Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dibromido{2-[(4-iodophenyl)iminomethyl]pyridine-κ^2N,N'}zinc(II)

Saeed Dehghanpour,[a]* Ali Mahmoudi,[b] Mehdi Khalaj[b] and Sadegh Salmanpour[c]

[a]Department of Chemistry, Alzahra University, PO Box 1993891176, Vanak, Tehran, Iran, [b]Department of Chemistry, Islamic Azad University, Karaj Branch, Karaj, Iran, and [c]Department of Chemistry, Islamic Azad University, Sari Branch, Sari, Iran
Correspondence e-mail: Dehganpour_farasha@yahoo.com

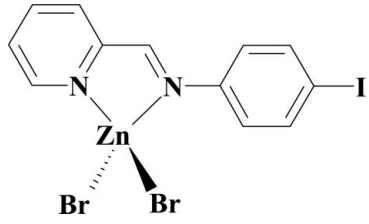
Received 15 October 2007; accepted 20 October 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.017; wR factor = 0.045; data-to-parameter ratio = 21.6.

The Zn^{II} centre in the title compound, $[ZnBr_2(C_{12}H_9IN_2)]$, is covalently bonded to two Br atoms and two N atoms of the diimine ligand in a distorted tetrahedral geometry.

Related literature

For related literature, see: Britovsek *et al.* (1999); Dehghanpour & Mahmoudi (2007*a*,*b*); Small *et al.* (1998).



Experimental

Crystal data

$[ZnBr_2(C_{12}H_9IN_2)]$
M_r = 533.30
Triclinic, $P\overline{1}$
a = 7.750 (2) Å
b = 8.831 (2) Å
c = 11.270 (3) Å
α = 89.44 (4)°
β = 71.66 (3)°
γ = 87.81 (4)°
V = 731.5 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 9.23 mm^{-1}
T = 100 (2) K
0.4 × 0.3 × 0.2 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.047, T_{max} = 0.160
13887 measured reflections
3520 independent reflections
3278 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.045
S = 1.00
3520 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −1.02 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—Br1	2.3422 (7)	Zn1—N1	2.0985 (19)
Zn1—Br2	2.3565 (7)	Zn1—N2	2.076 (2)
N2—Zn1—N1	80.87 (8)	N2—Zn1—Br2	109.60 (6)
N2—Zn1—Br1	122.39 (6)	N1—Zn1—Br2	109.69 (5)
N1—Zn1—Br1	117.40 (5)	Br1—Zn1—Br2	112.81 (2)

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

SD acknowledges the Alzahra University Research Council for partial support of this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2380).

References

Britovsek, G. J. P., Bruce, M., Gibson, V. C., Kimberley, B. S., Maddox, P. J., Mastroianni, S., Mctavish, S. J., Redshaw, C., Solan, G. A., Stromberg, S., White, A. J. P. & Williams, D. J. (1999). *J. Am. Chem. Soc.* **121**, 8728–8740.
Bruker (2005). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dehghanpour, S. & Mahmoudi, A. (2007*a*). *Acta Cryst.* E**63**, m1173–m1174.
Dehghanpour, S. & Mahmoudi, A. (2007*b*). *Synth. React. Inorg. Met.-Org. Chem.* **37**, 35–40.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Small, B. L., Brookhart, M. & Bennett, A. M. A. (1998). *J. Am. Chem. Soc.* **120**, 4049–4050.

  doi:10.1107/S1600536807051987

supplementary materials

Acta Cryst. (2007). E**63**, m2840 [**doi:10.1107/S1600536807051987**]

Dibromido{2-[(4-iodophenyl)iminomethyl]pyridine-κ^2N,N'}zinc(II)

S. Dehghanpour, A. Mahmoudi, M. Khalaj and S. Salmanpour

Comment

Pyridinecarbaldehyde and its substituted derivatives condense with amines to give a range of diimine compounds; iminopyridine ligands have been used to give adducts with transition metals. Among such complexes whose structures have been described are, for example, complexes of Cu^{I}, (Dehghanpour *et al.*, 2007), Co^{II}, (Small *et al.*, 2003) and Fe^{II}, (Britovsek *et al.*, 1999). The title complex, (I), was prepared by the reaction of $ZnBr_2$ with the bidentate ligand (4-iodo-phenyl)-pyridin-2-ylmethylene-amine.

Molecular structure of complex (I), as well as the atom-numbering scheme are shown in Fig. 1. A s one might expect for a four-coordinated zinc(II) complex, the metal center has a tetrahedral coordination. It shows signficant distortions mainly due to the presence of the 5-membered chelate cycle: the endocyclic N1—Zn1—N2 angle [80.87 (8)°] is much narrower than the ideal tetrahedral angle of 109.5°, whereas the N2—Zn1—Br1 angle [122.39 (6)°] is much wider than the ideal angle in the tetrahedron. The Zn1—Br1 and Zn1—Br2 bond lengths [2.3422 (7) and 2.3565 (7) Å respectively] are in good agreement with the Zn—Br distances in other tetrahedral zinc complexes, *e.g.* (Dehghanpour *et al.*, 2007*a*,b).

Experimental

To a solution of (4-iodo-phenyl)-pyridin-2-ylmethylene-amine (30.8 mg, 0.1 mmol) in 20 ml acetonitrile was added zinc bromide (22.5 mg, 0.1 mmol). The mixture was heated to dissolve the reactants. The solution was filtered and the volume of solvent removed under vacuum to about 5 ml. Diffusion of diethyl ether vapor into the solution gave yellow crystals. The crystals were collected and washed with diethylether-dichloromethane (9:1 *v*/*v*); yield 86%. Calc. for $C_{12}H_9Br_2IN_2Zn$: C 27.02, H 1.70, N 5.25%; found: C 27.01, H 1.72, N 5.26%.

Refinement

The H(C) atom positions were calculated. All hydrogen atoms were refined in isotropic approximation in riding model with the U_{iso}(H) parameters equal to 1.2 U_{eq}(Ci), for methyl groups equal to 1.5 U_{eq}(Cii), where U(Ci) and U(Cii) are respectively the equivalent thermal parameters of the carbon atoms to which corresponding H atoms are bonded.

Figures

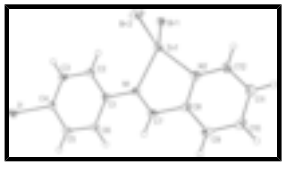


Fig. 1. Molecular structure of (I) showing the atom-labelling scheme with thermal ellipsoids drawn at the 50% probability level.

Dibromido{2-[(4-iodophenyl)iminomethyl]pyridine-κ^2N,N'}zinc(II)

Crystal data

$[ZnBr_2(C_{12}H_9IN_2)]$	$Z = 2$
$M_r = 533.30$	$F_{000} = 496$
Triclinic, $P\overline{1}$	$D_x = 2.421$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.750$ (2) Å	Cell parameters from 2531 reflections
$b = 8.831$ (2) Å	$\theta = 3$–29º
$c = 11.270$ (3) Å	$\mu = 9.23$ mm^{-1}
$\alpha = 89.44$ (4)º	$T = 100$ (2) K
$\beta = 71.66$ (3)º	Prism, yellow
$\gamma = 87.81$ (4)º	0.4 × 0.3 × 0.2 mm
$V = 731.5$ (3) Å^3	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	3520 independent reflections
Radiation source: fine-focus sealed tube	3278 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 100(2)$ K	$\theta_{max} = 28.0$º
φ and ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (APEX2; Bruker, 2005)	$h = -10 \rightarrow 10$
$T_{min} = 0.047$, $T_{max} = 0.160$	$k = -11 \rightarrow 11$
13887 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.017$	H-atom parameters constrained
$wR(F^2) = 0.045$	$w = 1/[\sigma^2(F_o^2) + (0.026P)^2 + 0.2955P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.029$
3520 reflections	$\Delta\rho_{max} = 0.85$ e Å^{-3}
163 parameters	$\Delta\rho_{min} = -1.02$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	1.162788 (19)	0.189540 (15)	−0.037792 (12)	0.01576 (5)
Br1	0.37752 (3)	0.15813 (2)	0.634148 (19)	0.01502 (6)
Zn1	0.60460 (3)	0.31017 (3)	0.65953 (2)	0.01325 (6)
Br2	0.81041 (3)	0.17579 (3)	0.74107 (2)	0.02209 (6)
N2	0.5476 (3)	0.5242 (2)	0.74024 (17)	0.0157 (4)
N1	0.7488 (2)	0.4397 (2)	0.50568 (16)	0.0132 (3)
C4	1.0254 (3)	0.2704 (2)	0.14462 (18)	0.0132 (4)
C7	0.7588 (3)	0.5783 (2)	0.53842 (19)	0.0140 (4)
H7	0.8354	0.6443	0.4833	0.017*
C9	0.6424 (3)	0.7819 (2)	0.6999 (2)	0.0159 (4)
H9	0.7115	0.8528	0.6457	0.019*
C5	1.0244 (3)	0.4260 (2)	0.1664 (2)	0.0163 (4)
H5	1.0843	0.4904	0.1021	0.020*
C3	0.9352 (3)	0.1728 (2)	0.2394 (2)	0.0152 (4)
H3	0.9352	0.0696	0.2236	0.018*
C1	0.8450 (3)	0.3866 (2)	0.38228 (19)	0.0129 (4)
C12	0.4418 (3)	0.5666 (3)	0.8544 (2)	0.0184 (4)
H12	0.3739	0.4940	0.9073	0.022*
C8	0.6478 (3)	0.6307 (2)	0.66368 (19)	0.0134 (4)
C6	0.9332 (3)	0.4841 (2)	0.2848 (2)	0.0157 (4)
H6	0.9307	0.5878	0.2993	0.019*
C2	0.8443 (3)	0.2307 (2)	0.35850 (19)	0.0152 (4)
H2	0.7833	0.1660	0.4222	0.018*
C11	0.4295 (3)	0.7156 (3)	0.8972 (2)	0.0201 (5)
H11	0.3543	0.7416	0.9770	0.024*
C10	0.5314 (3)	0.8245 (3)	0.8187 (2)	0.0184 (4)
H10	0.5254	0.9245	0.8453	0.022*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01789 (8)	0.01469 (8)	0.01293 (7)	−0.00300 (5)	−0.00197 (5)	−0.00125 (5)

Br1	0.01511 (11)	0.01407 (11)	0.01579 (10)	−0.00331 (8)	−0.00439 (8)	−0.00009 (8)
Zn1	0.01469 (12)	0.01014 (12)	0.01407 (12)	−0.00238 (9)	−0.00313 (9)	0.00119 (9)
Br2	0.02248 (12)	0.01486 (11)	0.03382 (13)	−0.00357 (9)	−0.01568 (10)	0.00575 (9)
N2	0.0154 (9)	0.0155 (9)	0.0167 (9)	−0.0014 (7)	−0.0055 (7)	0.0001 (7)
N1	0.0125 (8)	0.0125 (9)	0.0135 (8)	0.0003 (7)	−0.0029 (7)	0.0015 (7)
C4	0.0114 (9)	0.0157 (10)	0.0118 (9)	−0.0004 (8)	−0.0026 (8)	−0.0015 (7)
C7	0.0140 (10)	0.0131 (10)	0.0152 (10)	−0.0016 (8)	−0.0049 (8)	0.0035 (8)
C9	0.0178 (11)	0.0132 (10)	0.0189 (10)	−0.0033 (8)	−0.0089 (8)	0.0024 (8)
C5	0.0173 (11)	0.0139 (10)	0.0156 (10)	−0.0023 (8)	−0.0020 (8)	0.0032 (8)
C3	0.0188 (11)	0.0088 (10)	0.0175 (10)	−0.0019 (8)	−0.0049 (8)	−0.0009 (8)
C1	0.0121 (10)	0.0126 (10)	0.0140 (9)	−0.0013 (8)	−0.0038 (8)	0.0002 (7)
C12	0.0175 (11)	0.0178 (11)	0.0174 (10)	−0.0040 (9)	−0.0017 (8)	−0.0009 (8)
C8	0.0137 (10)	0.0125 (10)	0.0157 (10)	0.0000 (8)	−0.0072 (8)	0.0006 (8)
C6	0.0179 (11)	0.0098 (10)	0.0170 (10)	−0.0013 (8)	−0.0022 (8)	0.0017 (8)
C2	0.0166 (10)	0.0141 (10)	0.0132 (9)	−0.0027 (8)	−0.0021 (8)	0.0029 (8)
C11	0.0180 (11)	0.0219 (12)	0.0187 (11)	−0.0007 (9)	−0.0030 (9)	−0.0040 (9)
C10	0.0205 (11)	0.0134 (10)	0.0229 (11)	0.0004 (9)	−0.0088 (9)	−0.0033 (8)

Geometric parameters (Å, °)

Zn1—Br1	2.3422 (7)	C9—H9	0.9300
Zn1—Br2	2.3565 (7)	C5—C6	1.391 (3)
Zn1—N1	2.0985 (19)	C5—H5	0.9300
Zn1—N2	2.076 (2)	C3—C2	1.396 (3)
I1—C4	2.112 (2)	C3—H3	0.9300
N2—C12	1.338 (3)	C1—C6	1.404 (3)
N2—C8	1.360 (3)	C1—C2	1.405 (3)
N1—C7	1.294 (3)	C12—C11	1.395 (3)
N1—C1	1.430 (3)	C12—H12	0.9300
C4—C3	1.389 (3)	C6—H6	0.9300
C4—C5	1.398 (3)	C2—H2	0.9300
C7—C8	1.471 (3)	C11—C10	1.391 (3)
C7—H7	0.9300	C11—H11	0.9300
C9—C10	1.391 (3)	C10—H10	0.9300
C9—C8	1.395 (3)		
N2—Zn1—N1	80.87 (8)	C4—C3—C2	119.6 (2)
N2—Zn1—Br1	122.39 (6)	C4—C3—H3	120.2
N1—Zn1—Br1	117.40 (5)	C2—C3—H3	120.2
N2—Zn1—Br2	109.60 (6)	C6—C1—C2	119.60 (19)
N1—Zn1—Br2	109.69 (5)	C6—C1—N1	122.62 (19)
Br1—Zn1—Br2	112.81 (2)	C2—C1—N1	117.74 (18)
C12—N2—C8	118.44 (19)	N2—C12—C11	122.6 (2)
C12—N2—Zn1	130.10 (16)	N2—C12—H12	118.7
C8—N2—Zn1	111.26 (14)	C11—C12—H12	118.7
C7—N1—C1	121.34 (18)	N2—C8—C9	122.2 (2)
C7—N1—Zn1	111.01 (14)	N2—C8—C7	116.11 (19)
C1—N1—Zn1	127.26 (14)	C9—C8—C7	121.6 (2)
C3—C4—C5	120.86 (19)	C5—C6—C1	120.1 (2)
C3—C4—I1	121.24 (16)	C5—C6—H6	119.9

C5—C4—I1	117.88 (16)	C1—C6—H6	119.9
N1—C7—C8	119.40 (19)	C3—C2—C1	120.1 (2)
N1—C7—H7	120.3	C3—C2—H2	119.9
C8—C7—H7	120.3	C1—C2—H2	119.9
C10—C9—C8	118.7 (2)	C10—C11—C12	118.9 (2)
C10—C9—H9	120.6	C10—C11—H11	120.5
C8—C9—H9	120.6	C12—C11—H11	120.5
C6—C5—C4	119.7 (2)	C11—C10—C9	119.1 (2)
C6—C5—H5	120.1	C11—C10—H10	120.5
C4—C5—H5	120.1	C9—C10—H10	120.5
N1—Zn1—N2—C12	176.7 (2)	Zn1—N1—C1—C2	0.4 (3)
Br1—Zn1—N2—C12	60.0 (2)	C8—N2—C12—C11	0.6 (3)
Br2—Zn1—N2—C12	−75.5 (2)	Zn1—N2—C12—C11	174.89 (17)
N1—Zn1—N2—C8	−8.61 (14)	C12—N2—C8—C9	−0.6 (3)
Br1—Zn1—N2—C8	−125.35 (13)	Zn1—N2—C8—C9	−175.99 (16)
Br2—Zn1—N2—C8	99.15 (14)	C12—N2—C8—C7	−178.84 (19)
N2—Zn1—N1—C7	10.45 (15)	Zn1—N2—C8—C7	5.8 (2)
Br1—Zn1—N1—C7	132.31 (14)	C10—C9—C8—N2	0.4 (3)
Br2—Zn1—N1—C7	−97.20 (15)	C10—C9—C8—C7	178.5 (2)
N2—Zn1—N1—C1	−176.65 (18)	N1—C7—C8—N2	3.5 (3)
Br1—Zn1—N1—C1	−54.80 (18)	N1—C7—C8—C9	−174.7 (2)
Br2—Zn1—N1—C1	75.70 (17)	C4—C5—C6—C1	1.0 (3)
C1—N1—C7—C8	175.94 (18)	C2—C1—C6—C5	−2.1 (3)
Zn1—N1—C7—C8	−10.7 (2)	N1—C1—C6—C5	−179.8 (2)
C3—C4—C5—C6	0.6 (3)	C4—C3—C2—C1	−0.3 (3)
I1—C4—C5—C6	179.06 (16)	C6—C1—C2—C3	1.8 (3)
C5—C4—C3—C2	−0.9 (3)	N1—C1—C2—C3	179.57 (19)
I1—C4—C3—C2	−179.36 (16)	N2—C12—C11—C10	−0.3 (4)
C7—N1—C1—C6	−9.6 (3)	C12—C11—C10—C9	0.1 (3)
Zn1—N1—C1—C6	178.16 (16)	C8—C9—C10—C11	−0.1 (3)
C7—N1—C1—C2	172.7 (2)		

Fig. 1