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Bis[4-*n*-propyl-*N*-(8-quinolyl)benzenesulfonamidato-κ^2N,N']zinc(II) dimethylformamide solvate

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.040
wR factor = 0.116
Data-to-parameter ratio = 13.6

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

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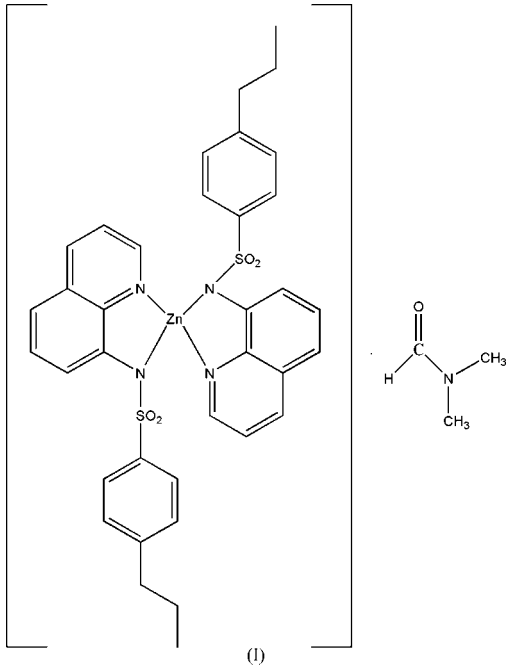
In the title compound, $[Zn(C_{18}H_{17}N_2O_2S)_2]\cdot C_3H_7NO$, the Zn atom is four-coordinated by the N atoms of sulfonamide and quinoline groups. Two intermolecular C—H···O hydrogen bonds connect the molecules into a three-dimensional network.

Comment

The zinc(II) ion is the second most abundant transition metal essential for the human body. Recent work showed that Zn^{II} is closely associated with severe pathological diseases, such as Alzheimer's disease and familial amyotrophic lateral sclerosis (Frederickson *et al.*, 2005). Moreover, it is believed that the fluorescence method is likely to be the most effective way to detect zinc, and so far many types of probes have been reported (Fahrni & O'Halloran, 1999). Thus, several quinoline-based compounds have been employed to detect zinc in living systems (Hendrickson *et al.*, 2003). Our interest in such metal chelators as potential probes for neuroprotection in Alzheimer's disease (Zheng *et al.*, 2005) led to the X-ray crystallographic study of the title compound, (I).



(I)

The Zn atom is four-coordinated by the N atoms of sulfonamide and quinoline groups, forming a distorted tetrahedral geometry. Table 1 shows selected bond distances and angles around the central Zn atom. The Zn—N(quinoline) bonds are slightly longer than the Zn—N(sulfonamide) bonds, which are in the usual range. Quinolinesulfomidate coordinates through

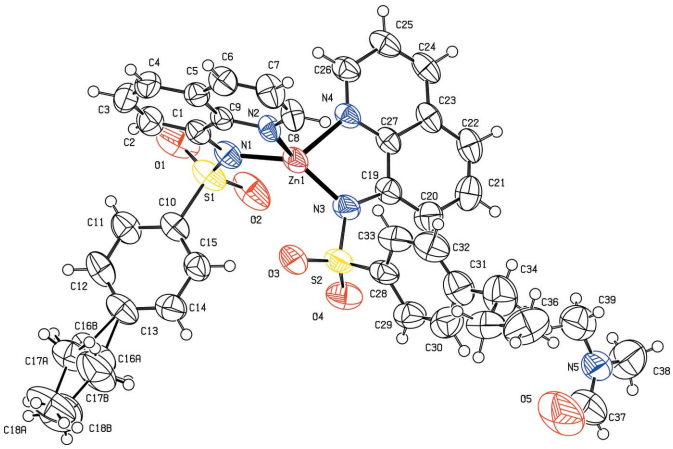


Figure 1
The asymmetric unit of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level. Both disorder components are shown.

the sulfonamide and quinoline N atoms, forming a five-membered ring with the Zn cation. The molecular structure of the title compound, (I), with the disorder and displacement ellipsoids, is shown Fig. 1. In the crystal structure, the molecules are linked through intermolecular C—H···O hydrogen bonds, as shown in the packing diagram (Fig. 2) and detailed in Table 2.

Experimental

Compound (I) was prepared according to a literature procedure (Macías *et al.*, 2003). Single crystals of (I) suitable for X-ray data collection appeared after a few days from a methanol–dimethylformamide (1:1) solution.

Crystal data

$[Zn(C_{18}H_{17}N_2O_2S)_2]\cdot C_3H_7NO$
M_r = 789.26
Monoclinic, $P2_1/n$
a = 15.385 (2) Å
b = 16.928 (2) Å
c = 16.170 (2) Å
β = 115.30 (1)°
V = 3807.3 (8) Å^3
Z = 4
D_x = 1.377 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 2.33 mm^{-1}
T = 299 (2) K
Prism, green
0.65 × 0.35 × 0.30 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.474, T_{max} = 0.592
(expected range = 0.399–0.498)
9944 measured reflections
6784 independent reflections
5817 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 67.0°
3 standard reflections
frequency: 120 min
intensity decay: 0.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.116
S = 1.05
6784 reflections
498 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2 + 1.3631P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.00120 (9)

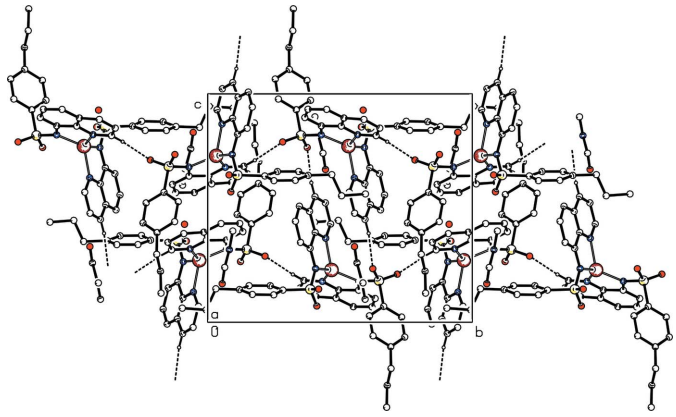


Figure 2
The molecular packing of (I), with hydrogen bonds shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

Table 1
Selected geometric parameters (Å, °).

Zn1—N3	1.953 (2)	Zn1—N2	2.0377 (19)
Zn1—N1	1.970 (2)	Zn1—N4	2.0663 (18)
N3—Zn1—N1	136.44 (9)	N3—Zn1—N4	81.79 (8)
N3—Zn1—N2	128.30 (9)	N1—Zn1—N4	121.48 (8)
N1—Zn1—N2	82.40 (8)	N2—Zn1—N4	107.79 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1^{i}	0.93	2.24	3.151 (3)	167
C24—H24···O2^{ii}	0.93	2.37	3.286 (3)	168

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

H atoms were positioned with idealized geometry and refined using a riding model with C—H = 0.93 (aromatic), 0.96 (methyl) and 0.97 Å (methylene); U_{iso}(H) values were set at 1.2 times U_{eq} of the parent atom (1.5 times for methyl groups). One propyl group (C16–C18) is disordered and these atoms were refined with a split model. The corresponding site-occupation factors were refined so that their sum was unity [0.705 (17) and 0.295 (17)].

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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