-3}
S = 1.068	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
4778 reflections	Absolute structure: Flack (1983), 2205 Friedel pairs
325 parameters	Flack parameter = 0.52 (3)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Ru1—N1	2.011 (3)	Ru1—P1^{i}	2.4071 (5)
Ru1—N1^{i}	2.011 (3)	C1—C2	1.435 (4)
Ru1—N2^{i}	2.051 (3)	C1—C1^{i}	1.457 (5)
Ru1—N2	2.051 (3)	C2—C3	1.354 (5)
Ru1—P1	2.4071 (5)	C3—C3^{i}	1.444 (7)
N1—Ru1—N1^{i}	77.63 (15)	P1—Ru1—P1^{i}	179.22 (5)
N1^{i}—Ru1—N2	94.05 (10)		

Symmetry code: (i) $-x, -y, z$.

The structure appears to be a racemic twin.

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 purchased with funds from NSERC Canada. We would like to acknowledge Proyectos FONDECYT 2980026 and 1970354.

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