Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

A redetermination of (acetonitrile-*κN*)diiodozinc(II)

Gaurav Bhosekar, Inke Jess and Christian Näther*

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

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

Received 10 May 2006
Accepted 12 May 2006

Key indicators

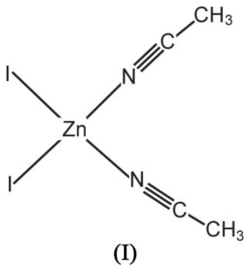
Single-crystal X-ray study
T = 220 K
Mean σ(C–C) = 0.008 Å
R factor = 0.032
wR factor = 0.088
Data-to-parameter ratio = 23.5

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

In the title compound, $[Zn(C_2H_3N)_2I_2]$ each Zn atom is coordinated by two symmetry-related I atoms and two symmetry-related acetonitrile ligands within a distorted tetrahedron to form a discrete complex. All non-H atoms are located in special positions, that for Zn having *m*2*m* symmetry.

Comment

Recently, we have reported two polymorphs of dibromobis(acetonitrile-*N*)zinc(II) (Bhosekar, Jess & Näther, 2006). Form 1 crystallizes in the orthorhombic space group *Pnma*, whereas form 2 crystallizes in space group *Cmcm*. We have proven that form 2 is the thermodynamically more stable form between 233 and 353 K and that form 1 is metastable. In continuation of this work, we have investigated the reaction of zinc(II) iodide with acetonitrile. Surprisingly, only one form can be prepared, which is isotypic with the more stable form 2 of dibromobis(acetonitrile-*N*)zinc(II). A search of the CSD database [Version 1.8; Allen, 2002 using *ConQuest* (Version 1.8; Bruno *et al.*, 2002)] showed that this structure is known, but was reported in space group $P2_1/m$ (Raubacher & Weller, 1996). However, this structure can easily be transformed into the orthorhombic cell and space group *Cmcm* was used in the refinement of the present compound.



(I)

The asymmetric unit of the title compound, (I), consists of one zinc cation located on a position of site symmetry *m*2*m*, as well as one iodide anion and one acetonitrile ligand which are located on perpendicular crystallographic mirror planes. The zinc cations are each coordinated by two symmetry-related iodide anions and two N atoms of two symmetry-related acetonitrile ligands within a distorted tetrahedron (Fig. 1). The Zn—I distance of 2.5315 (6) Å and the Zn—N distance of 2.046 (5) Å are comparable to those in related structures retrieved from the CSD. The crystal packing is shown in Fig. 2.

Experimental

ZnI_2 was obtained from Acros and acetonitrile from Fluka. Large amounts of crystalline powder can be prepared if a crystalline suspension of 1 mmol (319.2 mg) of zinc(II) iodide is stirred in 1 ml of acetonitrile for 2 d. Single crystals are obtained if 1 mmol (319.2 mg) zinc(II) iodide is dissolved in 6.0 ml acetonitrile and 0.3 ml of water. After slow evaporation of the solvent, colourless plates formed. The homogeneity of the product was checked by X-ray powder diffraction.

Crystal data

$[Zn(C_2H_3N)_2I_2]$
$M_r = 401.28$
Orthorhombic, *Cmcm*
$a = 8.7049\ (7)$ Å
$b = 11.3913\ (11)$ Å
$c = 10.5121\ (11)$ Å
$V = 1042.38\ (17)$ Å^3

$Z = 4$
$D_x = 2.557$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 8.22$ mm^{-1}
$T = 220\ (2)$ K
Plate, colourless
0.15 × 0.10 × 0.04 mm

Data collection

Stoe IPDS-1 diffractometer
φ scans
Absorption correction: numerical
X-SHAPE (Stoe & Cie, 1998)
$T_{min} = 0.381$, $T_{max} = 0.725$

4886 measured reflections
704 independent reflections
628 reflections with $I > 2\sigma(I)$
$R_{int} = 0.065$
$\theta_{max} = 28.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.088$
$S = 1.06$
704 reflections
30 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.059P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.86$ e Å^{-3}
$\Delta\rho_{min} = -1.06$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0041 (5)

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.046 (5)	Zn1—I1	2.5316 (5)
N1^i—Zn1—N1	96.3 (3)	I1^{ii}—Zn1—I1	120.50 (3)
N1—Zn1—I1	109.33 (5)		

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

One of the H atoms was located in a difference map and its bond length was set to ideal values. Afterwards the positions of the two missing H atoms were calculated. In the end, all H atoms were treated as riding, with C—H = 0.97 Å and with $U_{iso}(H) = 1.5U_{eq}(C)$.

Data collection: *IPDS Software* (Stoe & Cie, 1998); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; 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* (Bruker, 1998).

This work is supported by the state of Schleswig-Holstein and the Deutsche Forschungsgemeinschaft (Projekt No. NA 720/1–1). We are very grateful to Professor Dr. Wolfgang Bensch for the opportunity to use his experimental equipment.

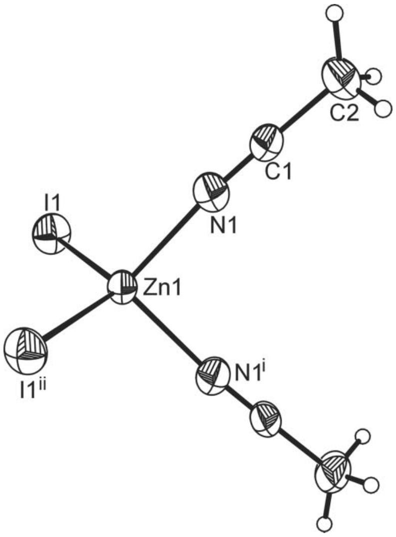


Figure 1
The structure of (I) with the atom-labelling and displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (i) $x, y, -z+\frac{1}{2}$; (ii) $-x, y, -z+\frac{1}{2}$.

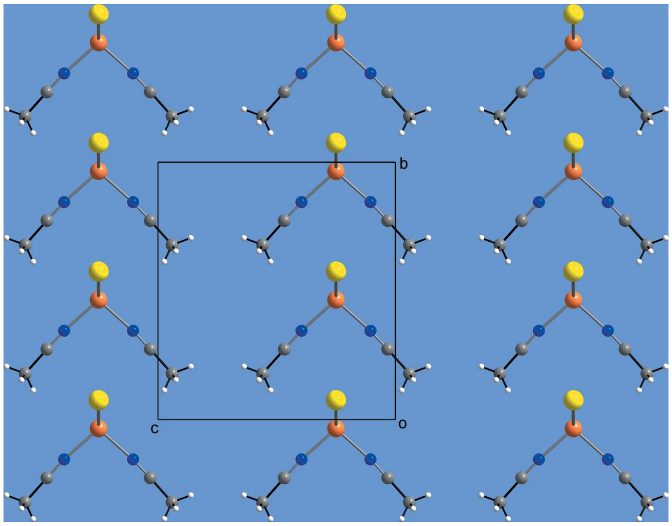


Figure 2
Packing of (I), viewed along the *a* axis.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bhosekar, G., Jess, I. & Näther, C. (2006). *Z. Naturforsch. Teil B* In the press.
Bruker (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.
Raubacher, F. & Weller, F. (1996). *Z. Kristallogr.* **211**, 576.
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.

m1316 Bhosekar *et al.* • $[Zn(C_2H_3N)_2I_2]$ *Acta Cryst.* (2006). E**62**, m1315–m1316