

(6,6'-Dimethyl-2,2'-bipyridine- κ^2N,N')- diiodidozinc(II)

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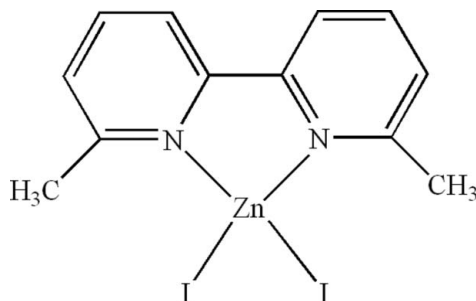
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.043; wR factor = 0.127; data-to-parameter ratio = 25.3.

The complete molecule of the title compound, $[\text{ZnI}_2(\text{C}_{12}\text{H}_{12}\text{N}_2)]$, is generated by crystallographic twofold symmetry, with the Zn^{II} atom lying on the rotation axis. The Zn^{II} atom is coordinated by the N,N -bidentate 6,6'-dimethyl-2,2'-bipyridine ligand and two iodide ions, resulting in a distorted ZnN_2I_2 tetrahedral geometry for the metal. In the crystal, there are weak π - π contacts between the pyridine rings [centroid-centroid distance = 3.978 (3) Å].

Related literature

For related structures, see: Ahmadi *et al.* (2008, 2009); Alizadeh, Heidari *et al.* (2009); Alizadeh, Kalateh *et al.* (2009); Alizadeh, Khoshtarkib *et al.* (2009); Blake *et al.* (2007); Khalighi *et al.* (2008); Khan & Tuck (1984); Khavasi *et al.* (2008); Khoshtarkib *et al.* (2009); Kwak *et al.* (2008); Lee *et al.* (2007); Marjani *et al.* (2009); Reimann *et al.* (1966); Seebacher *et al.* (2004); Wriedt *et al.* (2008).



Experimental

Crystal data

$[\text{ZnI}_2(\text{C}_{12}\text{H}_{12}\text{N}_2)]$
 $M_r = 503.43$
 Monoclinic, $C2/c$
 $a = 13.421$ (2) Å

$b = 8.441$ (2) Å
 $c = 13.752$ (3) Å
 $\beta = 105.140$ (14)°
 $V = 1503.8$ (5) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 5.72$ mm⁻¹

$T = 298$ K
 $0.48 \times 0.12 \times 0.11$ mm

Data collection

Bruker SMART CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
 $T_{\text{min}} = 0.425$, $T_{\text{max}} = 0.539$

5694 measured reflections
 1997 independent reflections
 1748 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.076$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.127$
 $S = 1.12$
 1997 reflections

79 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.23$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.85$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1—N1	2.058 (3)	Zn1—I1	2.5501 (6)
N1—Zn1—N1 ⁱ	81.9 (2)		

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We are grateful to the Damghan University of Basic Sciences and Islamic Azad University, Shahr-e-Rey Branch, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5152).

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supplementary materials

Acta Cryst. (2009). E65, m1439-m1440 [doi:10.1107/S1600536809043049]

(6,6'-Dimethyl-2,2'-bipyridine- κ^2N,N')diiodidozinc(II)

R. Alizadeh, K. Kalateh, Z. Khoshtarkib, R. Ahmadi and V. Amani

Comment

Recently, we reported the synthesis and crystal structure of [ZnCl₂(phen)], (II), (Khoshtarkib *et al.*, 2009), [HgBr₂(2,9-dmphen)], (III), (Alizadeh, Heidari *et al.*, 2009) and [Pb₄(NO₃)₈(6-mbpy)₄], (IV), (Ahmadi, Kalateh, Alizadeh *et al.*, 2009) [where phen is phenanthridine, 2,9-dmphen is 2,9-dimethyl-1,10-phenanthroline and 6-mbpy is 6-methyl-2,2'-bipyridine].

There are several Zn^{II} complexes, with formula, [ZnX₂(N—N)], (X = Cl, Br and I), such as [ZnCl₂(bipy)], (V), (Khan & Tuck, 1984), [ZnCl₂(phen)], (VI), (Reimann *et al.*, 1966), [ZnCl₂(dm4bt)], (VII), (Khavasi *et al.*, 2008), [ZnCl₂(5,5'-dmbpy)], (VIII), (khalighi *et al.*, 2008), [ZnCl₂(6-mbpy)], (IX), (Ahmadi, Kalateh, Ebadi *et al.*, 2008), [ZnCl₂(6,6'-dmbpy)], (X), (Alizadeh, Kalateh *et al.*, 2009), [ZnCl₂(PBD)], (XI), (Marjani *et al.*, 2009), [ZnBr₂(4,4'-(dtbpy))·(Et₂O)], (XII), (Blake *et al.*, 2007), {ZnBr₂[NH(py)₂]}, (XIII), (Lee *et al.*, 2007), {ZnBr₂[S(py)₂]}, (XIV) (Wriedt *et al.*, 2008), [ZnBr₂(6,6'-dmbpy)], (XV), (Alizadeh, Khoshtarkib *et al.*, 2009), [ZnI₂(2,9-dmphen)], (XVI), (Seebacher *et al.*, 2004) and {ZnI₂[NH(py)₂]}, (XVII) (Kwak *et al.*, 2008) [where bipy is 2,2'-bipyridine, phen is 1,10-phenanthroline, dm4bt is 2,2'-dimethyl-4,4'-bithiazole, 5,5'-dmbpy is 5,5'-dimethyl-2,2'-bipyridine, 6,6'-dmbpy is 6,6'-dimethyl-2,2'-bipyridine, PBD is *N*-(pyridin-2-ylmethylene)benzene-1,4-diamine, dtbpy is 4,4'-di-*tert*-butyl-2,2'-bipyridine, NH(py)₂ is bis(2-pyridyl)amine, S(py)₂ is bis(2-pyridyl)sulfide and NH(py)₂ is bis(2-pyridyl)amine] have been synthesized and characterized by single-crystal X-ray diffraction methods. We report herein the synthesis and crystal structure of the title compound (I).

In the molecule of the title compound, (I), (Fig. 1), the Zn^{II} atom is four-coordinated in distorted tetrahedral configurations by two N atoms from one 6,6'-dimethyl-2,2'-bipyridine and two terminal I atoms. The Zn—I and Zn—I bond lengths and angles (Table 1) are within normal range (XVI).

The π - π contacts between the pyridine rings, Cg2...Cg2ⁱ [symmetry cods: (i) -X,1-Y,1-Z, where, Cg2 is centroids of the ring (N1/C2—C6)] further stabilize the structure, with centroid-centroid distance of 3.978 (3) Å. It seems this π - π stacking is effective in the stabilization of the crystal structure (Fig. 2).

Experimental

A solution of 6,6'-dimethyl-2,2'-bipyridine (0.20 g, 1.10 mmol) in methanol (10 ml) was added to a solution of ZnI₂ (0.35 g, 1.10 mmol) in acetonitrile (10 ml) and the resulting colourless solution was stirred for 20 min at 313 K. This solution was left to evaporate slowly at room temperature. After one week, colourless needles of (I) were isolated (yield 0.41 g, 74.1%).

Refinement

All H atoms were positioned geometrically, with C—H = 0.93–0.96 Å and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

Figures

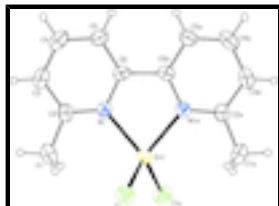


Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level.

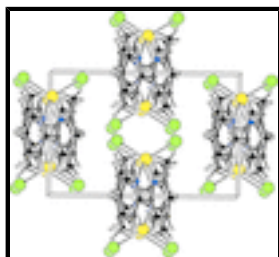


Fig. 2. Unit-cell packing diagram for (I).

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Crystal data

[ZnI₂(C₁₂H₁₂N₂)]

$M_r = 503.43$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 13.421\ (2)\ \text{\AA}$

$b = 8.441\ (2)\ \text{\AA}$

$c = 13.752\ (3)\ \text{\AA}$

$\beta = 105.140\ (14)^\circ$

$V = 1503.8\ (5)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 936$

$D_x = 2.224\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 896 reflections

$\theta = 2.9\text{--}29.2^\circ$

$\mu = 5.72\ \text{mm}^{-1}$

$T = 298\ \text{K}$

Needle, colourless

$0.48 \times 0.12 \times 0.11\ \text{mm}$

Data collection

Bruker SMART CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298\ \text{K}$

ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 1998)

$T_{\min} = 0.425$, $T_{\max} = 0.539$

5694 measured reflections

1997 independent reflections

1748 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.076$

$\theta_{\max} = 29.2^\circ$

$\theta_{\min} = 2.9^\circ$

$h = -18 \rightarrow 18$

$k = -9 \rightarrow 11$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.127$	$w = 1/[\sigma^2(F_o^2) + (0.0623P)^2 + 3.240P]$
$S = 1.12$	where $P = (F_o^2 + 2F_c^2)/3$
1997 reflections	$(\Delta/\sigma)_{\max} < 0.001$
79 parameters	$\Delta\rho_{\max} = 1.23 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.85 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1171 (5)	0.2312 (7)	0.4901 (4)	0.0650 (14)
H1A	0.1495	0.1657	0.4501	0.078*
H1B	0.0518	0.1858	0.4914	0.078*
H1C	0.1607	0.2378	0.5575	0.078*
C2	0.1003 (4)	0.3936 (6)	0.4452 (3)	0.0498 (9)
C3	0.1376 (4)	0.5282 (8)	0.5028 (4)	0.0624 (13)
H3	0.1737	0.5192	0.5702	0.075*
C4	0.1190 (5)	0.6766 (8)	0.4564 (5)	0.0677 (14)
H4	0.1435	0.7680	0.4925	0.081*
C5	0.0640 (4)	0.6862 (6)	0.3567 (4)	0.0581 (11)
H5	0.0499	0.7842	0.3251	0.070*
C6	0.0304 (4)	0.5486 (5)	0.3045 (3)	0.0466 (9)
N1	0.0498 (3)	0.4055 (4)	0.3488 (3)	0.0429 (7)
Zn1	0.0000	0.22134 (8)	0.2500	0.0467 (2)
I1	0.15441 (3)	0.07347 (4)	0.21872 (3)	0.06177 (17)

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.061 (3)	0.082 (4)	0.049 (3)	0.010 (3)	0.010 (2)	0.017 (2)
C2	0.045 (2)	0.062 (3)	0.043 (2)	0.0025 (19)	0.0125 (17)	-0.0009 (18)
C3	0.051 (2)	0.086 (4)	0.047 (2)	-0.001 (3)	0.0064 (19)	-0.017 (2)
C4	0.062 (3)	0.068 (3)	0.073 (3)	-0.009 (3)	0.017 (3)	-0.030 (3)
C5	0.058 (3)	0.046 (2)	0.068 (3)	-0.003 (2)	0.011 (2)	-0.011 (2)
C6	0.050 (2)	0.0395 (19)	0.052 (2)	-0.0028 (16)	0.0149 (18)	-0.0068 (16)
N1	0.0444 (17)	0.0428 (17)	0.0406 (16)	0.0000 (14)	0.0097 (13)	-0.0026 (13)
Zn1	0.0570 (4)	0.0354 (3)	0.0469 (4)	0.000	0.0121 (3)	0.000
II	0.0680 (3)	0.0582 (2)	0.0608 (2)	0.01460 (14)	0.01977 (18)	-0.00003 (13)

Geometric parameters (\AA , $^\circ$)

C1—C2	1.496 (8)	C4—H4	0.9300
C1—H1A	0.9600	C5—C6	1.378 (6)
C1—H1B	0.9600	C5—H5	0.9300
C1—H1C	0.9600	C6—N1	1.347 (6)
C2—N1	1.327 (6)	C6—C6 ⁱ	1.508 (9)
C2—C3	1.400 (8)	Zn1—N1	2.058 (3)
C3—C4	1.398 (9)	Zn1—N1 ⁱ	2.058 (3)
C3—H3	0.9300	Zn1—II ⁱ	2.5501 (6)
C4—C5	1.379 (8)	Zn1—II	2.5501 (6)
C2—C1—H1A	109.5	C6—C5—C4	119.0 (5)
C2—C1—H1B	109.5	C6—C5—H5	120.5
H1A—C1—H1B	109.5	C4—C5—H5	120.5
C2—C1—H1C	109.5	N1—C6—C5	121.5 (5)
H1A—C1—H1C	109.5	N1—C6—C6 ⁱ	116.1 (2)
H1B—C1—H1C	109.5	C5—C6—C6 ⁱ	122.4 (3)
N1—C2—C3	121.2 (5)	C2—N1—C6	120.5 (4)
N1—C2—C1	117.7 (4)	C2—N1—Zn1	126.6 (3)
C3—C2—C1	121.2 (5)	C6—N1—Zn1	112.8 (3)
C4—C3—C2	118.3 (5)	N1—Zn1—N1 ⁱ	81.9 (2)
C4—C3—H3	120.8	N1—Zn1—II ⁱ	113.38 (10)
C2—C3—H3	120.8	N1 ⁱ —Zn1—II ⁱ	110.04 (10)
C5—C4—C3	119.5 (5)	N1—Zn1—II	110.04 (10)
C5—C4—H4	120.3	N1 ⁱ —Zn1—II	113.38 (10)
C3—C4—H4	120.3	II ⁱ —Zn1—II	121.39 (3)
N1—C2—C3—C4	0.9 (7)	C5—C6—N1—C2	1.6 (7)
C1—C2—C3—C4	-179.8 (5)	C6 ⁱ —C6—N1—C2	-178.1 (5)
C2—C3—C4—C5	0.8 (8)	C5—C6—N1—Zn1	-175.7 (4)
C3—C4—C5—C6	-1.3 (8)	C6 ⁱ —C6—N1—Zn1	4.7 (6)
C4—C5—C6—N1	0.1 (8)	C2—N1—Zn1—N1 ⁱ	-178.8 (5)
C4—C5—C6—C6 ⁱ	179.8 (6)	C6—N1—Zn1—N1 ⁱ	-1.7 (2)

C3—C2—N1—C6	-2.1 (7)	C2—N1—Zn1—I1 ⁱ	72.8 (4)
C1—C2—N1—C6	178.6 (4)	C6—N1—Zn1—I1 ⁱ	-110.1 (3)
C3—C2—N1—Zn1	174.7 (3)	C2—N1—Zn1—I1	-66.8 (4)
C1—C2—N1—Zn1	-4.6 (6)	C6—N1—Zn1—I1	110.3 (3)

Symmetry codes: (i) $-x, y, -z+1/2$.

Fig. 1

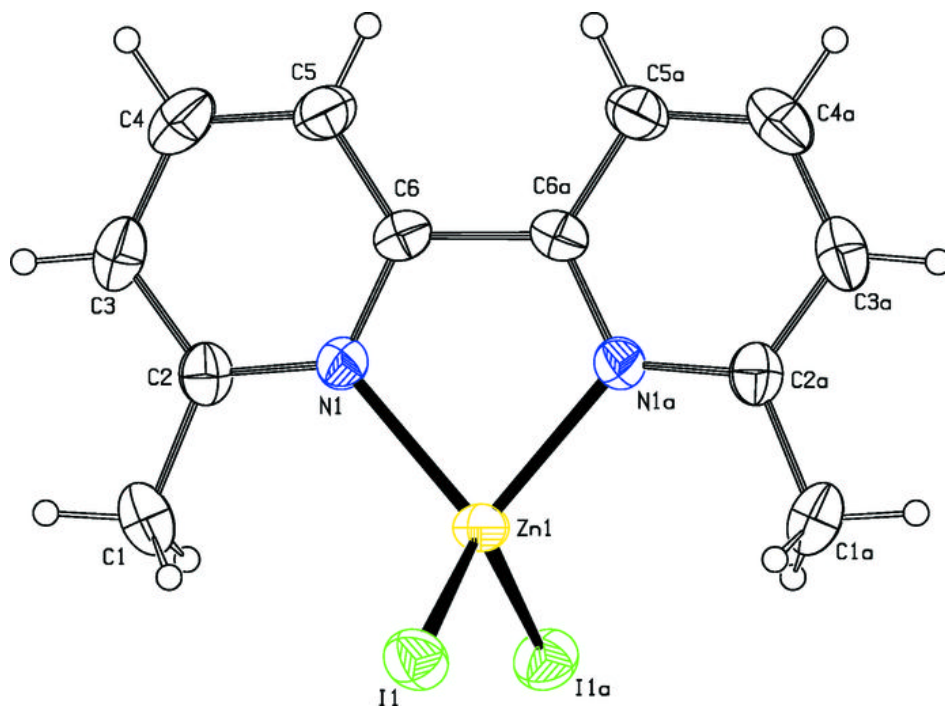


Fig. 2

