Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dibromido(2,2′:6′,2″-terpyridine-κ^3N,N',N'')zinc(II)

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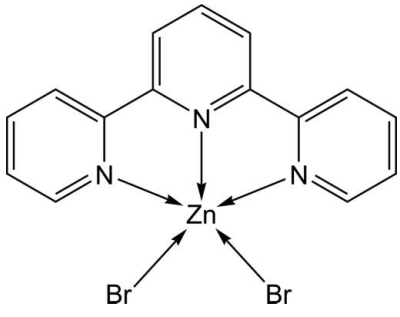
Received 5 May 2009; accepted 21 May 2009

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.015; wR factor = 0.039; data-to-parameter ratio = 15.0.

In the title compound, $[ZnBr_2(C_{15}H_{11}N_3)]$, the Zn^{II} ion is five-coordinated by the three N atoms from a 2,2′:6′,2″-terpyridine ligand (terpy) and two bromide anions in a distorted trigonal bipyramidal configuration. Each molecule is situated on a twofold rotational axis that passes through the Zn^{II} ion and the central ring of the terpy ligand. In the crystal structure, aromatic π–π interactions between terpy ligands [centroid–centroid distances = 3.6265 (9) Å] link molecules into stacks propagated in the [001] direction.

Related literature

For related structures, see: Alizadeh *et al.* (2009); Mahmoudi *et al.* (2009); Huang *et al.* (2009); Ma *et al.* (2009); Bai *et al.* (2009).



Experimental

Crystal data

$[ZnBr_2(C_{15}H_{11}N_3)]$
M_r = 458.46
Monoclinic, $C2/c$
a = 17.0972 (5) Å
b = 9.3528 (3) Å
c = 11.5334 (4) Å
β = 126.051 (1)°
V = 1491.08 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 7.00 mm^{-1}
T = 296 K
0.20 × 0.18 × 0.16 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.335, T_{max} = 0.401
(expected range = 0.273–0.326)
9665 measured reflections
1457 independent reflections
1371 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.039
S = 1.08
1457 reflections
97 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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*.

The authors are grateful to the Henan Administration of Science and Technology for financial support (grant No. 092300410031).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2561).

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supporting information

Acta Cryst. (2009). E**65**, m693 [doi:10.1107/S1600536809019266]

Dibromido(2,2′:6′,2″-terpyridine-κ^3N,N',N'')zinc(II)

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S1. Comment

As a contribution to structural characterization of 2,2′:6′,2″-terpyridine complexes (Alizadeh *et al.*, 2009; Huang *et al.*, 2009; Ma *et al.*, 2009; Bai *et al.*, 2009) we present here the title complex (I).

In (I) (Fig. 1), the Zn^{II} ion is five-coordinated in a distorted trigonal bipyramidal configuration by three N atoms from a 2,2′:6′,2″-terpyridine ligand and by two Br anions. The Zn–Br and Zn–N bond lengths are within normal ranges (Mahmoudi *et al.*, 2009).

In the crystal structure, the π–π stacking interactions between aromatic rings of *Cg*1 and *Cg*2 [*Cg*1 and *Cg*2 are (N1, C6 — C8, $C7^i$, $C6^i$) and (N2, C1 — C5) ring centroids, respectively, symmetry code: (i) $-x + 1, y, -z + 1/2$] are observed, with a centroid–centroid distances of 3.6265 (9) Å.

S2. Experimental

The title compound was synthesized hydrothermally in a Teflon-lined autoclave (25 mL) by heating a mixture of 2,2′:6′,2″-terpyridine (0.2 mmol), $ZnBr_2$ (0.2 mmol) and one drop of Et_3N (pH ≃ 8–9) in water (10 mL) at 393 K for 3 d. Crystals suitable for X-ray analysis were obtained.

S3. Refinement

All H atoms were included in calculated positions, with C—H distances fixed to 0.93 Å and were refined in the riding-model approximation, with $U_{iso}(H) = 1.2\ U_{eq}$ (C).

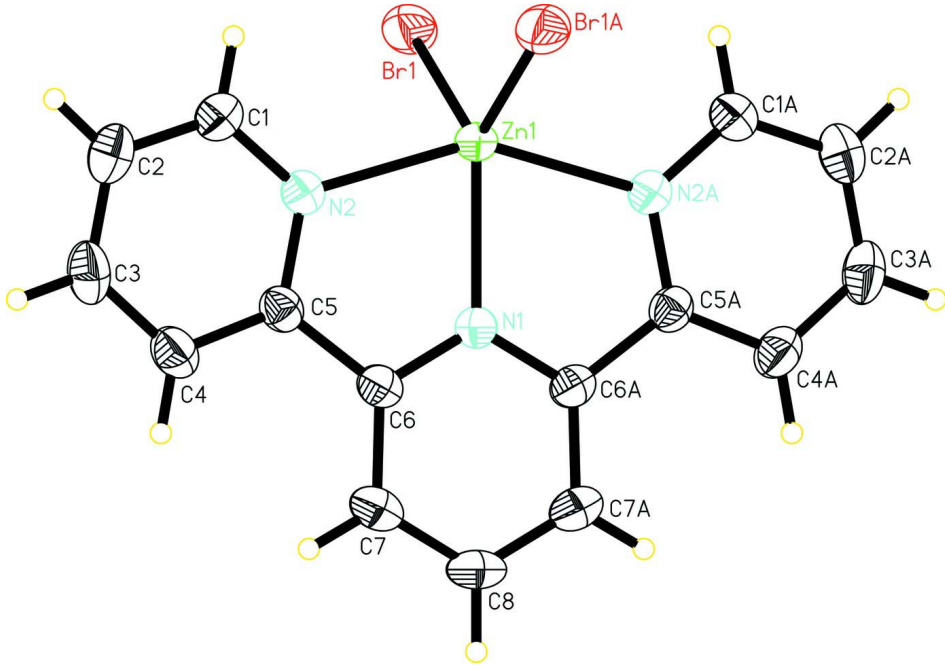

Figure 1

The molecular structure of the title compound with the atom-labelling scheme [symmetry code: (A) -*x*, + 1, *y*, -*z* + 1/2]. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

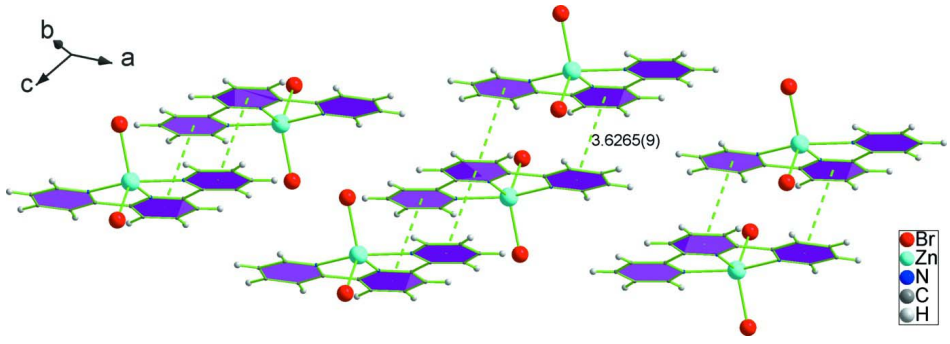

Figure 2

A portion of the crystal packing showing the π–π interactions (dashed lines) between the aromatic rings.

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Crystal data

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Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 17.0972 (5) Å
b = 9.3528 (3) Å
c = 11.5334 (4) Å
β = 126.051 (1)°
V = 1491.08 (8) Å^3
Z = 4
F(000) = 888
D_x = 2.042 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 1580 reflections
θ = 2.5–26.3°
μ = 7.00 mm^{-1}
T = 296 K
Block, colourless
0.20 × 0.18 × 0.16 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.335, T_{max} = 0.401
9665 measured reflections
1457 independent reflections
1371 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 26.0°, θ_{min} = 2.6°
h = −21→21
k = −11→11
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.039
S = 1.08
1457 reflections
97 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
$w = 1/[\sigma^2(F_o^2) + (0.0184P)^2 + 1.2604P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 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}
Br1	0.380531 (15)	0.11870 (2)	0.03979 (2)	0.04022 (8)
Zn1	0.5000	0.25499 (3)	0.2500	0.02736 (8)
N1	0.5000	0.4802 (2)	0.2500	0.0253 (4)
N2	0.58982 (11)	0.31649 (16)	0.18054 (15)	0.0288 (3)
C1	0.63375 (14)	0.2248 (2)	0.1474 (2)	0.0352 (4)
H1	0.6256	0.1272	0.1525	0.042*
C2	0.69093 (14)	0.2696 (2)	0.1056 (2)	0.0392 (4)
H2	0.7210	0.2033	0.0838	0.047*
C3	0.70254 (14)	0.4137 (2)	0.0970 (2)	0.0394 (4)
H3	0.7411	0.4461	0.0700	0.047*
C4	0.65606 (13)	0.5102 (2)	0.12890 (18)	0.0346 (4)
H4	0.6620	0.6081	0.1219	0.042*
C5	0.60056 (12)	0.45792 (18)	0.17152 (16)	0.0268 (4)
C6	0.54892 (12)	0.55136 (18)	0.21013 (16)	0.0263 (3)
C7	0.54910 (13)	0.69976 (19)	0.20701 (19)	0.0337 (4)
H7	0.5815	0.7485	0.1767	0.040*

C8	0.5000	0.7736 (3)	0.2500	0.0367 (6)
H8	0.5000	0.8730	0.2500	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.04910 (14)	0.03300 (12)	0.03959 (12)	−0.01116 (8)	0.02667 (10)	−0.00711 (7)
Zn1	0.03545 (17)	0.01984 (14)	0.03395 (16)	0.000	0.02441 (14)	0.000
N1	0.0293 (10)	0.0231 (10)	0.0253 (9)	0.000	0.0170 (9)	0.000
N2	0.0322 (8)	0.0264 (8)	0.0335 (7)	−0.0007 (6)	0.0224 (7)	0.0004 (6)
C1	0.0407 (11)	0.0311 (10)	0.0417 (10)	0.0025 (8)	0.0285 (9)	−0.0011 (8)
C2	0.0372 (11)	0.0487 (12)	0.0398 (10)	0.0025 (9)	0.0271 (9)	−0.0038 (9)
C3	0.0354 (10)	0.0545 (12)	0.0380 (10)	−0.0069 (9)	0.0271 (9)	−0.0022 (9)
C4	0.0367 (10)	0.0359 (10)	0.0339 (9)	−0.0072 (8)	0.0222 (8)	0.0005 (8)
C5	0.0268 (9)	0.0287 (9)	0.0235 (7)	−0.0027 (7)	0.0139 (7)	0.0004 (7)
C6	0.0274 (9)	0.0247 (8)	0.0237 (7)	−0.0027 (7)	0.0133 (7)	0.0007 (6)
C7	0.0360 (10)	0.0268 (9)	0.0351 (9)	−0.0042 (8)	0.0193 (8)	0.0030 (7)
C8	0.0426 (16)	0.0201 (12)	0.0409 (14)	0.000	0.0210 (13)	0.000

Geometric parameters (Å, º)

Br1—Zn1	2.4179 (2)	C2—H2	0.9300
Zn1—N1	2.106 (2)	C3—C4	1.388 (3)
Zn1—N2^{i}	2.1861 (14)	C3—H3	0.9300
Zn1—N2	2.1861 (14)	C4—C5	1.389 (2)
Zn1—Br1^{i}	2.4179 (2)	C4—H4	0.9300
N1—C6^{i}	1.3441 (19)	C5—C6	1.485 (2)
N1—C6	1.3441 (19)	C6—C7	1.388 (3)
N2—C1	1.336 (2)	C7—C8	1.385 (2)
N2—C5	1.348 (2)	C7—H7	0.9300
C1—C2	1.385 (3)	C8—C7^{i}	1.385 (2)
C1—H1	0.9300	C8—H8	0.9300
C2—C3	1.374 (3)		
N1—Zn1—N2^{i}	74.75 (4)	C3—C2—H2	120.5
N1—Zn1—N2	74.75 (4)	C1—C2—H2	120.5
N2^{i}—Zn1—N2	149.49 (8)	C2—C3—C4	119.27 (17)
N1—Zn1—Br1	121.815 (7)	C2—C3—H3	120.4
N2^{i}—Zn1—Br1	98.34 (4)	C4—C3—H3	120.4
N2—Zn1—Br1	97.60 (4)	C3—C4—C5	118.78 (18)
N1—Zn1—Br1^{i}	121.815 (7)	C3—C4—H4	120.6
N2^{i}—Zn1—Br1^{i}	97.60 (4)	C5—C4—H4	120.6
N2—Zn1—Br1^{i}	98.34 (4)	N2—C5—C4	121.69 (16)
Br1—Zn1—Br1^{i}	116.370 (14)	N2—C5—C6	114.99 (14)
C6^{i}—N1—C6	120.6 (2)	C4—C5—C6	123.32 (16)
C6^{i}—N1—Zn1	119.68 (10)	N1—C6—C7	121.01 (16)
C6—N1—Zn1	119.68 (10)	N1—C6—C5	114.25 (15)
C1—N2—C5	118.88 (15)	C7—C6—C5	124.74 (15)

C1—N2—Zn1	124.80 (12)	C8—C7—C6	118.57 (17)
C5—N2—Zn1	116.32 (11)	C8—C7—H7	120.7
N2—C1—C2	122.43 (18)	C6—C7—H7	120.7
N2—C1—H1	118.8	C7^{i}—C8—C7	120.2 (2)
C2—C1—H1	118.8	C7^{i}—C8—H8	119.9
C3—C2—C1	118.93 (18)	C7—C8—H8	119.9
N2^{i}—Zn1—N1—C6^{i}	0.68 (9)	C1—C2—C3—C4	−0.6 (3)
N2—Zn1—N1—C6^{i}	−179.32 (9)	C2—C3—C4—C5	1.3 (3)
Br1—Zn1—N1—C6^{i}	91.12 (8)	C1—N2—C5—C4	−0.1 (2)
Br1^{i}—Zn1—N1—C6^{i}	−88.88 (8)	Zn1—N2—C5—C4	179.88 (12)
N2^{i}—Zn1—N1—C6	−179.32 (9)	C1—N2—C5—C6	179.87 (15)
N2—Zn1—N1—C6	0.68 (9)	Zn1—N2—C5—C6	−0.19 (18)
Br1—Zn1—N1—C6	−88.88 (8)	C3—C4—C5—N2	−0.9 (3)
Br1^{i}—Zn1—N1—C6	91.12 (8)	C3—C4—C5—C6	179.12 (16)
N1—Zn1—N2—C1	179.71 (15)	C6^{i}—N1—C6—C7	−0.96 (12)
N2^{i}—Zn1—N2—C1	179.71 (15)	Zn1—N1—C6—C7	179.04 (12)
Br1—Zn1—N2—C1	−59.30 (14)	C6^{i}—N1—C6—C5	179.02 (15)
Br1^{i}—Zn1—N2—C1	58.90 (14)	Zn1—N1—C6—C5	−0.98 (15)
N1—Zn1—N2—C5	−0.23 (11)	N2—C5—C6—N1	0.74 (19)
N2^{i}—Zn1—N2—C5	−0.23 (11)	C4—C5—C6—N1	−179.33 (14)
Br1—Zn1—N2—C5	120.76 (11)	N2—C5—C6—C7	−179.29 (16)
Br1^{i}—Zn1—N2—C5	−121.05 (11)	C4—C5—C6—C7	0.6 (3)
C5—N2—C1—C2	0.8 (3)	N1—C6—C7—C8	1.9 (2)
Zn1—N2—C1—C2	−179.16 (14)	C5—C6—C7—C8	−178.10 (13)
N2—C1—C2—C3	−0.4 (3)	C6—C7—C8—C7^{i}	−0.91 (11)

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.