

Diiodobis(pyridazine- κN)zinc(II)

Gaurav Bhosekar, Inke Jess and Christian Näther*

Institut für Anorganische Chemie, Christian-Albrechts-Universität Kiel, Olshausenstrasse 40, D-24098 Kiel, Germany

Correspondence e-mail: cnaether@ac.uni-kiel.de

Key indicators

Single-crystal X-ray study
 $T = 170$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
 R factor = 0.028
 wR factor = 0.065
 Data-to-parameter ratio = 22.4

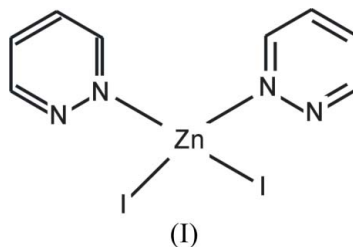
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the crystal structure of the molecular title compound, $[\text{ZnI}_2(\text{C}_4\text{H}_4\text{N}_2)_2]$, the Zn atom is coordinated by two I atoms and two pyridazine ligands, resulting in a slightly distorted ZnN_2I_2 tetrahedral geometry.

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Comment

We are interested in the synthesis, structures and thermal properties of coordination compounds containing zinc(II) cations, halide ions and N -donor ligands (Bhosekar *et al.*, 2006*a,b,c*). For a particular zinc(II) halide and a specific N -donor ligand, frequently several compounds of different stoichiometry are found, which differ in the ratio between the inorganic and organic components. We have found that most of the ligand-rich compounds can be transformed into ligand-poor compounds on heating. Starting from these findings, we have initiated systematic investigations on the structures and properties of zinc(II) halide coordination polymers. We report here the synthesis and structure of the molecular title compound, (I).



In the asymmetric unit of (I), all atoms are in general positions. The Zn atom is coordinated by two I atoms and two N atoms of two pyridazine ligands in a slightly distorted tetrahedral geometry (Fig. 1). The discrete complex molecules are stacked in the a -axis direction (Fig. 2). It should be noted that the title compound is not isotopic with the previously reported dibromobis(pyridazine- κN)zinc(II) compound, which crystallizes in the orthorhombic space group $P2_12_12_1$ (Bhosekar *et al.*, 2006*d*).

Concerning the thermal properties of (I), we have not found any evidence of the formation of a ligand-poor intermediate. On heating, the compound loses all its organic ligands in one step and transforms directly into zinc(II) iodide.

Experimental

A crystalline powder of (I) can be prepared if a suspension of 1 mmol (319.18 mg) of zinc(II) iodide and 1.0 mmol (80 mg) of pyridazine in 1 ml of acetonitrile is stirred for 2 d. Single crystals of (I) were

obtained by dissolving 0.1 mmol (31.9 mg) of zinc(II) iodide and 0.1 mmol (8.0 mg) of pyridazine in 1.0 ml of ethanol. After slow evaporation of the solvent, colourless crystals formed. The homogeneity of the product was confirmed by X-ray powder diffraction.

Crystal data

$[\text{ZnI}_2(\text{C}_4\text{H}_4\text{N}_2)_2]$	$Z = 4$
$M_r = 479.35$	$D_x = 2.468 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 7.9702 (5) \text{ \AA}$	$\mu = 6.67 \text{ mm}^{-1}$
$b = 12.9720 (7) \text{ \AA}$	$T = 170 (2) \text{ K}$
$c = 12.5449 (9) \text{ \AA}$	Block, colourless
$\beta = 95.928 (8)^\circ$	$0.09 \times 0.08 \times 0.07 \text{ mm}$
$V = 1290.07 (14) \text{ \AA}^3$	

Data collection

Stoe IPDS-1 diffractometer	8867 measured reflections
φ scans	3063 independent reflections
Absorption correction: numerical (<i>X-SHAPE</i> ; Stoe & Cie, 1998)	2402 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.561, T_{\max} = 0.632$	$R_{\text{int}} = 0.042$
	$\theta_{\text{max}} = 28.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.036P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.028$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.065$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 0.99$	$\Delta\rho_{\text{max}} = 0.84 \text{ e \AA}^{-3}$
3063 reflections	$\Delta\rho_{\text{min}} = -0.88 \text{ e \AA}^{-3}$
137 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.0020 (2)

Table 1

Selected bond lengths (\AA).

Zn1–N11	2.058 (4)	Zn1–I2	2.5463 (6)
Zn1–N1	2.065 (3)	Zn1–I1	2.5712 (6)

The H atoms were positioned with idealized geometry ($\text{C–H} = 0.95 \text{ \AA}$) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *IPDS* (Stoe & Cie, 1998); cell refinement: *IPDS*; data reduction: *IPDS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *CIFTAB* in *SHELXTL*.

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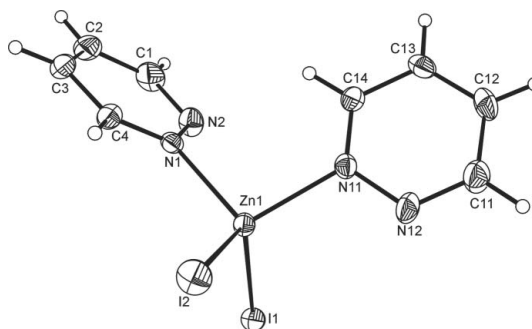


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level (arbitrary spheres for the H atoms).

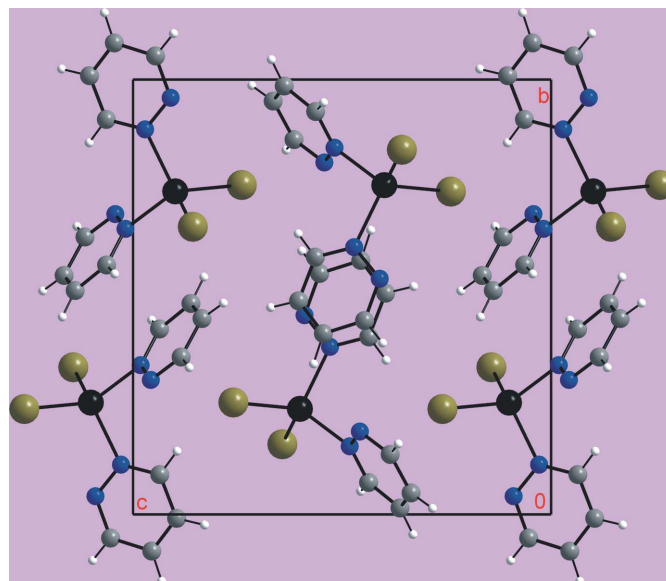


Figure 2
Packing of (I), viewed along the a axis.

References

- Bhosekar, G., Jess, I. & Näther, C. (2006a). *Acta Cryst.* **E62**, m1315–m1316.
 Bhosekar, G., Jess, I. & Näther, C. (2006b). *Z. Naturforsch. Teil B*, **61**, 721–726.
 Bhosekar, G., Jess, I. & Näther, C. (2006c). *Inorg. Chem.* **43**, 6508–6515.
 Bhosekar, G., Jess, I. & Näther, C. (2006d). *Acta Cryst.* **E62**, m1859–m1860.
 Bruker (1998). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
 Stoe & Cie (1998). *X-SHAPE* (Version 1.03) and *IPDS* (Version 2.89). Stoe & Cie, Darmstadt, Germany.