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Aquabis(benzonitrile)(*o*-benzoquinone diimine)(triphenylphosphine)-ruthenium(II) bis(tetrafluoroborate) hydrate

Diego Venegas-Yazigi,[a]* A. B. P. Lever,[b] Alan J. Lough,[c] Andrés Vega,[d] Verónica Paredes-García,[a] Juan Costamagna[e] and Ramón Latorre[f]

[a]Departamento de Química, Facultad de Ciencias, Universidad de Chile, Las Palmeras 3425, Nunoa, Santiago, Chile, and Departamento de Química, Fac. Cs. Nat., Mat. y del M. Amb., Universidad Tecnológica Metropolitana, Av. J.P. Alessandri 1242, Nunoa, Santiago, Chile, [b]Faculty of Pure and Applied Sciences, York University, 4700 Keele St., Toronto, Ontario, Canada M3J 1P3, [c]Department of Chemistry, University of Toronto, Toronto, Ontario, Canada M5S 3H6, [d]Departa-orgánica y Analítica, Facultad de Ciencias Químicas y Farmaceúticas, Universidad de Chile, Casilla 233, Santiago, Chile, [e]Facultad de Química y Biología, Universidad de Santiago, Santiago 33, Chile, and [f]Departamento de Química, Facultad de Ciencias, Universidad de Chile, Casilla 653, Santiago, Chile
Correspondence e-mail: diego@uchile.cl

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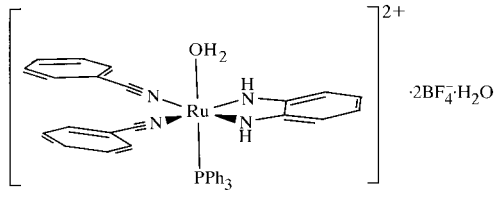
The Ru atom in the title compound, $[Ru(C_6H_5CN)_2\{P(C_6H_5)_3\}\{C_6H_4(NH)_2\}(H_2O)](BF_4)_2\cdot H_2O$, has six-coordinate octahedral geometry, with a *trans* arrangement of the triphenylphosphine ligand and the water molecule. The asymmetric unit contains one complex cation, two tetrafluoroborate anions and one solvent water molecule, which is disordered over two sites (ratio of occupancies 0.70:0.30).

Comment

In order to understand the bonding between ruthenium and redox-active (non-innocent) ligands and its implication for electrochemical behaviour (Lever, 1990; Masui *et al.*, 2000), we synthesized a family of ruthenium complexes containing *o*-benzoquinone diimine (BQDI) and other non-redox active ligands with different electron donor–acceptor behaviour. We have published complexes with ligands in a *trans* position to the benzoquinone dimine ring with: (i) donor character as two chlorines (Venegas-Yazigi *et al.*, 2000); (ii) acceptor behaviour as two acetonitriles (Venegas-Yazigi *et al.*, 2000*a*); (iii) one acceptor and one donor ligands as acetonitrile and chlorine (Venegas-Yazigi *et al.*, 2000*b*). In all these complexes, we could establish a quinone arrangement for the benzoquinone diimine ring which looks to be independent of the donor–acceptor behaviour of the ligands which are *trans* to it.

The Ru atom in the title complex, (I), shows an octahedral coordination. The benzonitrile ligands are in the same plane as the *o*-benzoquinone diimine ligand. Bond distances for the benzoquinone diimine ring establish a quinone arrangement showing that the highly acidic behaviour of the benzonitrile ligands does not have an influence on its arrangement.



(I)

Experimental

Crystal data

$[Ru(C_6H_6N_2)(C_7H_5N)_2(C_{18}H_{15}P)(H_2O)](BF_4)_2\cdot H_2O$
M_r = 885.36
Monoclinic, $P2_1/c$
a = 13.0428 (6) Å
b = 15.0530 (11) Å
c = 21.0245 (15) Å
β = 103.050 (4)°
V = 4021.2 (5) Å^3
Z = 4
D_x = 1.462 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24 821 reflections
θ = 4.08–25.03°
μ = 0.505 mm^{-1}
T = 100 (1) K
Plate, purple
0.30 × 0.15 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans with κ offsets
Absorption correction: multi-scan (*DENZO–SMN*; Otwinowski & Minor, 1997)
T_{min} = 0.863, T_{max} = 0.975
24 821 measured reflections
7016 independent reflections
4495 reflections with $I > 2\sigma(I)$
R_{int} = 0.072
θ_{max} = 25.03°
$h = -16 \rightarrow 15$
$k = -18 \rightarrow 17$
$l = -25 \rightarrow 24$
Intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.056
$wR(F^2)$ = 0.167
S = 1.022
7016 reflections
521 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0882P)^2 + 2.1510P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O*A*···F3	0.838 (5)	1.950 (8)	2.772 (5)	166.7 (13)
O1—H1O*B*···O1*W*	0.839 (5)	1.831 (10)	2.669 (9)	176.5 (6)
N1—H1*A*···F6	0.88	2.21	3.029 (6)	154
N1—H1*A*···F7	0.88	2.47	3.178 (6)	137
N2—H2*A*···F2	0.88	2.09	2.902 (6)	152

The asymmetric unit contains one solvent water molecule, which is disordered over two sites with a ratio of occupancies of 0.70:0.30. The H atoms of the disordered water molecule were not located and hence not included in the calculations.

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 thank Proyectos FONDECYT (2980026 and 1970354).

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