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Aquabis[4-nitro-*N*-(quinolin-8-yl)benzenesulfonamidato-κ^2N,N']zinc(II)

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.005 Å
R factor = 0.039
wR factor = 0.116
Data-to-parameter ratio = 12.7

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

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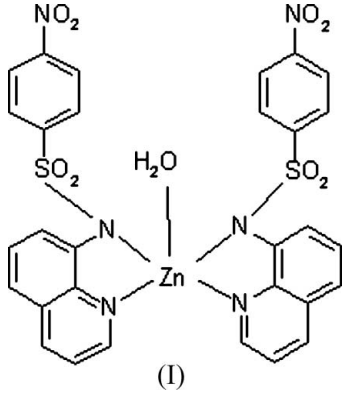
In the title compound, $[Zn(C_{15}H_{10}N_3O_4S)_2(H_2O)]$, the asymmetric unit contains one half-molecule. The coordination of the Zn^{II} ion, which occupies a special position on a twofold axis, is distorted trigonal bipyramidal.

Comment

There is increasing evidence that interactions between the amyloid beta peptide and metal ions such as copper and zinc may assist in the transformation of this healthy soluble peptide to a neurotoxic fibrillary form responsible for Alzheimer's disease (Miller *et al.*, 2005; Cardoso *et al.*, 2005, Ii, 1995). As part of our efforts to search for metal chelators as potential probes for neuroprotection in neurogenerative diseases (da Silva *et al.*, 2006*a*,*b*,*c*,*d*) the structure of the title compound, (I) (Fig. 1), has been determined.



(I)

The asymmetric unit of (I) contains one half-molecule. The other half of the complex is related by a C_2 axis running through the Zn^{II} ion and the water O atom. The Zn^{II} ion has a distorted trigonal–bipyramidal geometry formed by two quinoline N and two sulfonamide N atoms and the O atom of the water molecule (Table 1). The angle between the least-squares planes of the quinoline unit and the benzene ring is 89.27 (8)°. The water H atoms are shared between the water O atom and sulfonyl O atoms, linking the molecules in chains along the *c* axis (Fig. 2 and Table 2).

Experimental

The organic ligand was synthesized as reported previously (da Silva *et al.*, 2005) and the title compound was prepared according to the method of Macías *et al.* (2003). Single crystals of (I) suitable for X-ray data collection were obtained after two days from a methanol solution.

Crystal data

$[Zn(C_{15}H_{10}N_3O_4S)_2(H_2O)]$
M_r = 740.03
Monoclinic, $C2/c$
a = 31.407 (6) Å
b = 10.120 (1) Å
c = 10.342 (1) Å
β = 106.94 (2)°
V = 3144.5 (8) Å^3
Z = 4
D_x = 1.563 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 2.89 mm^{-1}
T = 299 (2) K
Needle, yellow
0.50 × 0.10 × 0.05 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.326, T_{max} = 0.869
3477 measured reflections
2798 independent reflections
2319 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 66.9°
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.116
S = 1.05
2798 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0708P)^2 + 2.3429P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.74 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—Zn1	2.187 (2)	Zn1—O1*W*	2.011 (3)
N2—Zn1	2.091 (2)		
O1*W*—Zn1—N2	124.48 (6)	N2^i—Zn1—N1	99.52 (8)
N2^i—Zn1—N2	111.04 (12)	N2—Zn1—N1	76.51 (8)
O1*W*—Zn1—N1	93.44 (6)	N1—Zn1—N1^i	173.12 (12)

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*
O1*W*—H1*W*···O1^{ii}	0.87 (2)	2.44 (3)	2.935 (2)	117 (3)

Symmetry code: (ii) $-x+1, -y, -z+2$.

The symmetry-independent water H atom was located in a difference Fourier map and was refined with restrained geometry, *viz*. O—H restrained to 0.85 (2) Å and H···H restrained to 1.365 (2) Å, thus leading to an H—O—H angle of 109 (3)°. All other H atoms were placed in calculated positions and treated as riding, with C—H = 0.93 Å. All H atoms were refined with U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *CAD-4-PC* Software (Nonius, 1996); cell refinement: *CAD-4-PC* Software; data reduction: *REDU4* (Stoe & Cie, 1987); 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*.

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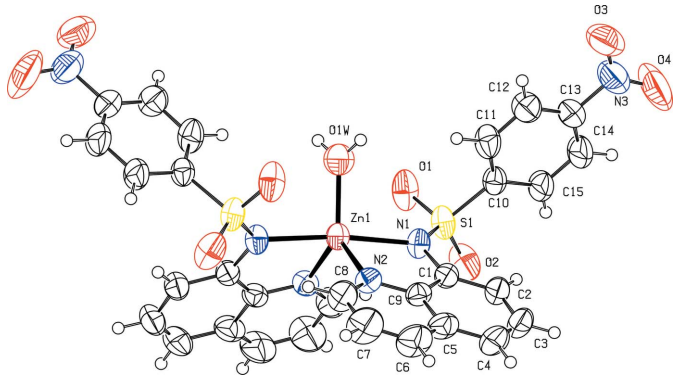

Figure 1
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operation $(-x+1, y, -z+\frac{3}{2})$.

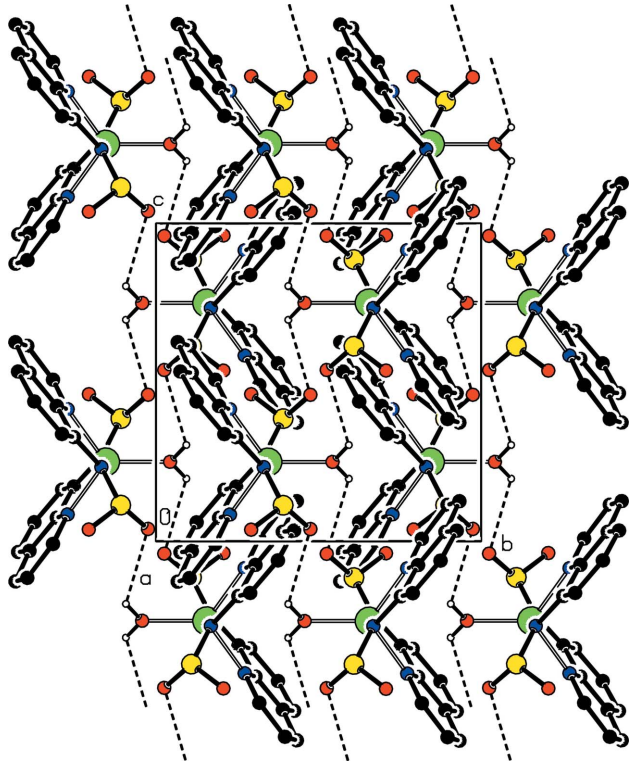

Figure 2
The molecular packing of the title compound, viewed along the *a*-axis direction, with hydrogen bonds shown as dashed lines. H atoms not involving in hydrogen bonding have been omitted.

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