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(Acetonitrile)(2,2′-bipyridine)tricarbonylrhenium(I) perchlorate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.024
wR factor = 0.061
Data-to-parameter ratio = 16.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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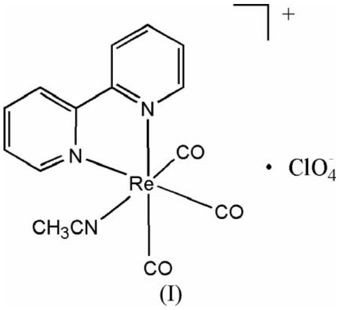
The title compound, $[Re(C_2H_3N)(C_{10}H_8N_2)(CO)_3]ClO_4$, was isolated from the reaction between $[ReCl(bpy)(CO)_3]$ (bpy is 2,2′-bipyridine) and $AgClO_4$ in acetonitrile. The Re atom adopts a distorted octahedral geometry.

Comment

Rhenium(I) tricarbonyl diimine systems are of great interest because of their rich photoluminescent properties and their possible effect in electrochemically promoted reductions of carbon dioxide (Yam *et al.*, 1997; Gibson *et al.*, 1998). Here, we report the crystal structure of the title rhenium(I) complex, $[Re(CO)_3(C_{10}H_8N_2)(CH_3CN)]ClO_4$, (I), which resulted from the reaction between $[Re(bpy)(CO)_3Cl]$ and $AgClO_4$ in acetonitrile (Fredericks *et al.*, 1979).



(I)

A perspective view of the complex cation of (I) with the atomic numbering scheme is shown in Fig. 1 and selected bonding parameters are listed in Table 1.

The three carbonyl ligands at the Re atom are arranged in a facial configuration. The Re atom adopts a slightly distorted octahedral geometry, with the C41—Re—N3 angle being 178.18 (12)°. The N2—Re—N1 [74.63 (10)°] angle is far from 90°, due to the steric effects of the chelating bipyridyl ligand (Yam *et al.*, 1995, 1996). The average bond distances for Re—N [2.172 (3) Å] and Re—C [1.922 (3) Å] are similar to those previously determined in rhenium(I) tricarbonyl diimine structures (Chen *et al.*, 1989, 2003; Yam *et al.*, 1997; Hevia *et al.*, 2002).

Experimental

An equimolar mixture of $[Re(bpy)(CO)_3Cl]$ and $AgClO_4$ in acetonitrile was refluxed under anaerobic conditions for 16 h, after which the resulting solution was filtered to give a yellow solution. The filtrate was evaporated under vacuum to afford a yellow solid, which was redissolved in dichloromethane and layered with diethyl ether to form well shaped yellow crystals of (I) suitable for an X-ray diffraction study.

Crystal data

$[Re(C_2H_3N)(C_{10}H_8N_2)(CO)_3]ClO_4$
$M_r = 566.92$
Monoclinic, $C2/c$
$a = 33.745$ (5) Å
$b = 6.3132$ (11) Å
$c = 18.793$ (4) Å
$\beta = 119.572$ (10)°
$V = 3482.1$ (11) Å^3
$Z = 8$
$D_x = 2.163$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4993 reflections
$\theta = 3.3$–27.5°
$\mu = 7.18$ mm^{-1}
$T = 293$ (2) K
Prism, yellow
0.55 × 0.40 × 0.30 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan, (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.043$, $T_{max} = 0.113$
12 732 measured reflections
3966 independent reflections
3745 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 27.5°$
$h = -43 \rightarrow 29$
$k = -8 \rightarrow 8$
$l = -24 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.061$
$S = 1.09$
3966 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2 + 5.548P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 2.50$ e Å^{-3}
$\Delta\rho_{min} = -2.44$ e Å^{-3}
Extinction correction: none

Table 1
Selected geometric parameters (Å, °).

Re—N1	2.172 (3)	Re—C21	1.925 (4)
Re—N2	2.172 (3)	Re—C31	1.931 (3)
Re—N3	2.140 (3)	Re—C41	1.921 (3)
N1—Re—N2	74.63 (10)	N2—Re—C41	92.92 (12)
N1—Re—N3	84.08 (10)	N3—Re—C21	91.37 (13)
N1—Re—C21	97.00 (13)	N3—Re—C31	91.09 (12)
N1—Re—C31	172.62 (12)	N3—Re—C41	178.18 (12)
N1—Re—C41	97.01 (12)	C21—Re—C31	88.68 (15)
N2—Re—N3	85.96 (10)	C21—Re—C41	89.94 (14)
N2—Re—C21	171.42 (13)	C31—Re—C41	87.68 (13)
N2—Re—C31	99.51 (12)		

H atoms were positioned geometrically, with C—H distances of 0.96 or 0.93 Å, and allowed to ride on their respective parent C atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. The highest peak and deepest hole are 1.077 Å from Re.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994) and *SAINT*; data reduction: *XPREP* in *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

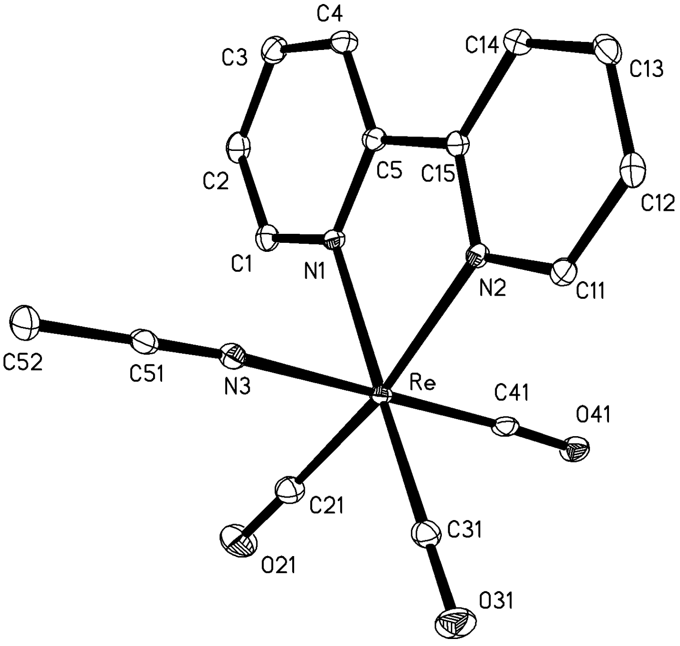


Figure 1
A view of the complex cation of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity..

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