Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis[2,4,6-triisopropyl-*N*-(quinolin-8-yl)benzenesulfonamidato-κ^2N,N']zinc(II)

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.102
Data-to-parameter ratio = 16.0

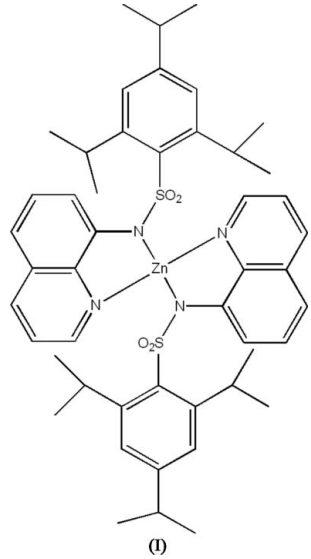
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 8 February 2006
Accepted 9 February 2006

In the title compound, $[Zn(C_{24}H_{29}N_2O_2S)_2]$, the Zn atom is four-coordinated by the N atoms of the sulfonamide and quinoline groups. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonds.

Comment

Metal-specific fluorescence probes are of increasing importance in understanding the neurobiology and general cell biology of zinc (Fahrni & O'Halloran, 1999). Several quinoline-based compounds, such as TSQ [6-methoxy-8-(4-tolylsulfonamido)quinoline] and zinquin, have been employed to detect zinc in living systems (Nasir *et al.*, 1999; Hendrickson *et al.*, 2003). As part of our study of the chemistry of quinoline-based fluorescence probes for the biological chemistry of zinc (da Silva *et al.*, 2005*a*,*b*,*c*,*d*), the structure of the title compound, (I), has been determined. As reported by Macías *et al.* (2003), the Zn atom is coordinated by four N atoms in a highly distorted tetrahedral geometry. The Zn—N(quinoline) bond lengths [2.074 (2) and 2.049 (2) Å] are slightly larger than the Zn—N(sulfonamide) bonds [1.972 (2) and 1.974 (2) Å], which are in the usual range. Table 1 shows selected bond distances and angles around the central Zn atom.



(I)

Quinolinesulfonamidate ligates through the sulfonamide and quinoline N atoms, forming a five-membered ring with the Zn cation. Intermolecular C—H···O hydrogen bonds connect the molecules into a three-dimensional network, as shown in the packing diagram (Fig. 2). Details of these hydrogen bonds are given in Table 2.

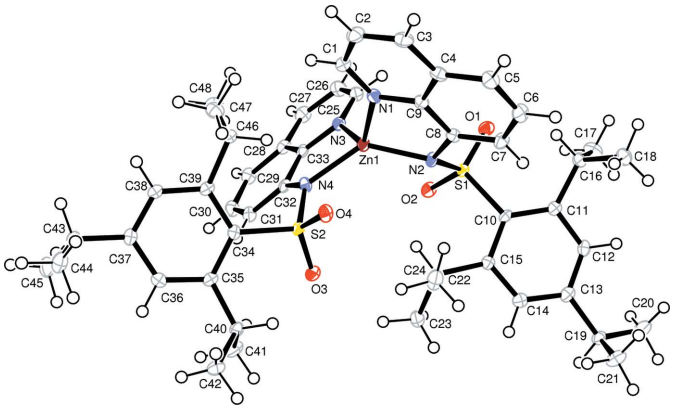


Figure 1
The molecular structure of (I), showing the atom labelling and with displacement ellipsoids drawn at the 50% probability level.

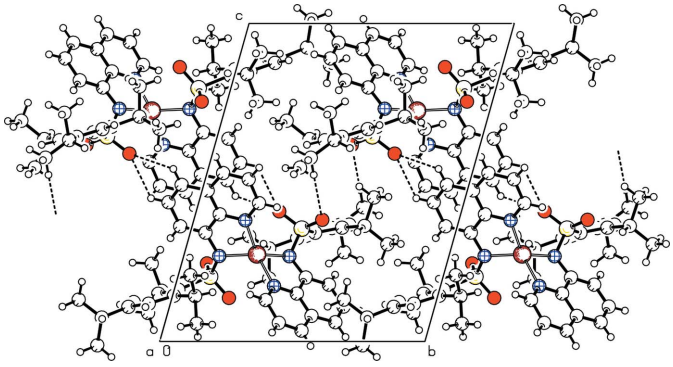


Figure 2
The molecular packing of (I), with hydrogen bonds shown as dashed lines.

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–dichloromethane (1:1) solution (m.p. 562 K).

Crystal data

$[Zn(C_{24}H_{29}N_2O_2S)_2]$
M_r = 884.47
Triclinic, $P\overline{1}$
a = 9.9732 (6) Å
b = 14.3281 (8) Å
c = 17.0425 (8) Å
α = 71.723 (5)°
β = 79.277 (4)°
γ = 69.875 (5)°
V = 2162.9 (2) Å^3
Z = 2
D_x = 1.358 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7555 reflections
θ = 2.2–27.6°
μ = 0.71 mm^{-1}
T = 100 (2) K
Prism, bright yellow
0.36 × 0.34 × 0.22 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
ω and φ scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2004)
T_{min} = 0.803, T_{max} = 0.900
15135 measured reflections
8527 independent reflections
7417 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 26.4°
$h = -11 \rightarrow 12$
$k = -13 \rightarrow 17$
$l = -20 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.102
S = 1.08
8527 reflections
532 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 1.6914P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—Zn1	2.0738 (18)	N3—Zn1	2.0487 (18)
N2—Zn1	1.9718 (17)	N4—Zn1	1.9742 (17)
N2—Zn1—N4	131.86 (7)	N2—Zn1—N1	82.95 (7)
N2—Zn1—N3	122.20 (7)	N4—Zn1—N1	119.23 (7)
N4—Zn1—N3	82.37 (7)	N3—Zn1—N1	123.93 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
C20—H20B···O1^{i}	0.98	2.55	3.533 (3)	179
C29—H29···O2^{ii}	0.95	2.55	3.158 (3)	123
C30—H30···O2^{ii}	0.95	2.54	3.165 (3)	123

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y, -z+1$.

H atoms were positioned with idealized geometry, with C—H = 0.95 (aromatic), 0.98 (methyl) or 1.00 Å (methine), and were refined as riding, with isotropic displacement parameters set at 1.2 times U_{eq} of the parent atom.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); 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*.

The autors thank Professor Dr Hartmut Fuess, Technische Universität Darmstadt, for diffractometer time.

References

Fahrni, C. J. & O'Halloran, T. V. (1999). *J. Am. Chem. Soc.* **121**, 11448–11458.
Hendrickson, K. M., Geue, J. P., Wyness, O., Lincoln, S. F. & Ward, A. D. (2003). *J. Am. Chem. Soc.* **123**, 3889–3895.
Macías, B., García, I., Villa, M. V., Borrás, J., Castiñeiras, A. & Sanz, F. (2003). *Z. Anorg. Allg. Chem.* **629**, 255–260.
Nasir, M. S., Fahrni, C. J., Suhy, D. A., Kolodsick, K. J., Singer, C. P. & O'Halloran, T. V. (1999). *J. Biol. Inorg. Chem.* **4**, 775–783.
Oxford Diffraction (2004). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd., Köln, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Silva, L. E. da, Joussef, A. C., Foro, S. & Schmidt, B. (2005*a*). *Acta Cryst.* E**61**, o3435–3436.
Silva, L. E. da, Joussef, A. C., Foro, S. & Schmidt, B. (2005*b*). *Acta Cryst.* E**61**, o3778–3779.
Silva, L. E. da, Joussef, A. C., Foro, S. & Schmidt, B. (2005*c*). *Acta Cryst.* E**61**, o3780–3781.
Silva, L. E. da, Joussef, A. C., Foro, S. & Schmidt, B. (2005*d*). *Acta Cryst.* E**61**, o3782–3783.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.