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Dibromobis(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 σ(C–C) = 0.009 Å
R factor = 0.038
wR factor = 0.090
Data-to-parameter ratio = 20.7

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

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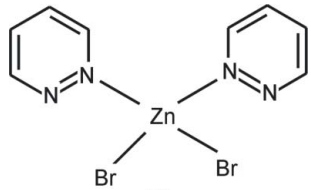
In the crystal structure of the title compound, $[ZnBr_2(C_4H_4N_2)_2]$, each Zn atom is coordinated by two Br atoms and two pyridazine ligands within a distorted tetrahedron to form a discrete complex.

Comment

Recently, we have become interested in the synthesis, structures and thermal properties of coordination compounds based on zinc(II) halides and *N*-donor ligands because we have found that such ligand-rich coordination compounds can be transformed into new ligand-poor compounds (Bhosekar *et al.*, 2006*a*,*b*,*c*). In further investigations, we have prepared such compounds using pyridazine as ligand. For the corresponding compound with zinc(II) chloride, we have found three different modifications of dichlorobis(pyridazine)-zinc(II), which consist of tetrahedral discrete complexes in which the zinc atom is coordinated by two pyridazine ligands and two chlorine atoms. On heating, these compounds transform into a ligand-poor compound. In a continuation of this work, we have investigated the reaction of zinc(II) bromide with pyridazine. In contrast to the chloro compound, we have found no signs of further modifications and also no sign of a ligand-poor compound. Here we report the structure of this compound, (I).



(I)

In the crystal structure of (I), all atoms are in general positions. The Zn^{II} atom is coordinated by two Br atoms and two N atoms of two pyridazine ligands in a distorted tetrahedral geometry (Fig. 1 and Table 1). The Zn—Br and Zn—N bond lengths are comparable to those in related structures retrieved from the Cambridge Structural Database (*Conquest* Version 1.8 of 2006; Allen, 2002).

Experimental

$ZnBr_2$ and pyridazine were obtained from Alfa Aesar, and acetonitrile was obtained from Fluka. Large amounts of crystalline powder can be prepared if a suspension of 1 mmol of $ZnBr_2$ and 1 mmol of pyridazine is stirred in 1 ml of acetonitrile for 2 d. Single crystals of (I) are obtained if 0.25 mmol (56.3 mg) $ZnBr_2$ is dissolved in 1.5 mmol (120.12 mg) pyridazine.

Crystal data

$[ZnBr_2(C_4H_4N_2)_2]$	$Z = 4$
$M_r = 385.37$	$D_x = 2.143$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 8.8914$ (5) Å	$\mu = 8.72$ mm^{-1}
$b = 9.7191$ (7) Å	$T = 170$ (2) K
$c = 13.8189$ (8) Å	Block, colourless
$V = 1194.18$ (13) Å^3	0.10 × 0.08 × 0.06 mm

Data collection

Stoe IPDS-1 diffractometer	6650 measured reflections
φ scans	2833 independent reflections
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)	2354 reflections with $I > 2\sigma(I)$
$T_{min} = 0.447$, $T_{max} = 0.601$	$R_{int} = 0.049$
	$\theta_{max} = 28.0°$

Refinement

Refinement on F^2	$(\Delta/\sigma)_{max} = 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$\Delta\rho_{max} = 0.81$ e Å^{-3}
$wR(F^2) = 0.090$	$\Delta\rho_{min} = -0.84$ e Å^{-3}
$S = 1.02$	Extinction correction: *SHELXL97*
2833 reflections	Extinction coefficient: 0.0071 (7)
137 parameters	Absolute structure: Flack (1983), 1163 Friedel pairs
H-atom parameters constrained	Flack parameter: 0.02 (2)
$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	

Table 1
Selected geometric parameters (Å, °).

Zn1—Br1	2.3735 (8)	Zn1—N1	2.041 (5)
Zn1—Br2	2.3541 (8)	Zn1—N11	2.056 (5)
N1—Zn1—N11	106.30 (19)	N1—Zn1—Br1	107.76 (13)
N1—Zn1—Br2	109.38 (13)	N11—Zn1—Br1	104.50 (13)
N11—Zn1—Br2	111.56 (13)	Br2—Zn1—Br1	116.75 (3)

H atoms were placed in calculated positions, with C—H = 0.95 Å, and refined in riding mode, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *IPDS* (Stoe & Cie, 1998b); 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: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

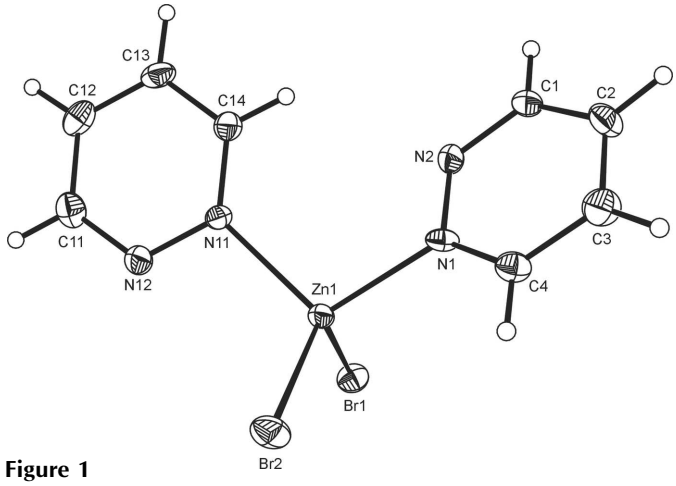


Figure 1
The molecular structure of (I) with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

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