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Bis[4-fluoro-*N*-(quinolin-8-yl)benzenesulfonamidato-κ^2N,N']zinc(II) hemihydrate

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.007 Å
H-atom completeness 96%
R factor = 0.056
wR factor = 0.143
Data-to-parameter ratio = 14.4

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

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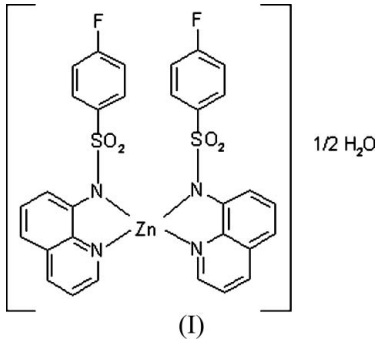
In the title compound, $[Zn(C_{15}H_{10}FN_2O_2S)_2]\cdot 0.5H_2O$, the Zn atom has a distorted tetrahedral geometry, formed by the N atoms of the quinoline and the sulfonamide groups. The water molecule occupies a special position on a twofold axis. Intermolecular C—H···O hydrogen bonds to the sulfonyl O atoms link the molecules into a three-dimensional network.

Comment

Metal-chelator therapy is a potential target for Alzheimer neuropathology (Opazo *et al.*, 2006). There is evidence that metals such as zinc and copper contribute to the aggregation of β-amyloid (Aβ) protein and the deposition of amyloid plaques in Alzheimer's disease, and the interactions between Aβ and these metals may benefit patients with Alzheimer's. In addition, the search for metal-specific fluorescence compounds is of importance in understanding the neurobiological role of these metals in the brain and it is currently a research field in development (Miller *et al.*, 2005; Cardoso *et al.*, 2005). As part of our efforts in the search for metal chelators as potential probes for neuroprotection in neurogenerative diseases (da Silva *et al.*, 2006*a*,*b*,*c*,*d*,*e*), the structure of the title compound, (I), has been determined.



(I)

Compound (I) features highly distorted tetrahedral coordination. Zn–ligand bonding takes place through the N atoms of the sulfonamide and quinoline groups. Bond distances are slightly longer to the quinoline N atoms than to the sulfonamide N atoms (Table 1). The bond angles N1—Zn1—N2 and N3—Zn1—N4 are quite small compared with the 109.5° angle of an ideal tetrahedral centre. The Zn1—O2 and Zn1—O3 distances are essentially non-bonding [3.039 (3) and 3.006 (3) Å, respectively].

The water molecule, lying on a twofold rotation axis, for which the H atoms were not found, is not coordinated to the metal atom in complex (I) and is not shown in Fig. 1. Two intermolecular C—H···O hydrogen bonds to the sulfonyl

atoms O2 and O3 link the molecules into a three-dimensional network (Fig. 2, Table 2).

Experimental

The ligand was prepared as described previously (da Silva *et al.*, 2005). The title compound was prepared according to a literature procedure (Macías *et al.*, 2003). Single crystals of (I) suitable for X-ray data collection appeared after two days from a methanol solution.

Crystal data

$[Zn(C_{15}H_{10}FN_2O_2S)_2]\cdot 0.5H_2O$
M_r = 677.00
Monoclinic, $C2/c$
a = 23.401 (1) Å
b = 16.843 (1) Å
c = 17.186 (1) Å
β = 123.710 (1)°
V = 5634.8 (5) Å^3
Z = 8
D_x = 1.596 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.08 mm^{-1}
T = 299 (2) K
Prism, light green
0.20 × 0.12 × 0.12 mm

Data collection

Oxford Xcalibur Sapphire CCD area-detector diffractometer
ω and φ scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2004)
T_{min} = 0.778, T_{max} = 0.900
20017 measured reflections
5667 independent reflections
3364 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.143
S = 1.07
5667 reflections
393 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N3	1.949 (3)	Zn1—N2	2.018 (3)
Zn1—N1	1.963 (3)	Zn1—N4	2.049 (3)
N3—Zn1—N1	133.55 (14)	N3—Zn1—N4	82.66 (12)
N3—Zn1—N2	130.46 (13)	N1—Zn1—N4	119.49 (13)
N1—Zn1—N2	83.12 (13)	N2—Zn1—N4	109.46 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1^{i}	0.93	2.33	3.256 (5)	171
C21—H21···O2^{ii}	0.93	2.52	3.373 (5)	153

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

All H atoms were included in the riding-model approximation, with C—H = 0.93 Å, and with U_{iso}(H) = 1.2U_{eq}(C). Due to the high displacement parameters of the the water O atom, its H atoms could not be located.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2004); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

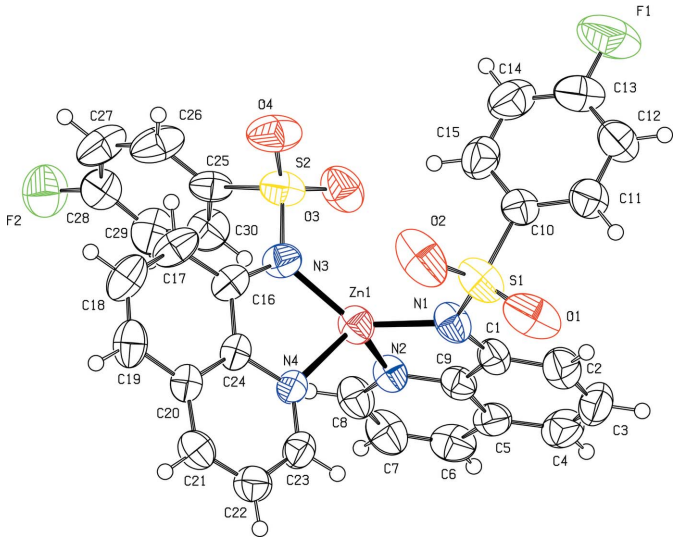


Figure 1
The molecular structure of (I), showing the atom-labelling scheme, and with displacement ellipsoids drawn at the 50% probability level.

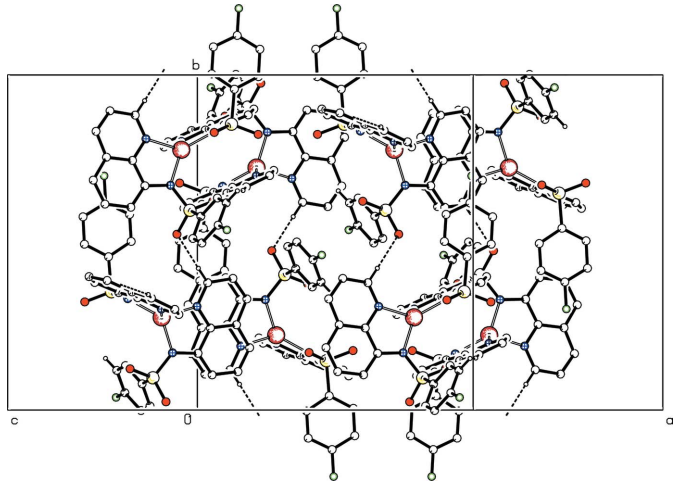


Figure 2
The molecular packing of (I), with hydrogen bonds shown as dashed lines. H atoms not involving in hydrogen bonding have been omitted.

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