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Dibromo(*N*,*N*,*N*′,*N*′-tetramethylethane-1,2-diamine)-zinc(II)

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Key indicators

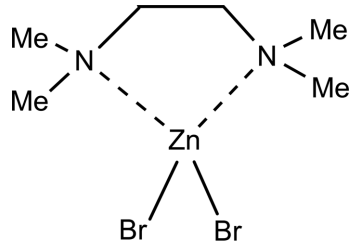
Single-crystal X-ray study
T = 101 K
Mean σ(C—C) = 0.009 Å
R factor = 0.045
wR factor = 0.112
Data-to-parameter ratio = 18.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The structure of the title compound, $[ZnBr_2(C_6H_{16}N_2)]$, which is interesting from the metal coordination point of view, was determined by direct methods on 15672 observed reflections with Mo $K\alpha$ radiation. The asymmetric unit contains two molecules on general positions.

Comment

It is interesting to note that in the title compound, (I), there are weak interactions between Br atoms and their neighboring H atoms, as evidenced by short Br···H distances, *e.g.* Br1···H4B^{i} = 3.00 (5), Br1···H7B^{ii} = 2.94 (7) Å [symmetry codes: (i) $\frac{3}{2}-x$, $-\frac{1}{2}+y$, $\frac{1}{2}-z$; (ii) $x+1$, $y-1$, z; sum of Pauling's (1960) van der Waals radii is 3.15 Å].



(I)

Experimental

Under an inert nitrogen atmosphere, *N*,*N*,*N*′,*N*′-tetramethylethylenediamine (tmeda) was added slowly to a vigorously stirred solution of zinc dibromide in ethanol, with a 1:1 stoichiometry. After overnight stirring, filtration and washing in ethanol, white crystals with the shape of thin needles were obtained. The melting point was determined to be 452 K (literature 455 K; Noltes, 1964).

Crystal data

$[ZnBr_2(C_6H_{16}N_2)]$
M_r = 341.40
Monoclinic, $P2_1/n$
a = 8.0995 (5) Å
b = 11.7771 (4) Å
c = 24.3528 (16) Å
β = 99.473 (3)°
V = 2291.3 (2) Å^3
Z = 8
D_x = 1.979 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5552 reflections
θ = 3.1–27.3°
μ = 9.07 mm^{-1}
T = 100 (2) K
Needle, colorless
0.56 × 0.10 × 0.06 mm

Data collection

Bruker Platform Diffractometer with 1K area-detector diffractometer
ω scans
Absorption correction: empirical by multipole expansion (Blessing, 1995)
T_{min} = 0.201, T_{max} = 0.496
15 672 measured reflections
5889 independent reflections
4111 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 29.7°
$h = -9 \rightarrow 10$
$k = -15 \rightarrow 15$
$l = -30 \rightarrow 32$

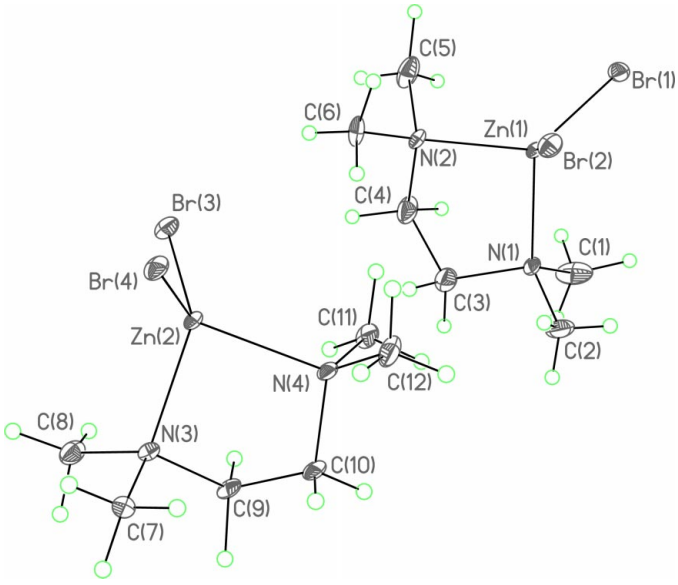


Figure 1
Plot (Bruker, 1998) of the two molecules of [Zn(tmeda)Br_2] in one asymmetric unit.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.112$
$S = 0.98$
5889 reflections
327 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0608P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.38$ e Å^{-3}
$\Delta\rho_{min} = -1.45$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—Zn1	2.3419 (8)	Zn1—N1	2.099 (5)
Br2—Zn1	2.3579 (8)	Zn1—N2	2.096 (5)
Br3—Zn2	2.3685 (8)	Zn2—N3	2.086 (5)
Br4—Zn2	2.3522 (8)	Zn2—N4	2.127 (4)
Br1—Zn1—Br2	117.57 (3)	Br3—Zn2—Br4	119.63 (3)
N1—Zn1—N2	88.10 (18)	N3—Zn2—N4	87.31 (18)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997; data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL* and the *Toledo Cifomatic*.

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