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[*N*,*N*′-Bis(2,6-dichlorobenzylidene)-propane-1,3-diamine-κ^2N,N']dibromidozinc

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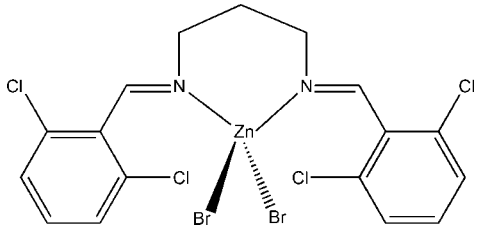
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.053; data-to-parameter ratio = 23.3.

In the title compound, $[ZnBr_2(C_{17}H_{14}Cl_4N_2)]$, the Zn^{II} ion is bonded to two bromide ions and two N atoms of the diimine ligand and displays a moderately distorted tetrahedral coordination geometry. The Schiff base ligand acts as a chelating ligand and coordinates to the Zn^{II} atom *via* two N atoms.

Related literature

For related structures, see: Khalaj *et al.* (2008, 2009); Salehzadeh *et al.* (2011); Khalaji *et al.* (2010, 2011, 2012). For properties and application of complexes of symmetric bidentate Schiff base ligands, see: Komatsu *et al.* (2007); Montazerozohori *et al.* (2011). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[ZnBr_2(C_{17}H_{14}Cl_4N_2)]$
M_r = 613.3
Monoclinic, $P2_1/c$
a = 17.0433 (3) Å
b = 9.3216 (2) Å
c = 13.6038 (2) Å
β = 97.313 (2)°
V = 2143.67 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.38 mm^{-1}
T = 120 K
0.33 × 0.28 × 0.10 mm

Data collection

Agilent Xcalibur diffractometer with an Atlas (Gemini ultra Cu) detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.5, T_{max} = 1
32456 measured reflections
5469 independent reflections
4344 reflections with $I > 3\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 3\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.053
S = 1.32
5469 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—Br1	2.3599 (3)	Zn1—N1	2.0662 (16)
Zn1—Br2	2.3371 (3)	Zn1—N2	2.0628 (16)

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *JANA2006* (Petříček *et al.*, 2006); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *JANA2006*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5947).

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supporting information

Acta Cryst. (2012). E**68**, m971 [https://doi.org/10.1107/S1600536812027997]

[*N*,*N*′-Bis(2,6-dichlorobenzylidene)propane-1,3-diamine-κ^2N,N']dibromidozinc

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S1. Comment

Complexes of symmetric bidentate Schiff base ligands with transition metals have attracted much attention because of their catalytic (Komatsu *et al.*, 2007) and thermal properties (Montazerozohori *et al.*, 2011). There is substantial interest in the coordination chemistry of the zinc(II) ion (Khalaj *et al.*, 2008, 2009; Salehzadeh *et al.*,2011; Khalaji *et al.*,2010, 2011, 2012).

The molecular structure of **1** with the atom-numbering scheme is presented in Fig. 1, and the bond lengths and angles are generally normal (Allen *et al*., 1987). The zinc(II) ion is coordinated by the bidentate Schiff-base ligand and two Br ions. Although a tetrahedral geometry might be expected for a four coordinated zinc(II) centre, the geometry around the zinc(II) ion is distorted by the bite angle N1—Zn1—N2 [90.24 (6)°] of the chelating ligand. On the contrary the Br1—Zn11—Br2 angle has opened up to 120.866 (11)°. The N—Zn—Br angles are also distorted from the tetrahedral values.

S2. Experimental

To a stirring solution of the (2,6-Cl-ba)$_2$en ligand (1 mmol, in 5 ml of chloroform) was added $ZnBr_2$ (1 mmol) in 10 ml of methanol and the mixture was stirred for 10 min in air at room temperature and was then left at 273 K for several days without disturbance yielding suitable crystals that subsequently were filtered off and washed with Et_2O.

S3. Refinement

All H atoms were positioned geometrically and treated as riding on their parent atoms. The displacement coefficients U_{iso}(H) were set to 1.2U_{eq}(C).

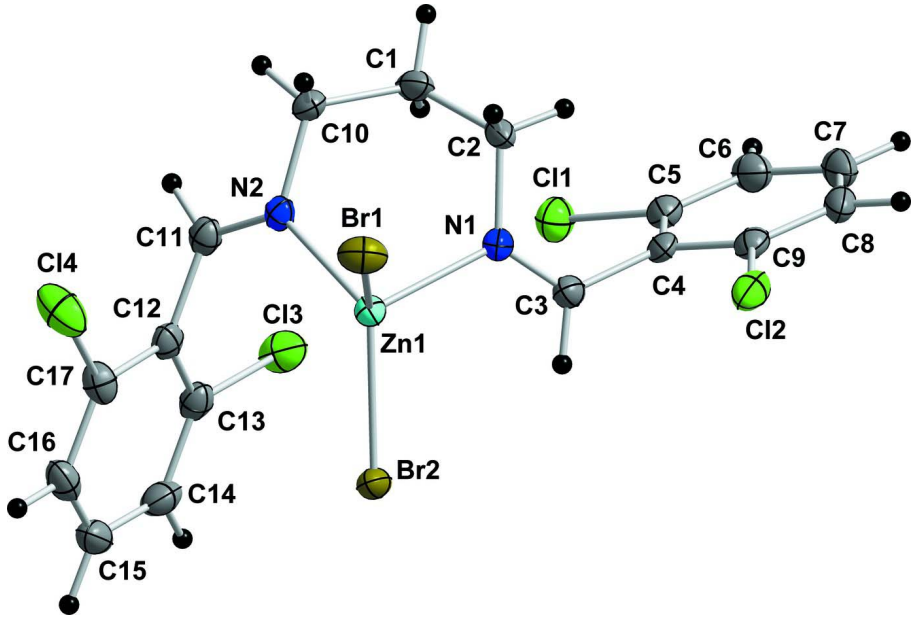

Figure 1

The molecular structure of 1. Displacement ellipsoids are drawn at the 50% probability level.

[*N*,*N*′-Bis(2,6-dichlorobenzylidene)propane-1,3- diamine-κ^2N,*N*′]dibromidozinc

Crystal data

$[ZnBr_2(C_{17}H_{14}Cl_4N_2)]$
M_r = 613.3
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 17.0433 (3) Å
b = 9.3216 (2) Å
c = 13.6038 (2) Å
β = 97.313 (2)°
V = 2143.67 (7) Å^3
Z = 4
$F(000)$ = 1192
D_x = 1.900 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.7107 Å
Cell parameters from 14022 reflections
θ = 3.0–29.3°
μ = 5.38 mm^{-1}
T = 120 K
Block, colourless
0.33 × 0.28 × 0.10 mm

Data collection

Agilent Xcalibur diffractometer with an Atlas (Gemini ultra Cu) detector
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 10.3784 pixels mm^{-1}
Rotation method data acquisition using ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.5, T_{max} = 1
32456 measured reflections
5469 independent reflections
4344 reflections with $I > 3\sigma(I)$
R_{int} = 0.032
θ_{max} = 29.4°, θ_{min} = 3.0°
h = −21→23
k = −12→12
l = −18→17

Refinement

Refinement on F^2
$R[F > 3\sigma(F)]$ = 0.023
$wR(F)$ = 0.053
S = 1.32
5469 reflections
235 parameters
0 restraints
56 constraints
H-atom parameters constrained

Weighting scheme based on measured s.u.'s $w = 1/(\sigma^2(I) + 0.0004I^2)$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

Special details

Experimental. Absorption correction: CrysAlisPro (Agilent Technologies, 2011) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Refinement. The refinement was carried out against all reflections. The conventional *R*-factor is always based on *F*. The goodness of fit as well as the weighted *R*-factor are based on *F* and F^2 for refinement carried out on *F* and F^2, respectively. The threshold expression is used only for calculating *R*-factors *etc*. and it is not relevant to the choice of reflections for refinement.
The program used for refinement, Jana2006, uses the weighting scheme based on the experimental expectations, see _refine_ls_weighting_details, that does not force *S* to be one. Therefore the values of *S* are usually larger than the ones from the *SHELX* program.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.778715 (13)	−0.01264 (2)	0.739863 (16)	0.01974 (7)
Br1	0.815993 (14)	−0.06312 (2)	0.909367 (15)	0.03043 (7)
Br2	0.768458 (12)	0.22386 (2)	0.682623 (15)	0.02510 (7)
Cl1	0.57897 (3)	−0.18717 (6)	0.46139 (4)	0.03164 (17)
Cl2	0.49527 (3)	−0.02131 (6)	0.81149 (4)	0.03069 (16)
Cl3	0.78647 (4)	−0.01110 (6)	0.42235 (4)	0.03640 (18)
Cl4	1.01713 (4)	−0.02162 (7)	0.73027 (4)	0.0435 (2)
N1	0.67043 (10)	−0.11134 (16)	0.70285 (12)	0.0204 (5)
N2	0.83223 (9)	−0.16701 (17)	0.66248 (11)	0.0190 (5)
C1	0.72353 (12)	−0.3466 (2)	0.66028 (16)	0.0272 (6)
C2	0.67041 (12)	−0.2659 (2)	0.72376 (16)	0.0273 (6)
C3	0.60879 (12)	−0.0487 (2)	0.66383 (14)	0.0216 (6)
C4	0.52967 (11)	−0.1151 (2)	0.63559 (15)	0.0219 (6)
C5	0.50947 (12)	−0.1818 (2)	0.54428 (15)	0.0252 (6)
C6	0.43508 (13)	−0.2408 (2)	0.51740 (17)	0.0321 (7)
C7	0.37960 (13)	−0.2328 (2)	0.58284 (17)	0.0342 (7)
C8	0.39751 (12)	−0.1666 (2)	0.67387 (17)	0.0306 (7)
C9	0.47174 (12)	−0.1085 (2)	0.69829 (15)	0.0240 (6)
C10	0.81108 (12)	−0.3168 (2)	0.68397 (14)	0.0218 (6)
C11	0.87837 (12)	−0.1473 (2)	0.59844 (14)	0.0232 (6)
C12	0.90508 (12)	−0.0029 (2)	0.57246 (14)	0.0223 (6)
C13	0.86796 (12)	0.0692 (2)	0.48978 (15)	0.0248 (6)
C14	0.89235 (13)	0.2026 (2)	0.46228 (17)	0.0308 (7)
C15	0.95599 (13)	0.2659 (2)	0.51856 (16)	0.0312 (7)
C16	0.99483 (13)	0.1988 (2)	0.60108 (16)	0.0300 (7)
C17	0.96911 (12)	0.0647 (2)	0.62674 (15)	0.0260 (6)
H1a	0.714222	−0.447812	0.664797	0.0326*
H1b	0.706896	−0.326754	0.591541	0.0326*
H2a	0.617401	−0.302232	0.710663	0.0327*
H2b	0.688664	−0.281934	0.792584	0.0327*
H3	0.613239	0.052004	0.650974	0.0259*

H6	0.422365	−0.286607	0.45416	0.0386*
H7	0.328059	−0.273674	0.564947	0.0411*
H8	0.358864	−0.161171	0.719285	0.0367*
H10a	0.827835	−0.337727	0.752531	0.0262*
H10b	0.840072	−0.381379	0.64704	0.0262*
H11	0.896906	−0.229113	0.56525	0.0278*
H14	0.865572	0.250488	0.405122	0.037*
H15	0.973645	0.35864	0.499922	0.0375*
H16	1.038872	0.244152	0.639989	0.036*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01828 (12)	0.01772 (12)	0.02378 (12)	−0.00064 (9)	0.00483 (9)	−0.00078 (9)
Br1	0.04287 (14)	0.02484 (11)	0.02295 (11)	−0.00147 (9)	0.00178 (9)	0.00022 (8)
Br2	0.02661 (12)	0.01722 (10)	0.03323 (12)	0.00196 (8)	0.01065 (9)	0.00062 (8)
Cl1	0.0296 (3)	0.0355 (3)	0.0303 (3)	0.0012 (2)	0.0057 (2)	−0.0026 (2)
Cl2	0.0303 (3)	0.0317 (3)	0.0313 (3)	0.0085 (2)	0.0086 (2)	0.0035 (2)
Cl3	0.0359 (3)	0.0301 (3)	0.0389 (3)	0.0017 (2)	−0.0119 (3)	−0.0036 (2)
Cl4	0.0394 (4)	0.0537 (4)	0.0335 (3)	−0.0191 (3)	−0.0102 (3)	0.0086 (3)
N1	0.0173 (8)	0.0191 (8)	0.0252 (8)	0.0008 (7)	0.0047 (7)	0.0012 (7)
N2	0.0159 (8)	0.0209 (8)	0.0194 (8)	0.0000 (7)	−0.0008 (7)	−0.0022 (7)
C1	0.0230 (11)	0.0162 (10)	0.0405 (12)	−0.0015 (8)	−0.0033 (9)	0.0002 (9)
C2	0.0165 (10)	0.0208 (10)	0.0439 (13)	−0.0020 (8)	0.0016 (9)	0.0114 (9)
C3	0.0220 (11)	0.0187 (10)	0.0251 (10)	0.0001 (8)	0.0067 (9)	−0.0002 (8)
C4	0.0161 (10)	0.0181 (10)	0.0312 (10)	0.0046 (8)	0.0019 (8)	0.0056 (8)
C5	0.0222 (11)	0.0218 (10)	0.0315 (11)	0.0032 (8)	0.0038 (9)	0.0042 (9)
C6	0.0275 (12)	0.0282 (11)	0.0387 (13)	−0.0011 (9)	−0.0034 (10)	0.0014 (10)
C7	0.0188 (11)	0.0308 (12)	0.0508 (15)	−0.0022 (9)	−0.0042 (10)	0.0084 (11)
C8	0.0193 (11)	0.0291 (11)	0.0444 (13)	0.0042 (9)	0.0078 (10)	0.0108 (10)
C9	0.0224 (11)	0.0212 (10)	0.0283 (10)	0.0059 (8)	0.0029 (9)	0.0060 (9)
C10	0.0210 (10)	0.0171 (9)	0.0270 (10)	0.0031 (8)	0.0015 (8)	0.0025 (8)
C11	0.0194 (10)	0.0253 (10)	0.0243 (10)	0.0003 (8)	0.0006 (8)	−0.0043 (9)
C12	0.0207 (10)	0.0235 (10)	0.0238 (10)	0.0017 (8)	0.0075 (8)	−0.0045 (8)
C13	0.0222 (11)	0.0244 (10)	0.0275 (10)	0.0028 (8)	0.0026 (9)	−0.0071 (9)
C14	0.0345 (13)	0.0234 (11)	0.0352 (12)	0.0092 (9)	0.0067 (10)	0.0022 (9)
C15	0.0307 (12)	0.0211 (10)	0.0444 (13)	−0.0022 (9)	0.0147 (11)	−0.0012 (10)
C16	0.0254 (12)	0.0305 (12)	0.0355 (12)	−0.0097 (9)	0.0090 (10)	−0.0074 (10)
C17	0.0230 (11)	0.0325 (11)	0.0228 (10)	−0.0038 (9)	0.0042 (9)	−0.0024 (9)

Geometric parameters (Å, º)

Zn1—Br1	2.3599 (3)	C6—C7	1.381 (3)
Zn1—Br2	2.3371 (3)	C6—H6	0.96
Zn1—N1	2.0662 (16)	C7—C8	1.383 (3)
Zn1—N2	2.0628 (16)	C7—H7	0.96
N1—C2	1.469 (2)	C8—C9	1.377 (3)
N1—C3	1.259 (2)	C8—H8	0.96

N2—C10	1.481 (2)	C10—H10a	0.96
N2—C11	1.259 (3)	C10—H10b	0.96
C1—C2	1.526 (3)	C11—C12	1.478 (3)
C1—C10	1.512 (3)	C11—H11	0.96
C1—H1a	0.96	C12—C13	1.391 (3)
C1—H1b	0.96	C12—C17	1.388 (3)
C2—H2a	0.96	C13—C14	1.379 (3)
C2—H2b	0.96	C14—C15	1.378 (3)
C3—C4	1.489 (3)	C14—H14	0.96
C3—H3	0.96	C15—C16	1.379 (3)
C4—C5	1.393 (3)	C15—H15	0.96
C4—C9	1.386 (3)	C16—C17	1.384 (3)
C5—C6	1.388 (3)	C16—H16	0.96

Br1—Zn1—Br2	120.866 (11)	C5—C6—H6	120.45
Br1—Zn1—N1	105.69 (5)	C7—C6—H6	120.45
Br1—Zn1—N2	106.14 (4)	C6—C7—C8	120.7 (2)
Br2—Zn1—N1	108.19 (4)	C6—C7—H7	119.65
Br2—Zn1—N2	120.47 (4)	C8—C7—H7	119.65
N1—Zn1—N2	90.24 (6)	C7—C8—C9	118.9 (2)
Zn1—N1—C2	114.32 (12)	C7—C8—H8	120.57
Zn1—N1—C3	124.61 (13)	C9—C8—H8	120.57
C2—N1—C3	121.05 (16)	C4—C9—C8	122.59 (19)
Zn1—N2—C10	115.00 (12)	N2—C10—C1	112.92 (15)
Zn1—N2—C11	127.37 (14)	N2—C10—H10a	109.47
C10—N2—C11	117.60 (17)	N2—C10—H10b	109.47
C2—C1—C10	115.44 (16)	C1—C10—H10a	109.47
C2—C1—H1a	109.47	C1—C10—H10b	109.47
C2—C1—H1b	109.47	H10a—C10—H10b	105.79
C10—C1—H1a	109.47	N2—C11—C12	122.46 (18)
C10—C1—H1b	109.47	N2—C11—H11	118.77
H1a—C1—H1b	102.77	C12—C11—H11	118.77
N1—C2—C1	111.04 (17)	C11—C12—C13	120.71 (17)
N1—C2—H2a	109.47	C11—C12—C17	122.07 (17)
N1—C2—H2b	109.47	C13—C12—C17	117.19 (18)
C1—C2—H2a	109.47	C12—C13—C14	122.22 (18)
C1—C2—H2b	109.47	C13—C14—C15	118.60 (19)
H2a—C2—H2b	107.85	C13—C14—H14	120.7
N1—C3—C4	126.59 (18)	C15—C14—H14	120.7
N1—C3—H3	116.71	C14—C15—C16	121.4 (2)
C4—C3—H3	116.71	C14—C15—H15	119.32
C3—C4—C5	121.91 (19)	C16—C15—H15	119.32
C3—C4—C9	121.04 (17)	C15—C16—C17	118.73 (19)
C5—C4—C9	117.01 (18)	C15—C16—H16	120.63
C4—C5—C6	121.7 (2)	C17—C16—H16	120.63
C5—C6—C7	119.1 (2)	C12—C17—C16	121.89 (18)