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Bis[2-(4,5-dihydro-1*H*-imidazol-2-yl)phenolato-κ^2N^3,O]zinc(II) methanol solvate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.041
wR factor = 0.107
Data-to-parameter ratio = 14.8

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

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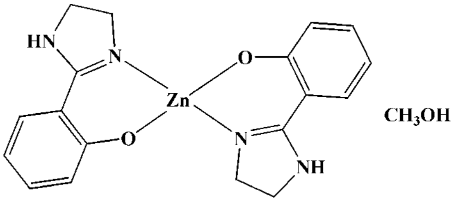
The title complex, $[Zn(C_{18}H_{18}N_4O_2)]\cdot CH_3OH$, comprises a Zn^{II} ion tetrahedrally coordinated by two bidentate 2-(4,5-dihydro-1*H*-imidazol-2-yl)phenolate ligands with average distances of Zn—N = 1.942 (3) Å and Zn—O = 1.942 (2) Å.

Comment

2-(1*H*-Imidazol-2-yl)phenol and 2-(4,5-dihydro-1*H*-imidazol-2-yl)phenol are two ligands that exhibit strong inhibition against several metalloproteinases with Zn catalytic centres (He & Rodgers, 2007). Their inhibitory action is thought to arise from their bonding to the catalytic Zn. It is important to understand how these ligands interact with Zn^{2+}. Previously, we reported the crystal structure of a zinc complex of 2-(1*H*-imidazol-2-yl)phenol (He, 2006) and the results revealed that two ligands coordinated to the Zn^{2+} ion in a tetrahedral geometry. During a modelling study of 2-(4,5-dihydro-1*H*-imidazol-2-yl)phenol with the model compound hydrotris(3,5-methylphenylpyrazol-1-yl)borate zinc hydroxide, [TP^{Me,Ph}Zn-OH], we obtained crystals of a different colour from those of the adduct of this ligand with the model complex. The course of the chemical reaction allowed two possibilities, either the product of a ligand substitution reaction between the tripodal ligand and 2-(4,5-dihydro-1*H*-imidazol-2-yl)phenol, or the interaction of an excess of 2-(4,5-dihydro-1*H*-imidazol-2-yl)phenol with Zn^{2+} from the decomposition of [TP^{Me,Ph}Zn-OH]. The latter reaction may have occurred as a result of the solution being allowed to stand for a long time at room temperature to give the title compound, (I).



(I)

Compound (I) is stable in air and crystallizes as a methanol solvate (Fig. 1, Table 1), with the two bidentate anionic 2-(4,5-dihydro-1*H*-imidazol-2-yl)phenolate ligands coordinating through the phenolate O and imidazolyl N atoms to the Zn^{II} ion to give a tetrahedral complex. The dihedral angles between the C1/C2/N1/N2/C3 imidazolyl and C4–C9 benzene rings, and between the C10/C11/N4/C12/N3 imidazolyl and the C13–C18 benzene rings, are 13.5 (3) and 5.67 (19)°, respectively.

The crystal packing of (I) is characterized by N—H···O and O—H···O hydrogen bonds (Table 2). Parallel benzene and imidazolyl rings are involved in stacking interactions (Fig. 2).

Experimental

2-(4,5-Dihydro-1*H*-imidazol-2-yl)phenol (48 mg, 0.29 mmol), prepared according to the literature method of Bishop *et al.* (2002), and [hydrotris(3,5-methylphenylpyrazol-1-yl)borate]zinc hydroxide (132.9 mg, 0.25 mmol) were dissolved separately in methanol (5 ml). The solutions were mixed and then stirred overnight. The clear solution was kept at room temperature. Crystals of (I) were obtained one year later.

Crystal data

$[Zn(C_9H_9N_2O)_2]\cdot CH_4O$
$M_r = 419.78$
Monoclinic, $P2_1/c$
$a = 7.8657\ (16)$ Å
$b = 26.140\ (5)$ Å
$c = 9.4918\ (19)$ Å
$\beta = 93.01\ (3)^\circ$
$V = 1948.9\ (7)$ Å^3
$Z = 4$
$D_x = 1.431$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.29$ mm^{-1}
$T = 293\ (2)$ K
Prism, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{min} = 0.738$, $T_{max} = 0.768$
14014 measured reflections
3810 independent reflections
2480 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 26.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.107$
$S = 1.02$
3810 reflections
257 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.7945P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N3	1.935 (3)	Zn1—O1	1.944 (2)
Zn1—O2	1.941 (2)	Zn1—N1	1.950 (3)
N3—Zn1—O2	95.63 (10)	N3—Zn1—N1	126.35 (12)
N3—Zn1—O1	117.85 (10)	O2—Zn1—N1	110.77 (10)
O2—Zn1—O1	112.97 (11)	O1—Zn1—N1	94.11 (10)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H20···O2^{i}	0.85 (3)	2.03 (4)	2.825 (4)	157 (3)
O3—H23···O1^{ii}	0.85 (5)	1.86 (5)	2.712 (4)	171 (5)
N4—H21···O3	0.76 (3)	2.18 (3)	2.915 (4)	163 (3)

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x+1, -y+1, -z+1$.

The H atoms on N2, N4 and O3 were refined freely, while the other H atoms were geometrically constrained and refined in riding mode as follows: methyl C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$; aromatic C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

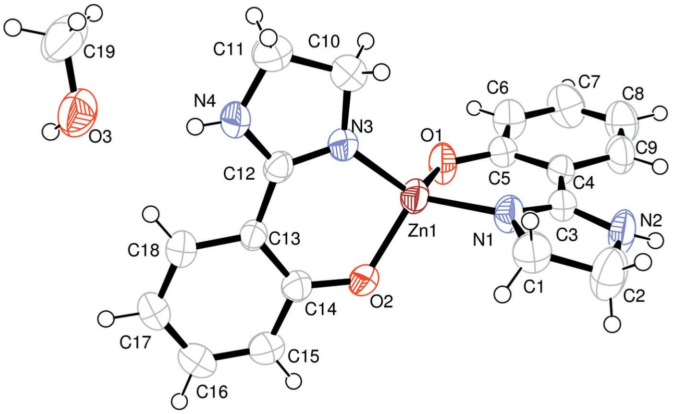


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small circles of arbitrary radii.

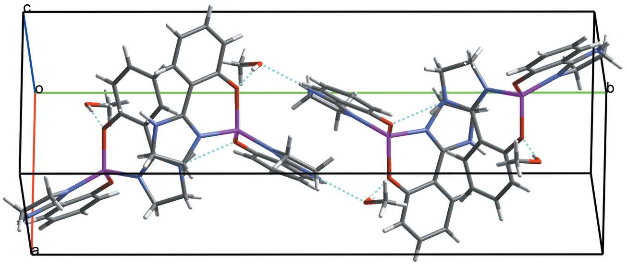


Figure 2
The molecular packing of (I), showing the chains formed by hydrogen bonds (dashed lines).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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