

Dibromido(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')zinc(II)

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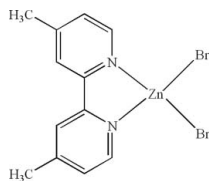
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Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(C-C) = 0.005$ Å; R factor = 0.039; wR factor = 0.099; data-to-parameter ratio = 22.8.

The asymmetric unit of the title compound, $[ZnBr_2(C_{12}H_{12}N_2)]$, contains two half-molecules; both are completed by crystallographic twofold axes running through the Zn^{II} atoms which are coordinated by an N,N' -bidentate 4,4'-dimethyl-2,2'-bipyridine ligand and two Br^- ions, resulting in distorted ZnN_2Br_2 tetrahedral coordination geometries. In the crystal, $C-H \cdots Br$ interactions link the molecules.

Related literature

For related structures, see: Ahmadi *et al.* (2008); Amani *et al.* (2009); Bellusci *et al.* (2008); Hojjat Kashani *et al.* (2008); Kalateh *et al.* (2008, 2010); Sakamoto *et al.* (2004); Sofetis *et al.* (2006); Willett *et al.* (2001); Yoshikawa *et al.* (2003); Yousefi *et al.* (2008).



Experimental

Crystal data

$[ZnBr_2(C_{12}H_{12}N_2)]$

$M_r = 409.43$

Monoclinic, $P2_1/c$

$a = 13.801$ (3) Å

$b = 8.2454$ (16) Å

$c = 13.716$ (3) Å

$\beta = 117.47$ (3)°

$V = 1384.9$ (6) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 7.52$ mm⁻¹

$T = 120$ K

$0.30 \times 0.22 \times 0.10$ mm

Data collection

Bruker SMART CCD diffractometer

Absorption correction: multi-scan

(*SADABS*; Bruker, 1998)

$T_{\min} = 0.157$, $T_{\max} = 0.479$

8352 measured reflections

3560 independent reflections

2963 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.050$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.099$

$S = 1.07$

3560 reflections

156 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.62$ e Å⁻³

$\Delta\rho_{\text{min}} = -1.04$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1–N1	2.053 (3)	Zn1–Br1	2.3428 (6)
Zn2–N2	2.050 (3)	Zn2–Br2	2.3356 (9)

N1–Zn1–N1 ⁱ	80.61 (17)	N2–Zn2–N2 ⁱⁱ	81.15 (17)
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Symmetry codes: (i) $-x + 1, y, -z + \frac{1}{2}$; (ii) $-x, y, -z + \frac{1}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C10–H10A \cdots Br1 ⁱⁱⁱ	0.96	2.89	3.772 (5)	152

Symmetry code: (iii) $x, y - 1, z$.

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5556).

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supplementary materials

Acta Cryst. (2010). E66, m996 [doi:10.1107/S1600536810028692]

Dibromido(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')zinc(II)

R. Alizadeh, P. Mohammadi Eshlaghi and V. Amani

Comment

4,4'-Dimethyl-2,2'-bipyridine (4,4'-dmbipy), is a good bidentate ligand, and numerous complexes with 4,4'-dmbipy have been prepared, such as that of mercury (Kalateh *et al.*, 2008; Yousefi *et al.*, 2008), indium (Ahmadi *et al.*, 2008), iron (Amani *et al.*, 2009), platinum (Hojjat Kashani *et al.*, 2008), manganese (Sakamoto *et al.*, 2004), silver (Bellusci *et al.*, 2008), gallium (Sofetis *et al.*, 2006), copper (Willett *et al.*, 2001), iridium (Yoshikawa *et al.*, 2003) and cadmium (Kalateh *et al.*, 2010). Here, we report the synthesis and structure of the title compound.

The asymmetric unit of the title compound, (Fig. 1), contains two half-molecule. The Zn^{II} atom is four-coordinated in distorted tetragonal configurations by two N atoms from one 4,4'-dimethyl-2,2'-bipyridine and two Br atoms. The Zn—Br and Zn—N bond lengths and angles are collected in Table 1.

In the crystal structure, intermolecular C—H \cdots Br hydrogen bonds (Table 2) may stabilize the structure (Fig. 2).

Experimental

A solution of 4,4'-dimethyl-2,2'-bipyridine (0.20 g, 1.10 mmol) in methanol (10 ml) was added to a solution of ZnBr₂ (0.25 g, 1.10 mmol) in methanol (5 ml) at room temperature. Colourless prisms of (I) were obtained by methanol diffusion to a colorless solution in DMSO. Suitable crystals were isolated after one week (yield; 0.35 g, 77.7%).

Refinement

All H atoms were positioned geometrically, with C—H = 0.93 Å and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

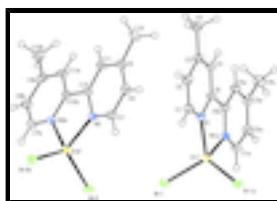


Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level. Atoms with suffix a are generated by (1-x, y, 1/2-z); those with suffix b are generated by (-x, y, 1/2-z).

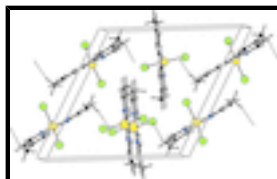


Fig. 2. Unit-cell packing diagram for (I). Hydrogen bonds are shown as dashed lines.

Dibromido(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')zinc(II)

Crystal data

$[ZnBr_2(C_{12}H_{12}N_2)]$	$F(000) = 792$
$M_r = 409.43$	$D_x = 1.964 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: $-P 2_1c$	Cell parameters from 984 reflections
$a = 13.801 (3) \text{ \AA}$	$\theta = 2.5\text{--}29.2^\circ$
$b = 8.2454 (16) \text{ \AA}$	$\mu = 7.52 \text{ mm}^{-1}$
$c = 13.716 (3) \text{ \AA}$	$T = 120 \text{ K}$
$\beta = 117.47 (3)^\circ$	Prism, colorless
$V = 1384.9 (6) \text{ \AA}^3$	$0.30 \times 0.22 \times 0.10 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD diffractometer	3560 independent reflections
Radiation source: fine-focus sealed tube graphite	2963 reflections with $I > 2\sigma(I)$
phi and ω scans	$R_{\text{int}} = 0.050$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$\theta_{\text{max}} = 29.2^\circ$, $\theta_{\text{min}} = 2.5^\circ$
$T_{\text{min}} = 0.157$, $T_{\text{max}} = 0.479$	$h = -13 \rightarrow 18$
8352 measured reflections	$k = -11 \rightarrow 11$
	$l = -18 \rightarrow 17$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.039$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.099$	H-atom parameters constrained
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 2.823P]$
3560 reflections	where $P = (F_o^2 + 2F_c^2)/3$
156 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.62 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -1.04 \text{ e \AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.3828 (3)	0.7308 (4)	0.0326 (3)	0.0225 (7)
H1	0.3650	0.8327	0.0001	0.027*
C2	0.3490 (3)	0.5946 (5)	-0.0343 (3)	0.0251 (8)
H2	0.3082	0.6056	-0.1101	0.030*
C3	0.3767 (3)	0.4417 (4)	0.0131 (3)	0.0234 (7)
C4	0.3428 (4)	0.2903 (5)	-0.0556 (4)	0.0313 (9)
H4A	0.2979	0.2252	-0.0345	0.038*
H4B	0.4065	0.2299	-0.0444	0.038*
H4C	0.3022	0.3191	-0.1318	0.038*
C5	0.4366 (3)	0.4324 (4)	0.1268 (3)	0.0220 (7)
H5	0.4562	0.3319	0.1611	0.026*
C6	0.4671 (3)	0.5733 (4)	0.1892 (3)	0.0185 (7)
C7	0.1273 (3)	0.7510 (4)	0.1512 (3)	0.0231 (7)
H7	0.1512	0.8521	0.1411	0.028*
C8	0.1556 (3)	0.6153 (5)	0.1110 (3)	0.0236 (7)
H8	0.1977	0.6260	0.0746	0.028*
C9	0.1209 (3)	0.4623 (4)	0.1250 (3)	0.0208 (7)
C10	0.1447 (4)	0.3130 (5)	0.0775 (4)	0.0287 (8)
H10C	0.1371	0.3370	0.0058	0.034*
H10B	0.0943	0.2289	0.0718	0.034*
H10A	0.2179	0.2774	0.1244	0.034*
C11	0.0594 (3)	0.4535 (4)	0.1817 (3)	0.0218 (7)
H11	0.0357	0.3534	0.1938	0.026*
C12	0.0334 (3)	0.5942 (4)	0.2202 (3)	0.0181 (7)
N1	0.4399 (3)	0.7211 (3)	0.1415 (3)	0.0186 (6)
N2	0.0668 (3)	0.7419 (3)	0.2042 (3)	0.0186 (6)
Zn1	0.5000	0.91089 (6)	0.2500	0.02024 (14)
Zn2	0.0000	0.93068 (6)	0.2500	0.01997 (14)
Br1	0.37461 (4)	1.05907 (4)	0.28513 (4)	0.02607 (11)
Br2	0.12396 (4)	1.07654 (4)	0.40271 (4)	0.02828 (11)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0274 (19)	0.0185 (15)	0.0221 (19)	0.0011 (14)	0.0119 (16)	0.0019 (13)
C2	0.0263 (19)	0.0284 (18)	0.0186 (18)	-0.0019 (15)	0.0085 (15)	-0.0024 (14)
C3	0.0261 (19)	0.0232 (16)	0.0232 (19)	-0.0021 (14)	0.0134 (16)	-0.0059 (14)

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C4	0.035 (2)	0.0265 (18)	0.026 (2)	-0.0044 (17)	0.0089 (18)	-0.0115 (16)
C5	0.0271 (19)	0.0141 (14)	0.0249 (19)	-0.0016 (13)	0.0121 (16)	-0.0035 (12)
C6	0.0262 (18)	0.0125 (13)	0.0187 (18)	-0.0021 (12)	0.0118 (15)	-0.0013 (12)
C7	0.0268 (19)	0.0184 (15)	0.025 (2)	-0.0015 (14)	0.0127 (16)	0.0010 (13)
C8	0.028 (2)	0.0240 (16)	0.025 (2)	0.0003 (15)	0.0171 (17)	0.0010 (14)
C9	0.0227 (18)	0.0196 (15)	0.0191 (18)	0.0039 (13)	0.0087 (15)	-0.0007 (13)
C10	0.033 (2)	0.0238 (17)	0.033 (2)	0.0066 (16)	0.0183 (19)	-0.0023 (15)
C11	0.0289 (19)	0.0138 (14)	0.0249 (19)	0.0006 (13)	0.0142 (16)	-0.0001 (12)
C12	0.0227 (17)	0.0133 (14)	0.0192 (18)	0.0012 (12)	0.0104 (15)	0.0003 (11)
N1	0.0222 (15)	0.0147 (12)	0.0177 (15)	-0.0004 (11)	0.0082 (12)	-0.0013 (10)
N2	0.0253 (16)	0.0129 (12)	0.0175 (15)	-0.0004 (11)	0.0097 (13)	0.0004 (10)
Zn1	0.0277 (3)	0.0107 (2)	0.0231 (3)	0.000	0.0123 (3)	0.000
Zn2	0.0274 (3)	0.0106 (2)	0.0212 (3)	0.000	0.0106 (3)	0.000
Br1	0.0329 (2)	0.01709 (16)	0.0322 (2)	0.00397 (14)	0.01838 (17)	0.00109 (14)
Br2	0.0317 (2)	0.01954 (17)	0.0281 (2)	-0.00180 (14)	0.00900 (17)	-0.00723 (14)

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

C1—N1	1.332 (5)	C8—H8	0.9300
C1—C2	1.388 (5)	C9—C11	1.394 (5)
C1—H1	0.9300	C9—C10	1.498 (5)
C2—C3	1.388 (5)	C10—H10C	0.9600
C2—H2	0.9300	C10—H10B	0.9600
C3—C5	1.390 (6)	C10—H10A	0.9600
C3—C4	1.503 (5)	C11—C12	1.389 (5)
C4—H4A	0.9600	C11—H11	0.9300
C4—H4B	0.9600	C12—N2	1.355 (4)
C4—H4C	0.9600	C12—C12 ⁱⁱ	1.488 (7)
C5—C6	1.387 (5)	Zn1—N1	2.053 (3)
C5—H5	0.9300	Zn2—N2	2.050 (3)
C6—N1	1.351 (4)	Zn1—N1 ⁱ	2.053 (3)
C6—C6 ⁱ	1.487 (8)	Zn1—Br1 ⁱ	2.3428 (6)
C7—N2	1.339 (5)	Zn1—Br1	2.3428 (6)
C7—C8	1.380 (5)	Zn2—N2 ⁱⁱ	2.050 (3)
C7—H7	0.9300	Zn2—Br2	2.3356 (9)
C8—C9	1.393 (5)	Zn2—Br2 ⁱⁱ	2.3356 (9)
N1—C1—C2	122.5 (3)	C9—C10—H10C	109.5
N1—C1—H1	118.7	C9—C10—H10B	109.5
C2—C1—H1	118.7	H10C—C10—H10B	109.5
C1—C2—C3	119.3 (4)	C9—C10—H10A	109.5
C1—C2—H2	120.4	H10C—C10—H10A	109.5
C3—C2—H2	120.4	H10B—C10—H10A	109.5
C2—C3—C5	117.9 (3)	C12—C11—C9	120.0 (3)
C2—C3—C4	121.4 (4)	C12—C11—H11	120.0
C5—C3—C4	120.6 (4)	C9—C11—H11	120.0
C3—C4—H4A	109.5	N2—C12—C11	121.5 (3)
C3—C4—H4B	109.5	N2—C12—C12 ⁱⁱ	115.6 (2)

H4A—C4—H4B	109.5	C11—C12—C12 ⁱⁱ	122.9 (2)
C3—C4—H4C	109.5	C1—N1—C6	119.0 (3)
H4A—C4—H4C	109.5	C1—N1—Zn1	126.8 (2)
H4B—C4—H4C	109.5	C6—N1—Zn1	114.1 (2)
C6—C5—C3	120.0 (3)	C7—N2—C12	118.8 (3)
C6—C5—H5	120.0	C7—N2—Zn2	127.2 (2)
C3—C5—H5	120.0	C12—N2—Zn2	113.5 (2)
N1—C6—C5	121.3 (4)	N1—Zn1—N1 ⁱ	80.61 (17)
N1—C6—C6 ⁱ	115.6 (2)	N1—Zn1—Br1 ⁱ	109.77 (9)
C5—C6—C6 ⁱ	123.1 (2)	N1 ⁱ —Zn1—Br1 ⁱ	117.20 (9)
N2—C7—C8	122.2 (3)	N1—Zn1—Br1	117.20 (9)
N2—C7—H7	118.9	N1 ⁱ —Zn1—Br1	109.77 (9)
C8—C7—H7	118.9	Br1 ⁱ —Zn1—Br1	117.13 (3)
C7—C8—C9	120.1 (3)	N2—Zn2—N2 ⁱⁱ	81.15 (17)
C7—C8—H8	119.9	N2—Zn2—Br2	114.76 (9)
C9—C8—H8	119.9	N2 ⁱⁱ —Zn2—Br2	111.31 (9)
C8—C9—C11	117.4 (3)	N2—Zn2—Br2 ⁱⁱ	111.31 (9)
C8—C9—C10	121.8 (3)	N2 ⁱⁱ —Zn2—Br2 ⁱⁱ	114.76 (9)
C11—C9—C10	120.8 (3)	Br2—Zn2—Br2 ⁱⁱ	118.01 (4)
N1—C1—C2—C3	-1.1 (6)	C6 ⁱ —C6—N1—Zn1	1.4 (5)
C1—C2—C3—C5	0.8 (6)	C8—C7—N2—C12	0.9 (6)
C1—C2—C3—C4	-179.6 (4)	C8—C7—N2—Zn2	-170.8 (3)
C2—C3—C5—C6	-0.2 (6)	C11—C12—N2—C7	-0.8 (6)
C4—C3—C5—C6	-179.9 (4)	C12 ⁱⁱ —C12—N2—C7	179.9 (4)
C3—C5—C6—N1	-0.2 (6)	C11—C12—N2—Zn2	172.0 (3)
C3—C5—C6—C6 ⁱ	-178.8 (4)	C12 ⁱⁱ —C12—N2—Zn2	-7.3 (5)
N2—C7—C8—C9	0.0 (6)	C1—N1—Zn1—N1 ⁱ	-177.6 (4)
C7—C8—C9—C11	-1.0 (6)	C6—N1—Zn1—N1 ⁱ	-0.5 (2)
C7—C8—C9—C10	176.7 (4)	C1—N1—Zn1—Br1 ⁱ	-62.0 (3)
C8—C9—C11—C12	1.0 (6)	C6—N1—Zn1—Br1 ⁱ	115.1 (3)
C10—C9—C11—C12	-176.7 (4)	C1—N1—Zn1—Br1	74.9 (3)
C9—C11—C12—N2	-0.2 (6)	C6—N1—Zn1—Br1	-108.0 (3)
C9—C11—C12—C12 ⁱⁱ	179.1 (4)	C7—N2—Zn2—N2 ⁱⁱ	174.8 (4)
C2—C1—N1—C6	0.7 (6)	C12—N2—Zn2—N2 ⁱⁱ	2.71 (19)
C2—C1—N1—Zn1	177.7 (3)	C7—N2—Zn2—Br2	-75.8 (3)
C5—C6—N1—C1	-0.1 (6)	C12—N2—Zn2—Br2	112.2 (3)
C6 ⁱ —C6—N1—C1	178.7 (4)	C7—N2—Zn2—Br2 ⁱⁱ	61.5 (3)
C5—C6—N1—Zn1	-177.4 (3)	C12—N2—Zn2—Br2 ⁱⁱ	-110.5 (3)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C10—H10A \cdots Br1 ⁱⁱⁱ	0.96	2.89	3.772 (5)	152

supplementary materials

Symmetry codes: (iii) $x, y-1, z$.

Fig. 1

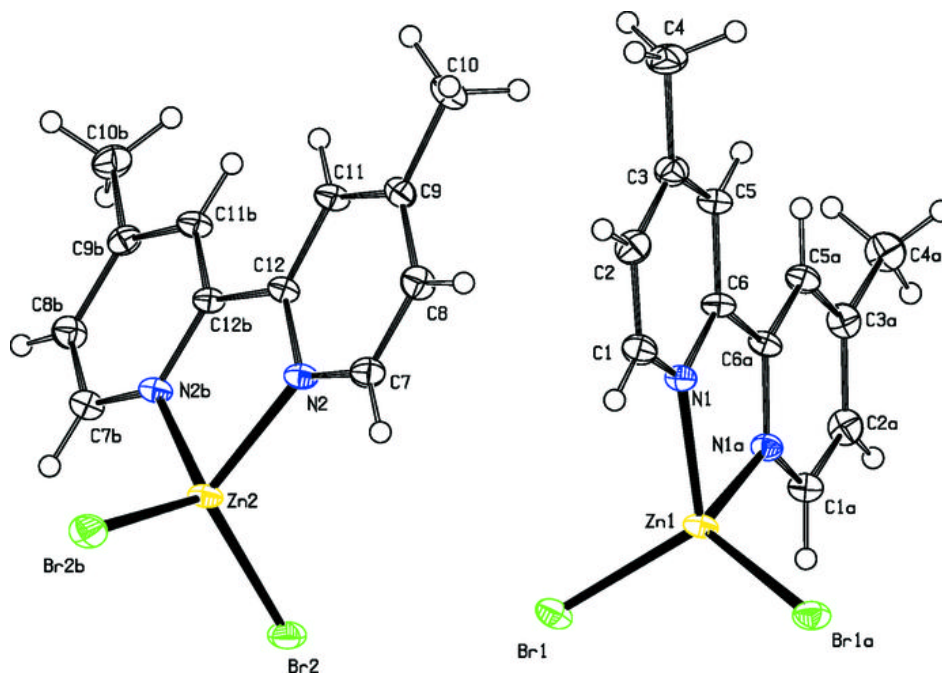


Fig. 2

