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Dibromido(6-methyl-2,2′-bipyridine-κ^2N,N')zinc(II)

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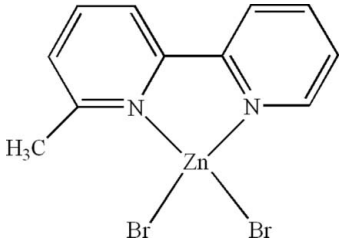
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.016 Å; R factor = 0.086; wR factor = 0.207; data-to-parameter ratio = 24.6.

In the title compound, $[ZnBr_2(C_{11}H_{10}N_2)]$, the Zn^{II} atom is four-coordinated in a distorted tetrahedral configuration by two N atoms from a 6-methyl-2,2′-bipyridine ligand and two terminal Br atoms. Weak intermolecular C—H···Br hydrogen bonds and π–π stacking interactions between the pyridine rings [centroid–centroid distances = 3.763 (5) and 3.835 (6) Å] contribute to crystal-packing effects.

Related literature

For unusual coordination geometries on transition metal atoms, see: Beeston *et al.* (1998), Meyer *et al.* (1999); For related literature, see: Ahmadi *et al.* (2009); Ahmadi, Ebadi *et al.* (2008); Ahmadi, Kalateh *et al.* (2008); Alizadeh *et al.* (2009); Amani *et al.* (2009); Newkome *et al.* (1982); Onggo *et al.* (1990, 2005).



Experimental

Crystal data

$[ZnBr_2(C_{11}H_{10}N_2)]$
M_r = 395.40
Monoclinic, $P2_1/n$
a = 7.6445 (7) Å
b = 9.7487 (11) Å
c = 17.8347 (18) Å
β = 96.972 (8)°
V = 1319.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 7.89 mm^{-1}
T = 298 K
0.46 × 0.30 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.076, T_{max} = 0.310
15389 measured reflections
3567 independent reflections
2498 reflections with $I > 2\sigma(I)$
R_{int} = 0.119

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.086
$wR(F^2)$ = 0.207
S = 1.13
3567 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.14 e Å^{-3}
$\Delta\rho_{min}$ = −1.14 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1*C*···Br1^{i}	0.96	2.86	3.805 (14)	169
C8—H8···Br1^{ii}	0.93	2.93	3.812 (12)	159

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

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: JJ2041).

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supporting information

Acta Cryst. (2010). E**66**, m1241 [doi:10.1107/S1600536810035658]

Dibromido(6-methyl-2,2′-bipyridine-κ^2N,N')zinc(II)

Khadijeh Kalateh, Roya Ahmadi and Vahid Amani

S1. Comment

Sterically hindered ligands such as 6-Methyl-2, 2′-bipyridine (6-mbipy) often convey unusual coordination geometries or oxidation states on transition metal centers (Beeston *et al.*, 1998; Meyer *et al.* 1999). Numerous complexes with 6-mbipy have been prepared, such as that of mercury (Ahmadi, Ebadi *et al.*, 2008), platin (Amani *et al.*, 2009), lead (Ahmadi *et al.*, 2009), palladium (Newkome *et al.*, 1982), ruthenium (Onggo, Scudder *et al.*, 2005) and iron (Onggo, Hook *et al.*, 1990). Here, we report the synthesis and structure of the title compound, $[Zn(C_{11}H_{10}N_2)Br_2]$.

In the title compound (Fig. 1), the Zn^{II} atom is four-coordinated in a distorted tetrahedral configuration by two N atoms from one 6-methyl-2,2′-bipyridine and two terminal Br atoms. The Zn—N and Zn—Br bond lengths and angles are within the normal range of $[ZnCl_2(6\text{-mbpy})]$, (Ahmadi, Kalateh *et al.*, 2008) and $[ZnBr_2(6,6'\text{-dmbpy})]$, (Alizadeh *et al.*, 2009) [where 6,6′-dmbpy is 6,6′-dimethyl-2, 2′-bipyridine] respectively.

In the crystal structure, weak intermolecular C—H···Br hydrogen bonds (Table 2) and $\pi\cdots\pi$ stacking interactions (Fig. 2, Table 1) between the pyridine rings,*Cg*1—*Cg*2 and *Cg*2—*Cg*3 contribute to crystal packing effects [where *Cg*1, *Cg*2 and *Cg*3 are centroids of the rings (Zn1/N1/C6—C7/N2), (N1/C2—C6) and (N2/C7—C11), respectively].

S2. Experimental

For the preparation of the title compound, a solution of 6-methyl-2,2′-bipyridine (0.16 g, 0.15 ml 0.94 mmol) in methanol (10 ml) was added to a solution of $ZnBr_2$ (0.21 g, 0.94 mmol) in acetonitrile (30 ml) and the resulting colorless solution was stirred for 20 min at 313 K. This solution was left to evaporate slowly at room temperature. After one week, colorless prismatic crystals of the title compound were isolated (yield 0.28 g, 75.3%).

S3. Refinement

All H atoms were positioned geometrically, with C—H = 0.93Å for aromatics H, C—H = 0.96Å for methyl and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}$. High values for $\Delta\rho$ are related to the poor quality of the crystals.

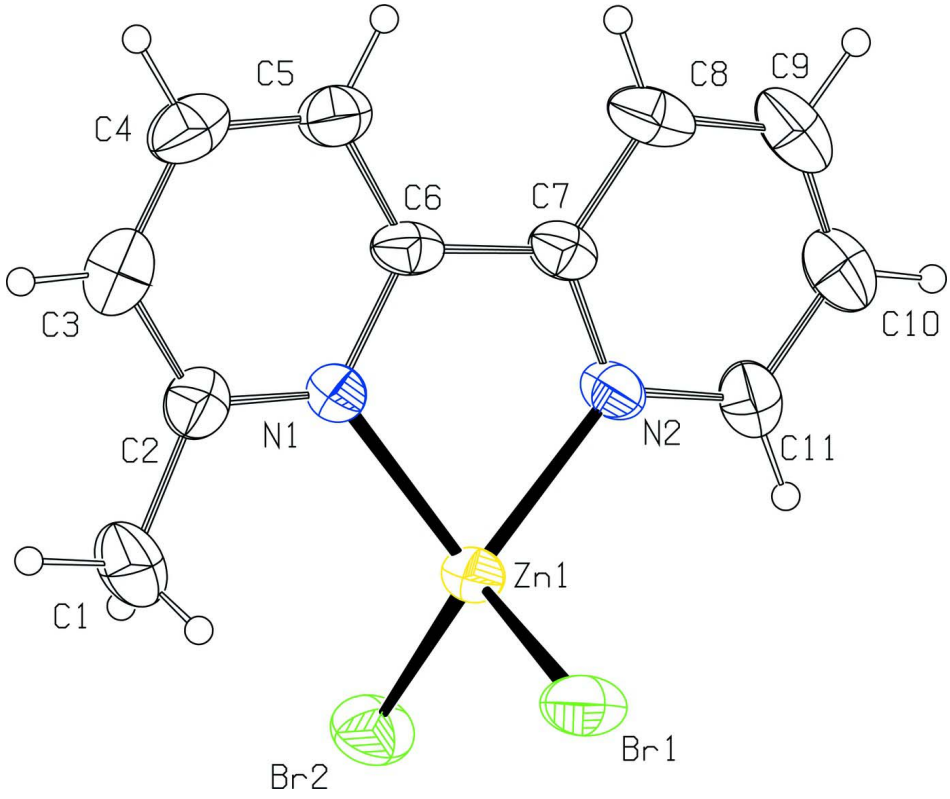

Figure 1

The molecular structure of the title molecule, [Zn($C_{11}H_{10}N_2$)Br_2], with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

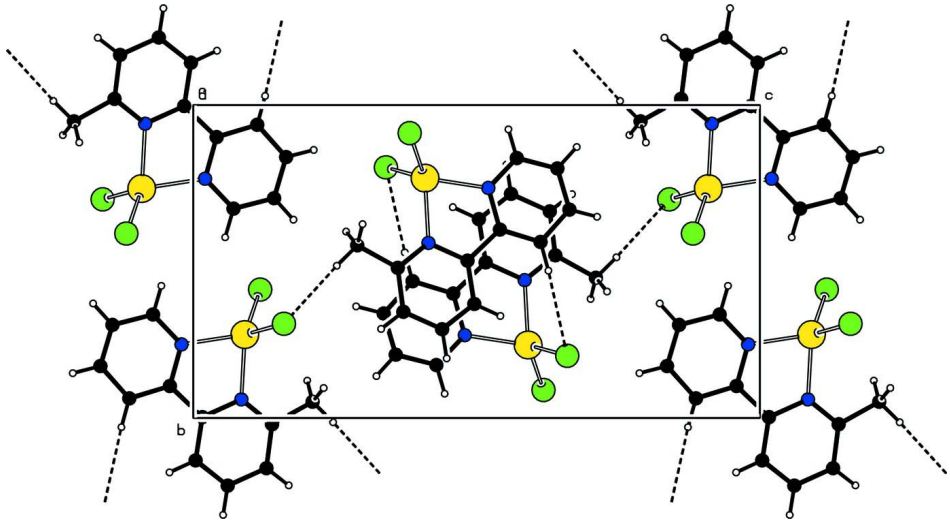

Figure 2

Unit-cell packing diagram for [Zn($C_{11}H_{10}N_2$)Br_2]. Dashed lines indicate weak C—H···Br intermolecular interactions.

Dibromido(6-methyl-2,2′-bipyridine-κ^2N,N')zinc(II)

Crystal data

$[ZnBr_2(C_{11}H_{10}N_2)]$
$M_r = 395.40$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.6445$ (7) Å
$b = 9.7487$ (11) Å
$c = 17.8347$ (18) Å
$\beta = 96.972$ (8)°
$V = 1319.3$ (2) Å^3
$Z = 4$
$F(000) = 760$
$D_x = 1.991$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 985 reflections
$\theta = 2.3$–$29.4°$
$\mu = 7.89$ mm^{-1}
$T = 298$ K
Prism, colorless
0.46 × 0.30 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.076$, $T_{max} = 0.310$
15389 measured reflections
3567 independent reflections
2498 reflections with $I > 2\sigma(I)$
$R_{int} = 0.119$
$\theta_{max} = 29.4°$, $\theta_{min} = 2.3°$
$h = -8 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.086$
$wR(F^2) = 0.207$
$S = 1.13$
3567 reflections
145 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 8.4252P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 2.14$ e Å^{-3}
$\Delta\rho_{min} = -1.14$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.651 (2)	0.9482 (15)	0.2106 (6)	0.099 (5)
H1A	0.7590	0.9042	0.2302	0.119*
H1B	0.5594	0.8805	0.2012	0.119*
H1C	0.6183	1.0135	0.2468	0.119*

C2	0.6740 (14)	1.0200 (10)	0.1390 (6)	0.063 (2)
C3	0.6519 (15)	1.1604 (12)	0.1292 (7)	0.074 (3)
H3	0.6227	1.2153	0.1685	0.089*
C4	0.6738 (15)	1.2162 (11)	0.0608 (8)	0.075 (3)
H4	0.6559	1.3097	0.0527	0.090*
C5	0.7221 (13)	1.1355 (10)	0.0041 (6)	0.063 (2)
H5	0.7415	1.1739	−0.0419	0.076*
C6	0.7415 (11)	0.9971 (9)	0.0160 (5)	0.051 (2)
C7	0.7873 (11)	0.8977 (10)	−0.0412 (5)	0.0509 (19)
C8	0.8184 (14)	0.9373 (12)	−0.1129 (6)	0.070 (3)
H8	0.8168	1.0293	−0.1268	0.084*
C9	0.8523 (16)	0.8339 (15)	−0.1639 (6)	0.080 (3)
H9	0.8735	0.8568	−0.2126	0.096*
C10	0.8542 (18)	0.7025 (14)	−0.1426 (6)	0.080 (3)
H10	0.8736	0.6339	−0.1768	0.097*
C11	0.8280 (15)	0.6692 (12)	−0.0710 (6)	0.072 (3)
H11	0.8344	0.5776	−0.0563	0.087*
N1	0.7182 (10)	0.9406 (7)	0.0849 (4)	0.0508 (17)
N2	0.7930 (10)	0.7647 (8)	−0.0208 (4)	0.0530 (17)
Br1	1.04853 (15)	0.69883 (13)	0.15998 (7)	0.0756 (4)
Br2	0.54078 (15)	0.58954 (13)	0.11809 (7)	0.0767 (4)
Zn1	0.76827 (14)	0.73342 (11)	0.09099 (6)	0.0525 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.147 (13)	0.102 (10)	0.056 (6)	0.016 (9)	0.040 (8)	−0.011 (6)
C2	0.063 (6)	0.057 (5)	0.068 (6)	0.004 (5)	0.010 (5)	−0.004 (5)
C3	0.061 (6)	0.070 (7)	0.088 (8)	0.006 (5)	0.001 (5)	−0.018 (6)
C4	0.071 (7)	0.051 (5)	0.102 (9)	0.003 (5)	0.005 (6)	0.013 (6)
C5	0.063 (6)	0.056 (5)	0.070 (6)	0.003 (5)	0.008 (5)	0.015 (5)
C6	0.038 (4)	0.058 (5)	0.056 (5)	−0.005 (4)	−0.001 (3)	0.021 (4)
C7	0.045 (4)	0.063 (5)	0.043 (4)	−0.006 (4)	0.002 (3)	0.009 (4)
C8	0.060 (6)	0.089 (7)	0.058 (6)	−0.018 (5)	0.002 (5)	0.028 (5)
C9	0.076 (7)	0.122 (11)	0.046 (5)	−0.016 (7)	0.018 (5)	−0.005 (6)
C10	0.091 (8)	0.098 (9)	0.056 (6)	−0.006 (7)	0.021 (6)	−0.010 (6)
C11	0.081 (7)	0.073 (7)	0.068 (6)	0.007 (6)	0.029 (6)	−0.004 (5)
N1	0.052 (4)	0.050 (4)	0.052 (4)	0.004 (3)	0.015 (3)	0.008 (3)
N2	0.059 (4)	0.059 (4)	0.042 (3)	−0.001 (4)	0.012 (3)	0.008 (3)
Br1	0.0576 (6)	0.0870 (8)	0.0815 (7)	0.0001 (5)	0.0052 (5)	0.0382 (6)
Br2	0.0673 (7)	0.0768 (7)	0.0878 (8)	−0.0131 (5)	0.0173 (6)	0.0197 (6)
Zn1	0.0560 (6)	0.0509 (6)	0.0528 (6)	0.0038 (5)	0.0149 (4)	0.0129 (4)

Geometric parameters (Å, º)

C1—C2	1.486 (16)	C7—N2	1.346 (11)
C1—H1A	0.9600	C7—C8	1.383 (12)
C1—H1B	0.9600	C8—C9	1.402 (17)

C1—H1C	0.9600	C8—H8	0.9300
C2—N1	1.312 (12)	C9—C10	1.335 (18)
C2—C3	1.388 (15)	C9—H9	0.9300
C3—C4	1.364 (17)	C10—C11	1.355 (15)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.368 (16)	C11—N2	1.342 (13)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.370 (13)	N1—Zn1	2.057 (7)
C5—H5	0.9300	N2—Zn1	2.048 (7)
C6—N1	1.378 (10)	Br1—Zn1	2.3617 (16)
C6—C7	1.480 (13)	Br2—Zn1	2.3300 (15)
Cg1···Cg2^{i}	3.762 (5)	Cg2···Cg3^{ii}	3.835 (6)
C2—C1—H1A	109.5	C7—C8—C9	117.7 (10)
C2—C1—H1B	109.5	C7—C8—H8	121.2
H1A—C1—H1B	109.5	C9—C8—H8	121.2
C2—C1—H1C	109.5	C10—C9—C8	120.1 (10)
H1A—C1—H1C	109.5	C10—C9—H9	120.0
H1B—C1—H1C	109.5	C8—C9—H9	120.0
N1—C2—C3	121.8 (10)	C9—C10—C11	120.0 (11)
N1—C2—C1	115.0 (9)	C9—C10—H10	120.0
C3—C2—C1	123.2 (10)	C11—C10—H10	120.0
C4—C3—C2	118.7 (11)	N2—C11—C10	121.8 (11)
C4—C3—H3	120.7	N2—C11—H11	119.1
C2—C3—H3	120.7	C10—C11—H11	119.1
C3—C4—C5	120.3 (10)	C2—N1—C6	119.5 (8)
C3—C4—H4	119.8	C2—N1—Zn1	127.1 (6)
C5—C4—H4	119.8	C6—N1—Zn1	113.3 (6)
C4—C5—C6	119.1 (10)	C11—N2—C7	119.4 (8)
C4—C5—H5	120.5	C11—N2—Zn1	126.6 (7)
C6—C5—H5	120.5	C7—N2—Zn1	113.8 (6)
C5—C6—N1	120.5 (9)	N2—Zn1—N1	80.9 (3)
C5—C6—C7	124.6 (8)	N2—Zn1—Br2	116.8 (2)
N1—C6—C7	114.9 (8)	N1—Zn1—Br2	117.6 (2)
N2—C7—C8	121.0 (9)	N2—Zn1—Br1	110.1 (2)
N2—C7—C6	116.5 (7)	N1—Zn1—Br1	108.6 (2)
C8—C7—C6	122.4 (9)	Br2—Zn1—Br1	117.30 (6)
N1—C2—C3—C4	1.2 (17)	C5—C6—N1—Zn1	−176.7 (7)
C1—C2—C3—C4	−179.0 (12)	C7—C6—N1—Zn1	3.4 (9)
C2—C3—C4—C5	−2.1 (18)	C10—C11—N2—C7	−1.4 (17)
C3—C4—C5—C6	2.5 (17)	C10—C11—N2—Zn1	−175.1 (9)
C4—C5—C6—N1	−2.0 (15)	C8—C7—N2—C11	−0.5 (14)
C4—C5—C6—C7	177.9 (9)	C6—C7—N2—C11	177.8 (9)
C5—C6—C7—N2	−177.1 (9)	C8—C7—N2—Zn1	174.0 (7)
N1—C6—C7—N2	2.9 (11)	C6—C7—N2—Zn1	−7.7 (10)
C5—C6—C7—C8	1.2 (14)	C11—N2—Zn1—N1	−178.6 (9)

N1—C6—C7—C8	−178.8 (8)	C7—N2—Zn1—N1	7.4 (6)
N2—C7—C8—C9	1.3 (15)	C11—N2—Zn1—Br2	−62.2 (9)
C6—C7—C8—C9	−176.9 (9)	C7—N2—Zn1—Br2	123.7 (6)
C7—C8—C9—C10	−0.1 (17)	C11—N2—Zn1—Br1	74.8 (9)
C8—C9—C10—C11	−2 (2)	C7—N2—Zn1—Br1	−99.2 (6)
C9—C10—C11—N2	3 (2)	C2—N1—Zn1—N2	176.6 (9)
C3—C2—N1—C6	−0.8 (15)	C6—N1—Zn1—N2	−5.8 (6)
C1—C2—N1—C6	179.5 (10)	C2—N1—Zn1—Br2	61.0 (9)
C3—C2—N1—Zn1	176.7 (8)	C6—N1—Zn1—Br2	−121.3 (5)
C1—C2—N1—Zn1	−3.0 (14)	C2—N1—Zn1—Br1	−75.2 (8)
C5—C6—N1—C2	1.2 (13)	C6—N1—Zn1—Br1	102.5 (6)
C7—C6—N1—C2	−178.7 (8)		

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*; (ii) −*x*+2, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*C*···Br1^{iii}	0.96	2.86	3.805 (14)	169
C8—H8···Br1^{ii}	0.93	2.93	3.812 (12)	159

Symmetry codes: (ii) −*x*+2, −*y*+2, −*z*; (iii) −*x*+3/2, *y*+1/2, −*z*+1/2.