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Bis(2,6-dimethylpyrazine-κN^4)diiodidozinc(II)

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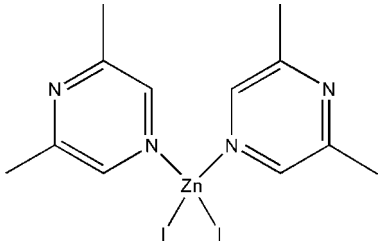
Key indicators: single-crystal X-ray study; T = 170 K; mean σ(C–C) = 0.007 Å; R factor = 0.032; wR factor = 0.069; data-to-parameter ratio = 19.0.

In the title compound, $[ZnI_2(C_6H_8N_2)_2]$, the Zn^{II} ion is coordinated by two iodide anions and two N atoms from 2,6-dimethylpyrazine in a distorted tetrahedral geometry.

Related literature

For background information, see: Batten & Robson (1998); Chi *et al.* (2006); Evans & Lin (2002); Hong *et al.* (2004); Janiak (2003); Janaik & Scharmann (2003); Kasai *et al.* (2000); Kitagawa *et al.* (2004); Luan *et al.* (2005, 2006); Moler *et al.* (2001); Moulton & Zaworotko (2001); Ryu *et al.* (2005); Wang *et al.* (2006); Blake *et al.* (1999); Saalfrank *et al.* (2001).



Experimental

Crystal data

$[ZnI_2(C_6H_8N_2)_2]$
M_r = 535.48
Monoclinic, $P2_1/c$
a = 9.1825 (7) Å
b = 13.8144 (10) Å
c = 13.6242 (10) Å
β = 98.381 (1)°
V = 1709.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.04 mm^{-1}
T = 170 (2) K
0.10 × 0.05 × 0.05 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
9413 measured reflections
3344 independent reflections
2518 reflections with $I > 2\sigma(I)$
R_{int} = 0.109

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.069
S = 0.81
3344 reflections
176 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −1.27 e Å^{-3}

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2320).

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supporting information

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Bis(2,6-dimethylpyrazine-κN^4)diiodidozinc(II)

Sun Hwa Lee, Sea-Hyun Kim, Pan-Gi Kim, Cheal Kim and Youngmee Kim

S1. Comment

Much interest has recently been focused on the rational design and construction of novel discrete and polymeric metal-organic complexes, not only due to their structural and topological novelty (Batten & Robson, 1998, Moler *et al.*, 2001, Moulton & Zaworotko, 2001), but also for their potential applications as functional materials such as catalysis, molecular recognition, separation, and nonlinear optics (Hong *et al.*, 2004, Evans & Lin, 2002, Kasai *et al.* 2000, Kitagawa *et al.*, 2004). It has shown that many factors such as the coordination geometry of metal ions (Chi *et al.*,2006), the structure of organic ligands (Wang *et al.*,2006), the solvent system (Ryu *et al.*, 2005), the counteranion (Luan *et al.*, 2006), and the ratio of ligands to metal ions (Blake *et al.*, 1999, Saalfrank *et al.*, 2001) influence highly on the structure of metal-organic complexes. In addition, it has been considered that the secondary forces such as hydrogen-bonding, pi-pi stacking, and host–guest interactions are of importance as well (Luan *et al.*, 2005, Janaik & Scharmann, 2003, Janiak, 2003). For obtaining novel structural motifs with predictable properties, therefore, a large number of organic ligands were designed and utilized. Among them, 2,6-dimethylpyrazine was often selected. We have also reacted ZnI_2 with 2,6-dimethylpyrazine to form a new zinc complex and report here on the crystal structure of diiodobis(2,6-dimethylpyrazine)zinc(II).

Asymmetric unit contains a whole molecule (Fig. 1). Zn^{II} ion is coordinated by two iodide anions and two nitrogen atoms from 2,6-dimethylpyrazine to form a distorted tetrahedral geometry (Fig. 1). Zn—I bond distances are 2.5393 (7) and 2.5442 (6) Å, and I—Zn—I and N—Zn—N bond angles are 122.78 (2) and 101.39 (14)°, respectively.

S2. Experimental

244.29 mg (0.75 mmol) of ZnI_2 were dissolved in 4 ml water and carefully layered by 4 ml e thanol solution of 2,6-dimethylpyrazine ligand (165.52 mg, 1.5 mmol). Suitable crystals of the title compound for X-ray analysis were obtained in a few weeks.

S3. Refinement

(type here to add refinement details)

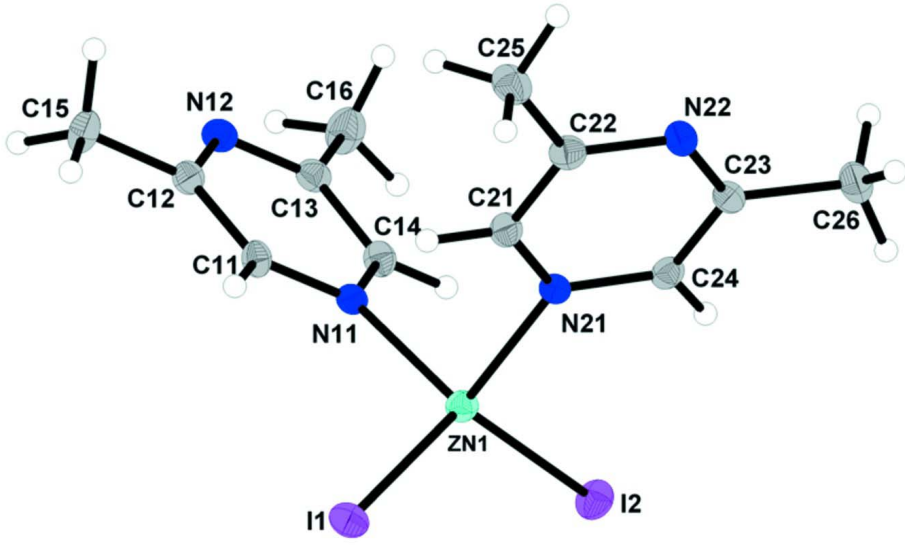

Figure 1

The structure of the title compound showing the atom-labeling scheme. Displacement ellipsoids are shown at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

Bis(2,6-dimethylpyrazine-κN^4)diiodidozinc(II)

Crystal data

$[ZnI_2(C_6H_8N_2)_2]$
$M_r = 535.48$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.1825\ (7)$ Å
$b = 13.8144\ (10)$ Å
$c = 13.6242\ (10)$ Å
$\beta = 98.381\ (1)°$
$V = 1709.8\ (2)$ Å^3
$Z = 4$
$F(000) = 1008$
$D_x = 2.080$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2888 reflections
$\theta = 2.7–25.6°$
$\mu = 5.04$ mm^{-1}
$T = 170$ K
Rod, colorless
0.10 × 0.05 × 0.05 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
9413 measured reflections
3344 independent reflections
2518 reflections with $I > 2\sigma(I)$
$R_{int} = 0.109$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.1°$
$h = -11\rightarrow11$
$k = -17\rightarrow16$
$l = -9\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.069$
$S = 0.81$
3344 reflections
176 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0147P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} = 0.001$
H-atom parameters constrained	$\Delta\rho_{max} = 0.81$ e Å^{-3}
	$\Delta\rho_{min} = -1.28$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.07870 (6)	0.24556 (4)	0.76694 (4)	0.02508 (15)
I1	0.07868 (4)	0.15009 (3)	0.60725 (2)	0.03357 (11)
I2	0.19801 (4)	0.41101 (3)	0.79495 (2)	0.03516 (11)
N11	−0.1362 (4)	0.2579 (3)	0.7987 (3)	0.0244 (9)
N12	−0.4102 (4)	0.2602 (3)	0.8610 (3)	0.0290 (10)
N21	0.1716 (4)	0.1540 (3)	0.8789 (3)	0.0247 (9)
N22	0.3046 (4)	0.0275 (3)	1.0237 (3)	0.0283 (10)
C11	−0.2359 (5)	0.1893 (4)	0.7695 (3)	0.0262 (11)
H11	−0.2115	0.1387	0.7276	0.031*
C12	−0.3750 (5)	0.1903 (4)	0.7992 (3)	0.0274 (11)
C13	−0.3120 (5)	0.3282 (4)	0.8896 (3)	0.0280 (12)
C14	−0.1739 (5)	0.3274 (4)	0.8575 (3)	0.0278 (11)
H14	−0.1058	0.3778	0.8781	0.033*
C15	−0.4843 (5)	0.1130 (4)	0.7682 (4)	0.0361 (13)
H15A	−0.5043	0.0768	0.8267	0.054*
H15B	−0.4450	0.0688	0.7222	0.054*
H15C	−0.5758	0.1422	0.7351	0.054*
C16	−0.3539 (5)	0.4070 (4)	0.9555 (4)	0.0438 (15)
H16A	−0.4566	0.4258	0.9340	0.066*
H16B	−0.2898	0.4631	0.9515	0.066*
H16C	−0.3429	0.3837	1.0241	0.066*
C21	0.1310 (5)	0.0616 (4)	0.8802 (3)	0.0278 (12)
H21	0.0566	0.0385	0.8299	0.033*
C22	0.1950 (5)	−0.0025 (4)	0.9535 (3)	0.0302 (12)
C23	0.3442 (5)	0.1193 (4)	1.0219 (3)	0.0277 (12)
C24	0.2793 (5)	0.1839 (4)	0.9502 (3)	0.0265 (11)
H24	0.3112	0.2494	0.9515	0.032*
C25	0.1460 (6)	−0.1051 (4)	0.9560 (4)	0.0391 (14)
H25A	0.1946	−0.1436	0.9098	0.059*
H25B	0.0390	−0.1085	0.9366	0.059*

H25C	0.1720	−0.1308	1.0234	0.059*
C26	0.4667 (6)	0.1544 (4)	1.1002 (3)	0.0406 (14)
H26A	0.4261	0.1714	1.1606	0.061*
H26B	0.5133	0.2115	1.0756	0.061*
H26C	0.5401	0.1030	1.1152	0.061*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0246 (3)	0.0250 (3)	0.0258 (3)	0.0006 (2)	0.0044 (2)	0.0019 (3)
I1	0.0398 (2)	0.0359 (2)	0.02578 (18)	0.00179 (16)	0.00728 (14)	−0.00169 (16)
I2	0.0342 (2)	0.0259 (2)	0.0448 (2)	−0.00311 (15)	0.00379 (16)	0.00327 (16)
N11	0.023 (2)	0.027 (2)	0.023 (2)	0.0031 (18)	0.0014 (17)	0.0060 (19)
N12	0.028 (2)	0.034 (3)	0.026 (2)	0.005 (2)	0.0062 (18)	0.001 (2)
N21	0.025 (2)	0.027 (3)	0.0217 (19)	−0.0010 (18)	0.0039 (16)	0.0008 (19)
N22	0.028 (2)	0.030 (3)	0.026 (2)	0.002 (2)	0.0014 (18)	0.000 (2)
C11	0.022 (3)	0.028 (3)	0.027 (2)	0.004 (2)	−0.001 (2)	−0.002 (2)
C12	0.023 (3)	0.029 (3)	0.028 (3)	0.003 (2)	0.000 (2)	0.007 (2)
C13	0.029 (3)	0.030 (3)	0.025 (3)	0.004 (2)	0.004 (2)	0.003 (2)
C14	0.028 (3)	0.026 (3)	0.028 (3)	0.001 (2)	0.000 (2)	0.000 (2)
C15	0.024 (3)	0.038 (3)	0.045 (3)	−0.006 (3)	0.003 (2)	−0.008 (3)
C16	0.032 (3)	0.049 (4)	0.051 (3)	0.001 (3)	0.009 (3)	−0.011 (3)
C21	0.029 (3)	0.028 (3)	0.026 (3)	−0.003 (2)	0.004 (2)	−0.004 (2)
C22	0.032 (3)	0.029 (3)	0.030 (3)	0.000 (2)	0.008 (2)	−0.001 (2)
C23	0.030 (3)	0.032 (3)	0.021 (2)	−0.003 (2)	0.004 (2)	−0.004 (2)
C24	0.023 (2)	0.029 (3)	0.029 (3)	−0.001 (2)	0.008 (2)	−0.002 (2)
C25	0.050 (3)	0.030 (3)	0.034 (3)	−0.002 (3)	−0.003 (3)	0.007 (3)
C26	0.041 (3)	0.045 (4)	0.033 (3)	−0.008 (3)	−0.006 (2)	0.002 (3)

Geometric parameters (Å, º)

Zn1—N21	2.068 (4)	C15—H15A	0.9800
Zn1—N11	2.088 (4)	C15—H15B	0.9800
Zn1—I2	2.5393 (7)	C15—H15C	0.9800
Zn1—I1	2.5442 (6)	C16—H16A	0.9800
N11—C14	1.328 (6)	C16—H16B	0.9800
N11—C11	1.337 (6)	C16—H16C	0.9800
N12—C13	1.321 (6)	C21—C22	1.398 (7)
N12—C12	1.351 (6)	C21—H21	0.9500
N21—C21	1.331 (6)	C22—C25	1.489 (7)
N21—C24	1.346 (5)	C23—C24	1.392 (6)
N22—C23	1.321 (6)	C23—C26	1.513 (6)
N22—C22	1.348 (6)	C24—H24	0.9500
C11—C12	1.395 (7)	C25—H25A	0.9800
C11—H11	0.9500	C25—H25B	0.9800
C12—C15	1.485 (7)	C25—H25C	0.9800
C13—C14	1.401 (7)	C26—H26A	0.9800
C13—C16	1.496 (7)	C26—H26B	0.9800

C14—H14	0.9500	C26—H26C	0.9800
N21—Zn1—N11	101.39 (14)	H15B—C15—H15C	109.5
N21—Zn1—I2	108.49 (11)	C13—C16—H16A	109.5
N11—Zn1—I2	107.19 (12)	C13—C16—H16B	109.5
N21—Zn1—I1	105.22 (11)	H16A—C16—H16B	109.5
N11—Zn1—I1	109.72 (10)	C13—C16—H16C	109.5
I2—Zn1—I1	122.78 (2)	H16A—C16—H16C	109.5
C14—N11—C11	117.7 (4)	H16B—C16—H16C	109.5
C14—N11—Zn1	121.4 (3)	N21—C21—C22	121.8 (4)
C11—N11—Zn1	120.5 (3)	N21—C21—H21	119.1
C13—N12—C12	118.6 (4)	C22—C21—H21	119.1
C21—N21—C24	117.6 (4)	N22—C22—C21	120.3 (5)
C21—N21—Zn1	120.7 (3)	N22—C22—C25	118.2 (4)
C24—N21—Zn1	121.7 (3)	C21—C22—C25	121.5 (5)
C23—N22—C22	117.5 (4)	N22—C23—C24	122.5 (4)
N11—C11—C12	121.5 (5)	N22—C23—C26	118.2 (4)
N11—C11—H11	119.2	C24—C23—C26	119.2 (5)
C12—C11—H11	119.2	N21—C24—C23	120.3 (5)
N12—C12—C11	120.0 (5)	N21—C24—H24	119.9
N12—C12—C15	118.6 (4)	C23—C24—H24	119.9
C11—C12—C15	121.3 (5)	C22—C25—H25A	109.5
N12—C13—C14	120.8 (5)	C22—C25—H25B	109.5
N12—C13—C16	118.1 (4)	H25A—C25—H25B	109.5
C14—C13—C16	121.1 (5)	C22—C25—H25C	109.5
N11—C14—C13	121.4 (5)	H25A—C25—H25C	109.5
N11—C14—H14	119.3	H25B—C25—H25C	109.5
C13—C14—H14	119.3	C23—C26—H26A	109.5
C12—C15—H15A	109.5	C23—C26—H26B	109.5
C12—C15—H15B	109.5	H26A—C26—H26B	109.5
H15A—C15—H15B	109.5	C23—C26—H26C	109.5
C12—C15—H15C	109.5	H26A—C26—H26C	109.5
H15A—C15—H15C	109.5	H26B—C26—H26C	109.5