Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

catena-Poly[[diiodozinc(II)]-*μ*-4,4′-bipyridine-$\kappa^2N:N'$]

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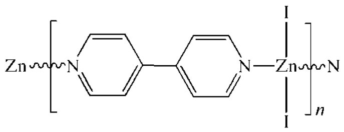
Received 21 September 2006
Accepted 28 September 2006
Online 31 October 2006

The title compound, $[ZnI_2(bipy)]_n$ (bipy is 4,4′-bipyridine, $C_{10}H_8N_2$), has been prepared by the hydrothermal reaction of ZnI_2 and bipy at 433 K. Each Zn atom is coordinated by two N atoms from two different bipy ligands and by two I atoms in a distorted tetrahedral geometry, with Zn—N distances ranging from 2.068 (7) to 2.101 (8) Å and Zn—I distances ranging from 2.5471 (13) to 2.5673 (13) Å. The molecular structure features a zigzag polymeric chain. Face-to-face π–π stacking interactions between adjacent bipy ligands stabilize the structure.

Comment

Over the past few years, considerable efforts have been devoted to the synthesis and structural characterization of coordination polymers. 4,4′-Bipyridine (bipy) has been used as a bridging ligand to construct supermolecular polymers (Hu & Englert, 2005; Nordell *et al.*, 2004; Pedireddi & Varughese, 2004; Vittal *et al.*, 2003; Yang *et al.*, 2004). It is not unusual that the backbone of these polymers is subject to considerable modification due to the influence of the coligands and the difference in reaction parameters. For example, according to the literature, it is found that the structures of polymers of type $[ZnX_2(bipy)]$ (X = Cl or Br) are influenced by the reaction conditions and coligands (Hu & Englert, 2001, 2005; Liang *et al.*, 2001; Fu *et al.*, 2001). Two isomorphic phases of the one-dimensional coordination polymer $[ZnCl_2(bipy)]$ were prepared by hydrothermal reactions with different stoichiometry ratios of the reactants. It is interesting that when the temperature is decreased to 130 K, both polymorphs can convert to a two-dimensional network and that the conversion is reversible (Hu & Englert, 2005). Polymeric $[ZnBr_2(bipy)]$ has a one-dimensional zigzag chain structure (Hu & Englert, 2001). However, according to the results of a search in the Cambridge Structural Database (Version 5.27; Allen, 2002), the structure and properties of polymeric $[ZnI_2(bipy)]$ have not been reported. We report here a new polymeric compound, $[ZnI_2(bipy)]_n$, (I), with a zigzag polymeric chain structure, obtained *via* hydrothermal synthesis.



(I)

In (I), there are two crystallographically independent Zn atoms in the asymmetric unit. Both are four-coordinated in a distorted tetrahedral environment by two N atoms from two different bipy ligands and two I atoms. The differences are their Zn—N and Zn—I distances (Table 1). As a result of this coordination, the molecular structure features a zigzag polymeric chain, which is similar to that in the polymers $[ZnX_2(bipy)]$ (X = Cl or Br), as shown in Fig. 1. In (I), an interesting phenomenon is that the two pyridine rings of the same bipy ligand are not coplanar [the dihedral angles between the two planes are 32.22 (13) and 38.42 (16)°]. In contrast, the two pyridine rings of the same bipy ligand in the polymers $[ZnX_2(bipy)]$ (X = Cl or Br) are coplanar. Figs. 2 and 3 show that zigzag chains stack on top of each other. As shown in Fig. 2, there are two different π–π stacking interactions. One relates bipy ring $R1$ (N1/C1–C3/C9/C10) to bipy ring $R2$ (N2/C4–C8) of an adjacent bipy ligand, denoted $R1^{i}\cdots R2$ [symmetry code: (i) $x, -y + \frac{3}{2}, z - \frac{1}{2}$]. The second is formed between bipy ring $R3$ (N3/C11–C13/C19/C20) and bipy ring

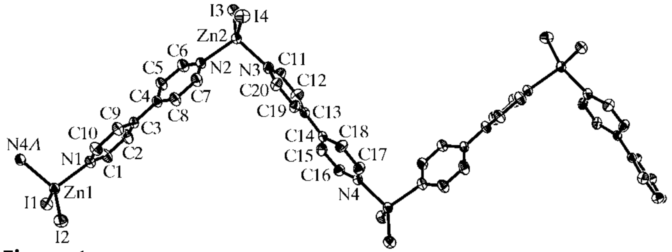


Figure 1
A view of the repeat unit of (I). Displacement ellipsoids are plotted at the 30% probability level and H atoms have been omitted for clarity. [Symmetry code: (A) $-1 + x, -y + \frac{3}{2}, z - \frac{1}{2}$.]

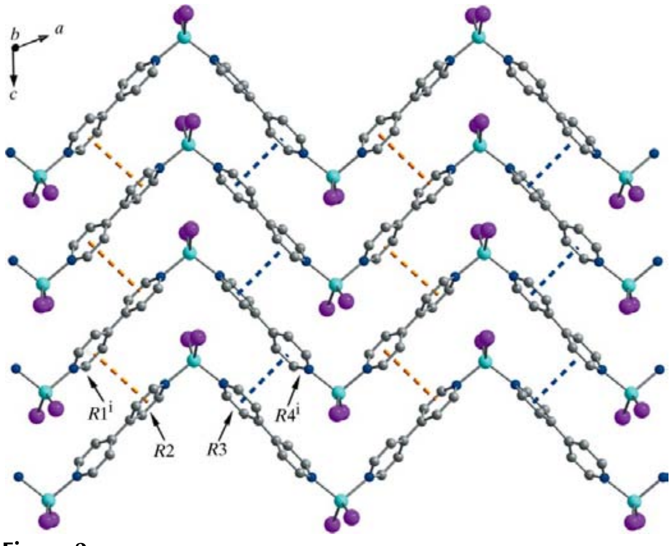


Figure 2
The π–π interactions between pairs of adjacent bipy ligands. [Symmetry code: (i) $x, -y + \frac{3}{2}, z - \frac{1}{2}$.]

DOI: 10.1107/S0108270106039965

*R*4 (N4/C14–C18) of an adjacent bipy ligand, denoted $R3\cdots R4^{i}$. The two bipy rings involved in each π–π stacking interaction are nearly parallel, with dihedral angles of 6.9 (3)° for $R1^{i}\cdots R2$ and 6.1 (4)° for $R3\cdots R4^{i}$, centroid-to-centroid distances of 4.282 (2) ($R1^{i}\cdots R2$) and 3.971 (2) Å ($R3\cdots R4^{i}$), and plane-to-plane distances of 3.61 (6) ($R2\cdots R1^{i}$) and 3.73 (6) Å ($R3\cdots R4^{i}$); the plane-to-plane distances are smaller than those in the isomorphic polymers [$ZnCl_2$(bipy)] [3.85 (7) Å; Fu *et al.*, 2001] and [$ZnBr_2$(bipy)] [4.17 (5) Å; Hu & Englert, 2001]. The face-to-face π–π stacking interactions between adjacent bipy ligands stabilize the structure.

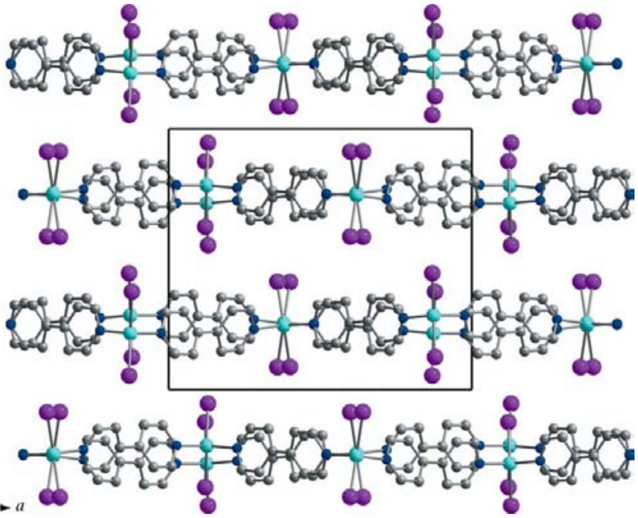


Figure 3
The packing diagram of (I), viewed down the *c* axis. H atoms have been omitted for clarity.

Experimental

A mixture of ZnI_2 (0.16 g, 0.5 mmol), bipy (0.78 g, 0.5 mmol) and water (13 ml) was sealed in a 25 ml Teflon-lined stainless steel reactor, heated to 443 K for 72 h, and then cooled slowly to room temperature. Block-shaped light-yellow crystals of (I) suitable for X-ray analysis were obtained by filtration (yield 23.2%).

Crystal data

[$ZnI_2(C_{10}H_8N_2)$]
M_r = 950.71
Monoclinic, $P2_1/c$
a = 17.140 (3) Å
b = 13.930 (3) Å
c = 11.950 (2) Å
β = 109.00 (3)°
V = 2697.7 (10) Å^3
Z = 4
D_x = 2.341 Mg m^{-3}
Mo *Kα* radiation
μ = 6.37 mm^{-1}
T = 293 (2) K
Block, light yellow
0.5 × 0.45 × 0.2 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: empirical (using intensity measurements) (*SADABS*; Sheldrick, 1996)
T_{min} = 0.632, T_{max} = 1.000 (expected range = 0.177–0.280)
14426 measured reflections
5080 independent reflections
3979 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.7°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.135
S = 1.04
5080 reflections
271 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2 + 24.4231P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.08 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.071 (7)	Zn2—N2	2.068 (7)
Zn1—N4^{ii}	2.101 (8)	Zn2—N3	2.088 (8)
Zn1—I1	2.5520 (13)	Zn2—I4	2.5471 (13)
Zn1—I2	2.5673 (13)	Zn2—I3	2.5483 (12)
N1—Zn1—N4^{ii}	101.5 (3)	N2—Zn2—N3	103.0 (3)
N1—Zn1—I1	108.4 (2)	N2—Zn2—I4	106.0 (2)
N4^{ii}—Zn1—I1	104.2 (2)	N3—Zn2—I4	105.7 (2)
N1—Zn1—I2	103.3 (2)	N2—Zn2—I3	107.9 (2)
N4^{ii}—Zn1—I2	108.2 (2)	N3—Zn2—I3	109.4 (2)
I1—Zn1—I2	128.33 (5)	I4—Zn2—I3	123.07 (5)

Symmetry code: (ii) $x - 1, -y + \frac{3}{2}, z - \frac{1}{2}$.

All H atoms were positioned geometrically and refined as riding atoms, with C—H distances of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1996); data reduction: *XPREP* in *SHELXTL* (Siemens, 1996) and *SAINT*; program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *ASP* (Chen, 2002); software used to prepare material for publication: *SHELXTL*.

This work was supported financially by the National Natural Science Foundation of China (Nos. 50572030 and 50372022).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK3060). Services for accessing these data are described at the back of the journal.

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