Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dianilinediiodozinc(II)

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Received 3 March 2004
Accepted 14 May 2004
Online 29 May 2004

Key indicators

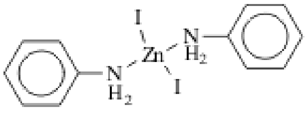
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.041
wR factor = 0.110
Data-to-parameter ratio = 31.6

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

In the title compound, [$ZnI_2(C_{12}H_{14}N)_2$], the Zn atom is located on a twofold axis and is coordinated in a distorted tetrahedral fashion by two I atoms and, *via* the N atoms, two aniline molecules. Molecules pack in a layer with the aromatic groups facing each other. A hydrogen-bonding network comprising N—H···I bonds extends parallel to the *bc* plane.

Comment

During the course of investigations focusing on the crystal engineering of organic–inorganic hybrid materials the title compound, (I), was crystallized. Its geometric parameters are compared here with those of previously reported analogues.



(I)

In (I), the asymmetric unit contains half a molecule, with the Zn atom located on a twofold rotation axis. The Zn atom is coordinated by two I atoms and by two N atoms of the aniline molecules in a distorted tetrahedral arrangement, as shown in Fig. 1.

The Zn—I bond length of 2.5850 (19) Å is marginally longer than the bond lengths observed for similar tetrahedral zinc complexes, with values of 2.530 (1) Å reported for bis(acetonitrile)diiodizinc [(II); Raubacher & Weller, 1996], 2.557 (1) Å for diiodobis(1-pyrroline)zinc(II) [(III); Freer *et al.*, 1993], and 2.543 (1) Å for bis(hexamethylenetetramine)diiodozinc(II) [(IV); Pickardt & Droas, 1989], as well as 2.553 (2) and 2.551 (1) Å found for diiododipyridinezinc(II) [(V); Le Querler et al., 1977]. The Zn—N bond length of 2.071 (3) Å in (I) falls within the range of equivalent values in the aforementioned structures, i.e. 2.038 (4) Å for (II), 2.029 (7) and 2.025 (7) Å for (III), 2.097 (3) Å for (IV), and

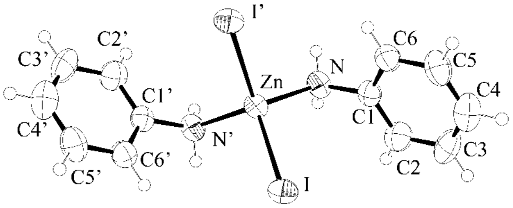


Figure 1
The molecular structure of (I), showing the atomic numbering scheme, with displacement ellipsoids drawn at the 50% probability level [symmetry code: (') $-x, y, \frac{1}{2} - z$].

DOI: 10.1107/S160053680401181X

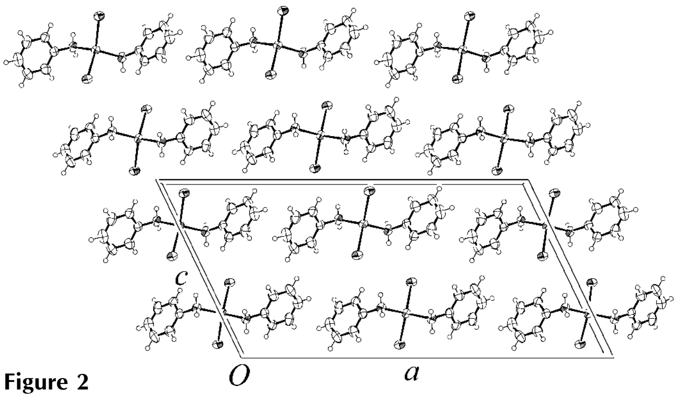


Figure 2
Packing diagram, viewed along the *b* axis.

2.05 (1) and 2.06 (1) Å for (V).

The I—Zn—I angle of 113.71 (6)° is smaller than corresponding angles reported for related structures. In addition, the N—Zn—N angle is 112.65 (18)°, indicating a small distortion from ideal tetrahedral coordination.

The atoms constituting the aromatic ring and atom N1 are coplanar, with an r.m.s. deviation of 0.004 Å. The dihedral angle between the two aromatic rings is 82.91 (13)°.

In the crystal structure, discrete molecules pack in layers with the aromatic groups facing each other, as shown in Fig. 2. The planes through the aromatic groups are parallel to the *ab* plane. However, no π–π stacking interactions are observed, the closest centroid-to-centroid distance being 5.232 (6) Å. Intermolecular N—H···I hydrogen bond interactions are also present in the structure. Thus, each N atom interacts with three I atoms through one normal (through H0*a*) and one bifurcated (through H0*b*) hydrogen bond; see Table 1. As a result of these interactions, a hydrogen-bonding network, extending parallel to the *bc* plane, is formed.

Experimental

Benzylammonium iodide was prepared by the dropwise addition of HI (47%, Acros Organics) to a solution of benzylamine (99%, Saarchem) in chloroform. The resulting precipitate was filtered off. The title compound, (I), was synthesized by dissolving stoichiometric amounts of benzylammonium iodide and ZnI_2 (98+%, Aldrich) (molar ratio 2:1) in water. The solution was heated slightly and allowed to cool to room temperature. Brown single crystals (m.p. 469–470 K) formed on evaporation at room temperature.

Crystal data

$[ZnI_2(C_{12}H_{14}N_2)]$
$M_r = 505.42$
Monoclinic, $C2/c$
$a = 25.073\ (13)$ Å
$b = 5.147\ (4)$ Å
$c = 13.296\ (12)$ Å
$\beta = 115.64\ (5)°$
$V = 1547\ (2)$ Å^3
$Z = 4$
$D_x = 2.170$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 963 reflections
$\theta = 2$–$32°$
$\mu = 5.56$ mm^{-1}
$T = 293\ (2)$ K
Block, brown
0.40 × 0.40 × 0.30 mm

Data collection

Oxford Excalibur2 diffractometer
ω–2θ scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{\min} = 0.142$, $T_{\max} = 0.189$
6914 measured reflections
2462 independent reflections
1839 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.074$
$\theta_{\max} = 31.9°$
$h = -35 \rightarrow 36$
$k = -7 \rightarrow 5$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.110$
$S = 0.96$
2462 reflections
78 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 1.90$ e Å^{-3}
$\Delta\rho_{\min} = -1.42$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N—H0a···I$^{\rm i}$	0.90	2.97	3.804 (4)	154
N—H0b···I$^{\rm ii}$	0.90	3.12	3.936 (5)	152
N—H0b···I$^{\rm iii}$	0.90	3.32	3.769 (4)	114

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

All H atoms were placed in calculated positions, with C—H distances of 0.93 Å and N—H distances of 0.90 Å, and were refined using a riding model, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(parent atom). The maximum electron-density peak is 2.02 Å from the N atom and 2.31 Å from the Zn atom, *i.e.* in a chemically non-sensible position. The minimum electron-density peak is located 1.30 Å from the I atom.

Data collection: *CrysAlis CCD* (Oxford Diffraction Ltd, 2003); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction Ltd, 2003); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2003).

The author acknowledges funding received for this work from the University of KwaZulu–Natal Research Office and the National Research Foundation (GUN:2054350).

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