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Dicarbonyldichlorido(*N*,*N*,*N*′,*N*′-tetramethylethylenediamine)ruthenium(II)

Ahmad O. Baghlaf,[a] Muhammad Ishaq,[a] Salih S. Al-Juaid,[a] Abdullah M. Asiri[b]‡ and Muhammad Nadeem Arshad[c]*

[a]Chemistry Department, Faculty of Science, King Abdul Aziz University, PO Box 80203, Jeddah 21589, Saudi Arabia, [b]The Center of Excellence for Advanced Materials Research, King Abdul Aziz University, Jeddah, PO Box 80203, Saudi Arabia, and [c]X-ray Diffraction and Crystallography Laboratory, Department of Physics, School of Physical Sciences, University of the Punjab, Quaid-e-Azam Campus, Lahore-54590, Pakistan
Correspondence e-mail: mnachemist@hotmail.com

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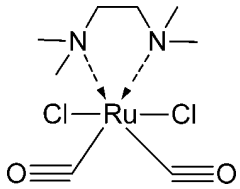
Key indicators: single-crystal X-ray study; T = 160 K; mean σ(C–C) = 0.004 Å; R factor = 0.023; wR factor = 0.061; data-to-parameter ratio = 15.6.

In the title compound, $[RuCl_2(C_6H_{16}N_2)(CO)_2]$, the geometry around the Ru^{II} atom is a distorted $RuC_2N_2Cl_2$ octahedron, with pairs of C and Cl atoms *trans* to each other and the N atoms of the bidentate ligand in a *cis* conformation. The five-membered chelate ring is puckered on the C—C bond.

Related literature

For background to ruthenium carbonyl derivatives, see: Manchot & Konig (1924); Stephenson & Wilkinson (1966); Kingston *et al.* (1967); Baghlaf *et al.* (2007); Campbell (1975); Padhey & Kaufman (1985). For a related structure, see: Bakar *et al.* (1993).



Experimental

Crystal data

$[RuCl_2(C_6H_{16}N_2)(CO)_2]$
M_r = 344.20
Monoclinic, $P2_1/c$
a = 7.463 (6) Å
b = 14.579 (6) Å
c = 12.718 (12) Å
β = 106.37 (8)°
V = 1327.7 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.57 mm^{-1}
T = 160 K
0.38 × 0.38 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.591, T_{max} = 0.69
3153 measured reflections
2877 independent reflections
2644 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
2 standard reflections every 100 reflections
intensity decay: 5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.061
S = 1.07
2877 reflections
184 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.06 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ru1—C1	1.872 (3)	Ru1—N1	2.220 (2)
Ru1—C2	1.872 (2)	Ru1—Cl1	2.413 (2)
Ru1—N2	2.211 (2)	Ru1—Cl2	2.408 (2)
N2—Ru1—N1	82.75 (9)		

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); 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: HB5901).

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‡ Chemistry Department, Faculty of Science, King Abdul Aziz University, PO Box 80203, Jeddah 21589, Saudi Arabia.