Bis(1,10-phenanthroline-$\kappa^2 N,N'$)(sulfato-$\kappa^2 O,O'$)-zinc(II) 1,2-ethenediol solvate

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In the title compound, [Zn(SO$_4$)(C$_{12}$H$_8$N$_2$)$_2$]·C$_2$H$_6$O$_2$, the Zn atom shows an octahedral geometry, composed of four N atoms from two phenanthroline groups and two O atoms from a bidentate sulfate ligand. It lies on a special position of site symmetry 2. The solvate features a pair of O—H···O hydrogen bonds.

Comment

The crystal structures of zinc–phenanthroline complexes with monodentate (Harvey *et al.*, 2000; 2003) and bidentate bridging (Harvey *et al.*, 2000) sulfate have been reported. The title zinc complex, (I), is isostructural with the recently reported cobalt(II) and cadmium(II) (Zhong *et al.*, 2006; Lu *et al.*, 2006) analogues.
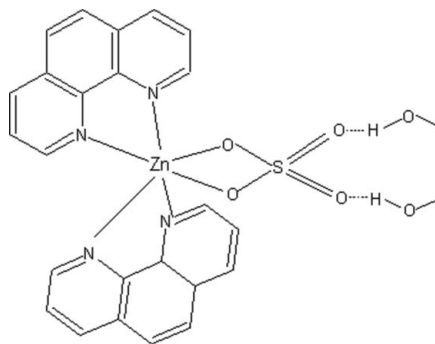
(I)

A twofold rotation axis passes through the Zn and S atoms, and also through the mid-point of the C—C bond of the solvent molcule. The Zn^{II} centre exists in an octahedral geometry, composed of four N atoms from two phenanthroline groups and two O atoms from a bidentate sulfate ligand (Fig. 1).

The ethane-1,2-diol solvent molecule is disordered over two positions. It is hydrogen bonded to the sulfate ligand (Table 2).

Experimental

Yellow block-shaped crystals of the title compound were obtained by a procedure similar to that described previously by Zhong *et al.* (2006), but with ZnSO$_4$·7H$_2$O in place of CoSO$_4$·7H$_2$O.

Crystal data

[Zn(SO$_4$)(C$_{12}$H$_8$N$_2$)$_2$]·C$_2$H$_6$O$_2$	$Z = 4$
$M_r = 583.91$	$D_x = 1.572$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 18.519$ (4) Å	$\mu = 1.13$ mm^{-1}
$b = 11.879$ (3) Å	$T = 293$ (2) K
$c = 12.840$ (3) Å	Block, yellow
$\beta = 119.121$ (4)°	$0.35 \times 0.30 \times 0.21$ mm
$V = 2467.6$ (9) Å^3	

Data collection

Bruker SMART CCD 1K area-detector diffractometer	8471 measured reflections
φ and ω scans	3069 independent reflections
Absorption correction: multi-scan	2505 reflections with $I > 2\sigma(I)$
($SADABS$; Sheldrick, 1996)	$R_{int} = 0.028$
$T_{min} = 0.693$, $T_{max} = 0.797$	$\theta_{max} = 28.3°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0569P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$+ 2.3359P]$
$wR(F^2) = 0.109$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
3069 reflections	$\Delta\rho_{max} = 0.56$ e Å^{-3}
182 parameters	$\Delta\rho_{min} = -0.49$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.142 (2)	S1—O1	1.4814 (19)
Zn1—N2	2.153 (2)	C13—O3	1.317 (5)
Zn1—O1	2.171 (2)	C13—C13^i	1.508 (4)
S1—O2	1.449 (2)		
N1—Zn1—N2	77.92 (8)	O1^i—S1—O1	103.55 (16)
O1—Zn1—O1^i	64.83 (10)	O3—C13—C13^i	127.4 (4)
O2^i—S1—O2	110.05 (19)		

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

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O3—H3⋯O2^i	0.82	2.04	2.688 (6)	136
O3′—H3′⋯O2^i	0.82	2.38	2.715 (6)	105

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

The H atoms of CH and CH$_2$ groups were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 and 0.97 Å, respectively, and with U_{iso}(H) = 1.2U_{eq}(C). The O atom of the ethane-1,2-diol solvent is disordered over two positions; the site-occupancy factors were 0.60 and 0.40, sharing a common atom C13. The disordered atoms were refined isotropically. The H atoms of the OH group were also positioned geometrically and then allowed to ride on their parent atoms, with O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine
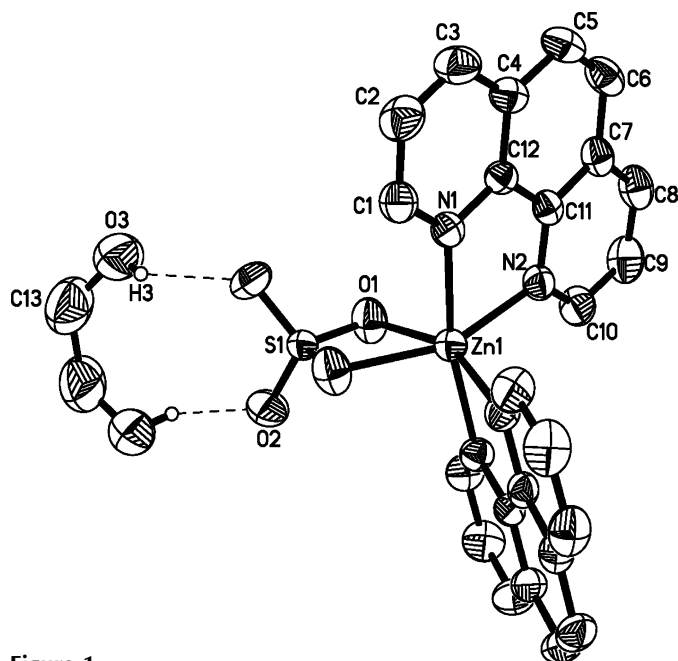

Figure 1
The molecular structure of (I), showing the atom-numbering scheme and with displacement ellipsoids drawn at the 50% probability level. The dashed lines represent O—H⋯O interactions. Other H atoms not involved in these interactions have been omitted. Unlabelled atoms are related to labelled atoms by the symmetry operator $(1 - x, y, \frac{3}{2} - z)$. Only one disorder component is shown.

structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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