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{2-[(2-Hydroxyphenyl)iminomethyl]phenolato}-(*N*-oxido-*N*-phenylbenzamide)oxovanadium(V)

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Key indicators

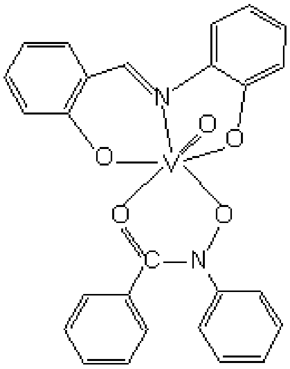
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.131
Data-to-parameter ratio = 16.5

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

The V^V atom in the title complex, $[V(C_{13}H_9NO_2)(C_{13}H_{10}NO_2)O]$, is coordinated by two O atoms and one N atom of the tridentate Schiff base ligand, and by two O atoms of the bidentate hydroxamate co-ligand, defining a distorted octahedral VO(ONO)(OO) geometry.

Comment

The presence of oxovanadium(V) at the active sites of some biological enzymes has resulted in increased interest in the study of the structural properties (Butler & Walker, 1993; Sangeetha & Pal, 2000). A tridentate Schiff base ligand is generally coordinated to a metal through the O and N atoms, giving coordination environments similar to those of the biological system; therefore, it is important to investigate vanadium(V) complexes with Schiff base ligands. To date, only three vanadium(IV/V) complexes containing the same H_2L^1 ligand as the title compound, (I), have been reported; in these, the V atoms have two structural forms, namely VO^{3+} (Caselato *et al.*, 1982; Clague *et al.*, 1993) and V^{4+} (Hefele *et al.*, 1995). In our previous work, we have reported the structures of oxovanadium(V) complexes containing hydrazone ligands (Gao *et al.*, 1998, 2004; Huo, Gao, Liu, Li & Ng, 2004; Huo, Gao, Liu, Zhao & Ng, 2004; Liu & Gao, 1998).



(I)

The molecular structure of (I) is illustrated in Fig. 1. The V atom is coordinated by five O atoms and one N atom, and forms a distorted octahedral O_5N configuration. The equatorial plane is defined by atoms O2, O3 and N1 of the fully deprotonated tridentate Schiff base ligand, and oxime atom O4 of the hydroxamate co-ligand has a deviation of 0.009 (4) Å from this plane. The axial oxo atom O1 is in a *trans* position relative to carbonyl atom O5 of the hydroxamate co-ligand. The V atom deviates by 0.28 (3) Å from the equatorial plane, towards the oxo atom. The V1—O1 bond distance is within the normal range in the structures of VO^{3+} complexes (Chen *et al.*, 1999). The bond distances in the equatorial plane follow the order: V1—O2 < V1—O4 < V1—O3 < V1—N1. The axial V1—O5 distance is longer than the equatorial V—O bond lengths, owing to the strong *trans* influence of the oxo group. The Schiff base ligand and the hydroxamate co-ligand combine with the V atom to give one six-membered and two five-membered chelate rings. The two five-membered chelate rings, involving atoms O3, C13, C8, N1 and V1, and O4, N2, C20, O5 and V1, are each basically planar, with mean deviations of 0.08 (3) and 0.06 (3) Å, respectively, whereas the six-membered chelate ring, involving atoms O2, C1, C6, C7, N1 and V1, is non-planar, with an r.m.s. deviation of 0.19 (2) Å. The dihedral angle between the two five-membered chelate rings is 72.9 (7)°, the dihedral angle between the benzene rings C1–C6 and C8–C13 is 34.2 (4)°, and that between the C14–C19 and C21–C26 rings is 58.2 (4)°.

Experimental

Solid vanadyl(IV) diacetate (1 mmol) was added to an ethanol solution (15 ml) of 2-(2′-hydroxyphenyl)iminomethylphenol (1 mmol) and the mixture was refluxed with stirring for 1.5 h. An ethanol solution containing *N*-hydroxy-*N*-phenylbenzamide (1 mmol) was added to the above solution with refluxing for 1.0 h and then filtered. The resulting dark-red solid was dissolved in dichloromethane and filtered. Dark-red crystals of (I) were obtained by slow diffusion of hexane into the filtrate over several days. Analysis calculated for $C_{26}H_{19}N_2O_5V$: C 63.68, H 3.91, N 5.71%; found: C 63.64, H 3.87, N 5.69%.

Crystal data

$[V(C_{13}H_9NO_2)(C_{13}H_{10}NO_2)O]$
$M_r = 490.37$
Triclinic, $P\overline{1}$
$a = 9.0795$ (18) Å
$b = 10.134$ (2) Å
$c = 12.624$ (3) Å
$\alpha = 104.84$ (3)°
$\beta = 91.11$ (3)°
$\gamma = 92.08$ (3)°
$V = 1121.6$ (4) Å^3

$Z = 2$
$D_x = 1.452$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9503 reflections
$\theta = 3.0$–27.5°
$\mu = 0.48$ mm^{-1}
$T = 296$ (2) K
Prism, dark red
0.38 × 0.26 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.837$, $T_{\max} = 0.918$
11 056 measured reflections

5076 independent reflections
4098 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.017$
$\theta_{\max} = 27.5$°
$h = -11 \rightarrow 11$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.131$
$S = 1.05$
5076 reflections
307 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0777P)^2 + 0.2634P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.79$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}

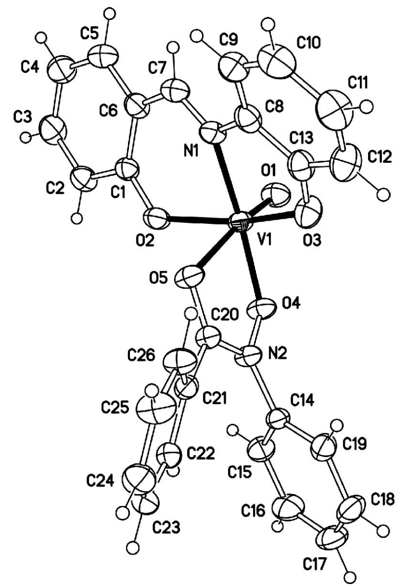


Figure 1
ORTEPII plot (Johnson, 1976) of the title complex, with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small circles of arbitrary radii.

Table 1
Selected geometric parameters (Å, °).

V1—N1	2.087 (2)	N1—C8	1.457 (3)
V1—O1	1.5901 (16)	N2—C20	1.338 (3)
V1—O2	1.8769 (16)	O2—C1	1.322 (2)
V1—O3	1.8958 (18)	O3—C13	1.347 (3)
V1—O4	1.8776 (15)	O4—N2	1.372 (2)
V1—O5	2.2016 (16)	O5—C20	1.250 (2)
V1—C7	1.257 (3)	N2—C14	1.430 (2)
N1—V1—O5	88.02 (7)	O2—V1—O4	101.03 (7)
O1—V1—N1	100.62 (8)	O2—V1—O5	81.98 (7)
O1—V1—O2	97.36 (9)	O3—V1—N1	77.75 (8)
O1—V1—O3	101.64 (9)	O3—V1—O5	81.61 (8)
O1—V1—O4	95.85 (8)	O4—V1—N1	162.36 (7)
O1—V1—O5	171.21 (7)	O4—V1—O3	92.85 (8)
O2—V1—N1	83.17 (8)	O4—V1—O5	75.75 (6)
O2—V1—O3	155.16 (8)		

All H atoms were placed in calculated positions and were allowed to ride on their parent C atoms, with C—H = 0.93 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$.

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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