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Bis(8-hydroxyquinolinato)oxopropoxovanadium(V)

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.007 Å
H-atom completeness 85%
R factor = 0.053
wR factor = 0.176
Data-to-parameter ratio = 17.3

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

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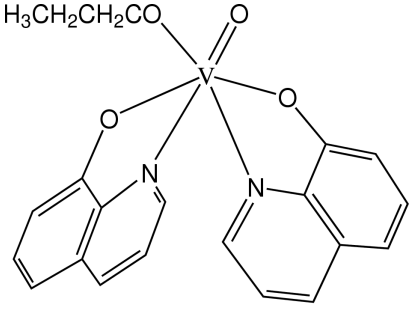
The title compound, $[VO(C_9H_6NO)_2(C_3H_7O)]$, contains a six-coordinate V^V atom. The central V^V atom has a distorted octahedral coordination geometry involving two O atoms of the oxo (V=O) and propoxo (V—O^{n}Pr) groups, two N and two O atoms of the two 8-hydroxyquinoline rings.

Comment

8-Hydroxyquinoline (8-quinolinol, oxine) is a well known analytical reagent for forming chelate complexes with metal ions. Its metal complexes with copper(II), zinc(II) and nickel(II) have remarkable antimicrobial or fungicidal activity (Okide *et al.*, 2000; Patel *et al.*, 1999). The bismuth(III) complex also has antitumor activity against leukemia (Smith *et al.*, 1998). On the other hand, vanadium(IV) and vanadium(V) salts have insulin-mimetic effects in living animals (Bhattacharyya & Tracey, 2001) or in intact cell systems (Kanamori *et al.*, 2001). Peroxovanadium(V) complexes also show antitumor activity (Djordjevic & Wampler, 1985). These findings drive the structural research on various 8-hydroxyquinoline derivatives, as well as vanadium compounds, because of their therapeutic value. For these reasons, we aimed to prepare compounds of 8-hydroxyquinoline and vanadium, and determine their structures.



(I)

Here, we report the structure of a vanadium(V) complex of 8-hydroxyquinoline, (I). The molecular structure of (I) is shown in Fig. 1. The crystal structures of similar vanadium(V) compounds have been reported, *e.g.* as the isopropyl ester, oxoisopropoxobis(8-hydroxyquinolinato)vanadium(V) with a VO(O^{i}Pr) group (Scheidt, 1973), and as the ethyl ester, oxoethoxobis(5,7-dichloro-8-hydroxquinolinato)vanadium(V) with a VO(OEt) group (González-Baró *et al.*, 1998). These species are considered to be inorganic esters (Baran, 2000). Both of the above esters were prepared by the esterification of oxohydroxobis(8-hydroxyqinolinato)vanadium(V)

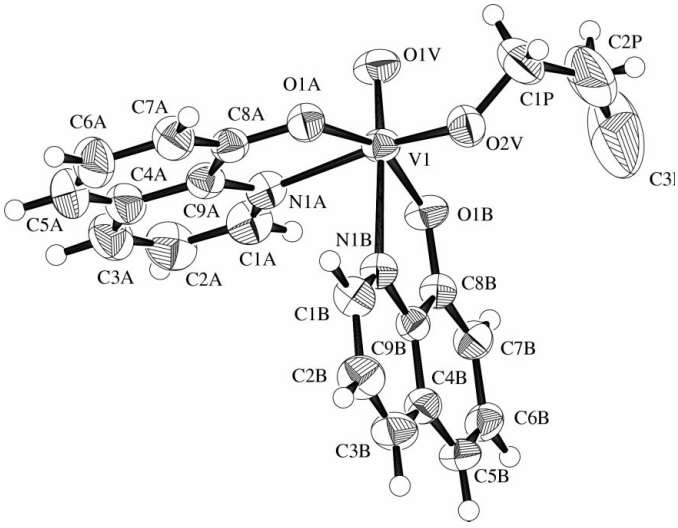


Figure 1
*ORTEP*II (Johnson, 1976) drawing of the title compound with the atomic numbering scheme. Displacement ellipsoids for non-H atoms correspond to 50% probability.

and oxohydroxobis(5,7-dichloro-8-hydroxyquinolinato)vanadium(V).

The O atoms of the oxo (V═O) and propoxo (V—O^{n}Pr) groups are in a *cis* configuration with respect to the VO(O^{n}Pr) group. Two N atoms of the 8-hydroxyquinoline molecules are located in mutually *cis* positions, but two O atoms at the 8-position are *trans*. The central V^V atom has a distorted octahedral coordination geometry. The overall atomic arrangement of the title compound is the same as in oxoisopropoxo(8-hydroxyquinolinato)vanadium(V) (Scheidt, 1973), although there are small differences in their geometrical parameters.

Experimental

A dark-brown plate-shaped crystal of (I) was obtained by slow evaporation from a propanol solution of a mixture of 8-hydroxyquinoline and $VOSO_4$ (8:1).

Crystal data

$C_{21}H_{19}N_2O_4V$
M_r = 414.33
Triclinic, $P\overline{1}$
a = 9.639 (3) Å
b = 12.751 (3) Å
c = 9.044 (3) Å
α = 95.76 (2)°
β = 110.97 (2)°
γ = 108.63 (2)°
V = 954.1 (5) Å^3
Z = 2
D_x = 1.442 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 14.7–15.0°
μ = 0.55 mm^{-1}
T = 296.2 K
Hexagonal plate, dark brown
0.20 × 0.20 × 0.07 mm

Data collection

Rigaku AFC-5*R* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.896, T_{max} = 0.962
4645 measured reflections
4391 independent reflections
2952 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 27.5°
$h = 0 \rightarrow 12$
$k = -16 \rightarrow 15$
$l = -11 \rightarrow 10$
3 standard reflections
every 150 reflections
intensity decay: 0.6%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.176
S = 1.14
4389 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = -0.002$
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

V1—O1*A*	1.924 (3)	V1—N1*B*	2.307 (3)
V1—O1*B*	1.888 (3)	O1*A*—C8*A*	1.328 (4)
V1—O1*V*	1.600 (3)	O1*B*—C8*B*	1.338 (5)
V1—O2*V*	1.775 (2)	O2*V*—C1*P*	1.420 (6)
V1—N1*A*	2.207 (3)		
O1*A*—V1—O1*B*	153.0 (1)	O1*V*—V1—N1*B*	169.6 (1)
O1*A*—V1—O1*V*	103.0 (1)	O2*V*—V1—N1*A*	164.8 (1)
O1*A*)—V1—O2*V*	93.7 (1)	O2*V*—V1—N1*B*	86.4 (1)
O1*A*)—V1—N1*A*	76.9 (1)	N1*A*—V1—N1*B*	80.52 (10)
O1*A*—V1—N1*B*	82.1 (1)	V1—O1*A*—C8*A*	120.8 (2)
O1*B*—V1—O1*V*	96.2 (1)	V1—O1*B*—C8*B*	123.0 (2)
O1*B*—V1—O2*V*	100.6 (1)	V1—O2*V*—C1*P*	129.7 (2)
O1*B*—V1—N1*A*	83.8 (1)	V1—N1*A*—C1*A*	130.5 (3)
O1*B*—V1—N1*B*	76.2 (1)	V1—N1*A*—C9*A*	111.2 (2)
O1*V*—V1—O2*V*	102.1 (1)	V1—N1*B*—C1*B*	132.9 (3)
O1*V*—V1—N1*A*	91.7 (1)	V1—N1*B*—C9*B*	108.5 (2)
V1—O1*A*—C8*A*—C7*A*	173.7 (3)	O1*V*—V1—O1*B*—C8*B*	−174.3 (2)
V1—O1*B*—C8*B*—C7*B*	−178.1 (2)	O1*V*—V1—O2*V*—C1*P*	−4.6 (4)
V1—O2*V*—C1*P*—C2*P*	−91.6 (5)	O2*V*—C1*P*—C2*P*—C3*P*	0 (1)
O1*A*—V1—O2*V*—C1*P*	−108.7 (4)	N1*A*—V1—O1*B*—C8*B*	−83.2 (2)
O1*A*—V1—N1*B*—C1*B*	−16.9 (3)	N1*B*—V1—O1*A*—C8*A*	−78.1 (2)
O1*B*—V1—O2*V*—C1*P*	94.2 (4)	N1*B*—V1—O2*V*—C1*P*	169.4 (4)
O1*V*—V1—O1*A*—C8*A*	92.7 (3)		

All H atoms, except those attached to C3*P*, were located in difference Fourier maps; they were then fixed at ideal positions and included in the refinement as riding atoms.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation and Rigaku Corporation, 1999); cell refinement: MSC/AFC Diffractometer Control Software; data reduction: *TEXSAN* (Molecular Structure Corporation and Rigaku Corporation, 1999); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997) and *DIRDIF*94 (Beurskens *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

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