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Bis(4-methylbenzylammonium) tetrabromidozincate

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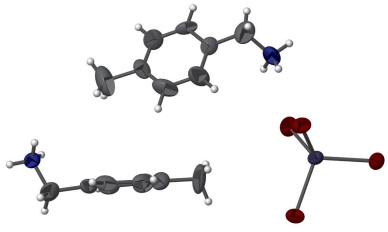
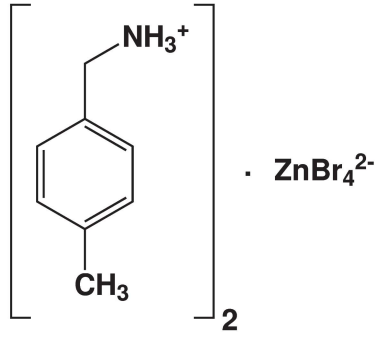
The structure of the non-centrosymmetric organic–inorganic hybrid material, $(C_8H_{12}N)_2[ZnBr_4]$, consists of two 4-methylbenzylammonium cations and one $[ZnBr_4]^{2-}$ anion connected by N—H···Br and C—H···Br hydrogen bonds. The Zn^{II} cation has a slightly distorted tetrahedral coordination environment. No π–π stacking interactions between the phenylene rings but C—H···π interactions towards them are observed. The structure was refined as a two-component inversion twin.

3D view



Chemical scheme



Structure description

Non-linear optical (NLO) materials play a vital role in the field of photonics as they generate coherent radiation at new frequencies that are not available with conventional laser sources. Organic crystals with non-linear optical properties frequently have poor mechanical and thermal properties due to the presence of weak van der Waals interactions and hydrogen bonds (Dolbecq *et al.*, 2010), whereas inorganic crystals possess good mechanical and thermal properties but have low NLO properties due to the presence of strong covalent or ionic interactions (Jiang & Fang, 1999). Hence, attempts have been made by several groups to synthesize new organic–inorganic materials with NLO properties, combining the features of both organic and inorganic crystals. In this context we report here the synthesis and crystal structure of a new organic–inorganic hybrid compound, bis(4-methylbenzylammonium) tetrabromidozincate. This salt crystallizes in the non-centrosymmetric space group type $Pna2_1$, and hence could be a potential candidate for second order non-linear optical properties.

The asymmetric unit of the title compound consists of an isolated tetrabromidozincate anion, $[ZnBr_4]^{2-}$, and two 4-methylbenzylammonium cations, $(C_8H_{12}N)^+$, as shown in

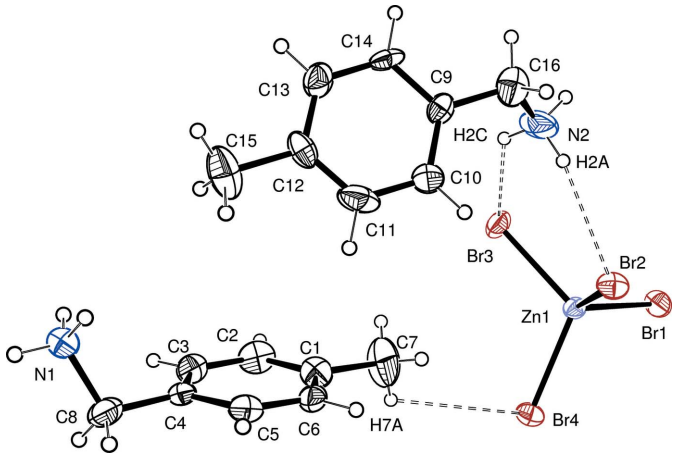


Figure 1
A view of the asymmetric unit, showing the atom numbering and displacement ellipsoids drawn at the 30% probability level. Dashed lines indicate hydrogen-bonding interactions.

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C9–C14 benzene rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···*Cg*2^{i}	0.93	2.94	3.73 (3)	143
C14—H14···*Cg*1^{ii}	0.93	2.94	3.72 (2)	143
C8—H8*B*···Br3^{iii}	0.97	2.88	3.81 (2)	161
C8—H8*A*···Br1^{iv}	0.97	2.91	3.82 (3)	157
C16—H16*B*···Br4^{v}	0.97	3.03	3.90 (3)	150
N1—H1*A*···Br1^{vi}	0.89	2.58	3.427 (17)	159
N1—H1*B*···Br2^{iv}	0.89	2.92	3.626 (17)	137
N1—H1*B*···Br4^{vi}	0.89	2.94	3.613 (16)	133
N1—H1*C*···Br2^{vii}	0.89	2.96	3.414 (17)	113
N1—H1*C*···Br4^{vii}	0.89	2.82	3.563 (17)	142
N2—H2*A*···Br2	0.89	2.61	3.46 (2)	159
N2—H2*B*···Br3^{viii}	0.89	2.47	3.34 (2)	166
N2—H2*C*···Br3	0.89	2.79	3.45 (3)	132

Symmetry codes: (i) $x, y, z-1$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+1$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z$; (iv) $-x+\frac{3}{2}, y-\frac{1}{2}, z-\frac{1}{2}$; (v) $x, y, z+1$; (vi) $-x+\frac{3}{2}, y-\frac{1}{2}, z+\frac{1}{2}$; (vii) $x-\frac{1}{2}, -y+\frac{1}{2}, z$; (viii) $-x+1, -y+1, z+\frac{1}{2}$.

Fig. 1. The Zn^{2+} cation is tetrahedrally coordinated by four bromide ligands with Zn—Br bond lengths ranging from 2.399 (3) to 2.426 (3) Å, and Br—Zn—Br bond angles varying between 104.90 (12) and 113.82 (13)°.

The crystal structure consists of layers of 4-methylbenzylammonium cations sandwiched between tetrabromidozincate layers extending parallel to the *ac* plane, as shown in Fig. 2. The cationic units are linked into a two-dimensional network by two weak C—H···π interactions (Fig. 3, Table 1). The crystal packing is assured by a complex hydrogen-bonding system, involving the positively charged ammonium groups and to a lesser extent the methylene groups of the cations as donors and the bromide ligands of the isolated tetrahedral $[ZnBr_4]^{2-}$ units as acceptors (Table 1), which reinforce the Coulombic interactions, as depicted in Fig. 2.

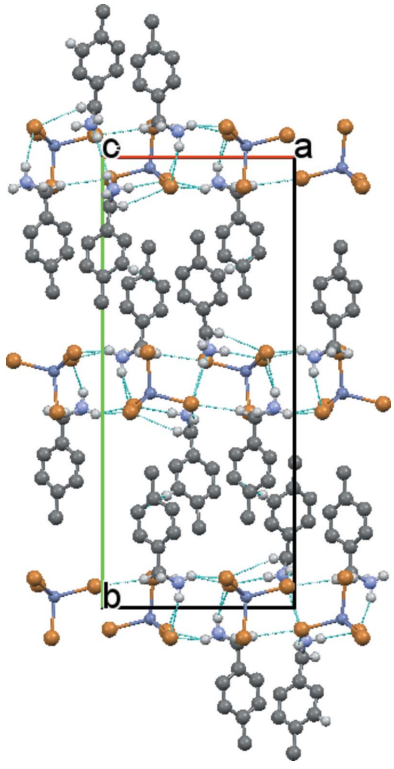


Figure 2
Packing diagram of the title compound viewed along the *c* axis, showing the alternate stacking, along the *b* axis, of organic and inorganic layers. Dashed lines indicate the hydrogen-bonding network.

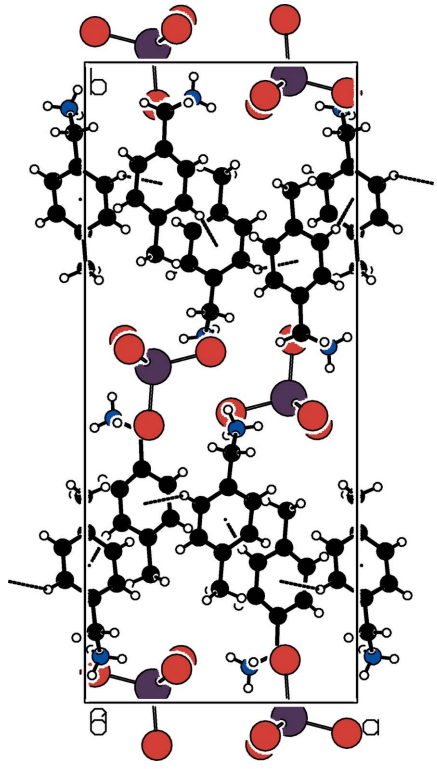


Figure 3
Partial packing diagram showing the C2—H2···π interaction involving the C9–C14 benzene ring and C14—H14···π interaction involving the C1–C6 benzene ring.

Table 2
Experimental details.

Crystal data	
Chemical formula	$(C_8H_{12}N)_2[ZnBr_4]$
M_r	629.38
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	296
a, b, c (Å)	11.0702 (5), 26.0585 (13), 7.7302 (3)
V (Å^3)	2229.95 (17)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	8.27
Crystal size (mm)	0.15 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker Kappa APEX3 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.309, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27881, 3809, 3481
R_{int}	0.056
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.074, 0.156, 1.36
No. of reflections	3809
No. of parameters	213
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.40, −1.01
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.18 (6)

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

Synthesis and crystallization

Bis(4-methylbenzylammonium) tetrabromidozincate single crystals were obtained by the solution growth solvent evaporation method. A mixture of 4-methylbenzylamine (2 mmol, 2.73 ml), zinc bromide (1 mmol, 1.125 g) and HBr (2 mmol, 2.73 ml) in water (20 ml) was well stirred using a magnetic stirrer for 3 h and left to stand at room temperature. After 15 d, colourless single crystals of the title compound were harvested.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The refinement was finalized under consideration of inversion twinning.

Acknowledgements

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full crystallographic data

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Bis(4-methylbenzylammonium) tetrabromidozincate

Crystal data

$(C_8H_{12}N)_2[ZnBr_4]$
M_r = 629.38
Orthorhombic, $Pna2_1$
a = 11.0702 (5) Å
b = 26.0585 (13) Å
c = 7.7302 (3) Å
V = 2229.95 (17) Å^3
Z = 4
$F(000)$ = 1216
D_x = 1.875 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9620 reflections
θ = 3.0–27.9°
μ = 8.27 mm^{-1}
T = 296 K
Block, colourless
0.15 × 0.15 × 0.10 mm

Data collection

Bruker Kappa APEX3 CMOS diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.309, T_{max} = 0.746
27881 measured reflections
3809 independent reflections
3481 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 25.0°, θ_{min} = 3.0°
h = −13→13
k = −30→30
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.156
S = 1.36
3809 reflections
213 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 30.013P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.40 e Å^{-3}
$\Delta\rho_{min}$ = −1.01 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.18 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refined as a two-component inversion twin All H atoms were placed geometrically and refined using a riding-model approximation, with C—H distances of 0.93 (aromatic), 0.97 (methylene) or 0.96 Å (methyl), and N—H distances of 0.89 Å. The torsion angles of the methyl and ammonium H atoms were allowed to refine to best fit the experimental electron density map, and the U_{iso}(H) values of the these groups were constrained to 1.5 times that of their carrier atom. For the other hydrogen atoms U_{iso} was set to 1.2 times U_{eq} of the carrier atom.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.732 (2)	0.2421 (9)	0.275 (3)	0.057 (6)
C2	0.636 (2)	0.2194 (11)	0.189 (3)	0.062 (7)
H2	0.578512	0.239423	0.133959	0.074*
C3	0.628 (2)	0.1666 (11)	0.187 (3)	0.056 (6)
H3	0.565268	0.151337	0.125072	0.067*
C4	0.7094 (17)	0.1354 (8)	0.274 (3)	0.042 (5)
C5	0.8041 (18)	0.1597 (9)	0.363 (3)	0.046 (5)
H5	0.859752	0.140149	0.424816	0.055*
C6	0.815 (2)	0.2123 (9)	0.359 (3)	0.049 (6)
H6	0.879008	0.227882	0.416005	0.059*
C7	0.742 (3)	0.2997 (9)	0.270 (5)	0.103 (12)
H7A	0.776947	0.310150	0.161771	0.154*
H7B	0.793394	0.310999	0.363177	0.154*
H7C	0.663715	0.314629	0.282620	0.154*
C8	0.705 (2)	0.0772 (9)	0.264 (4)	0.064 (7)
H8A	0.693924	0.066588	0.144981	0.077*
H8B	0.781694	0.063220	0.304081	0.077*
C9	0.5269 (16)	0.3365 (8)	0.850 (3)	0.043 (5)
C10	0.617 (2)	0.3142 (10)	0.755 (4)	0.070 (8)
H10	0.685325	0.332821	0.725302	0.084*
C11	0.604 (3)	0.2637 (12)	0.702 (4)	0.074 (8)
H11	0.664217	0.249089	0.633743	0.088*
C12	0.506 (2)	0.2346 (8)	0.747 (3)	0.053 (6)
C13	0.4183 (19)	0.2578 (9)	0.842 (4)	0.060 (6)
H13	0.350192	0.239050	0.872581	0.072*
C14	0.4268 (17)	0.3085 (9)	0.894 (3)	0.046 (6)
H14	0.365046	0.323451	0.958389	0.056*
C15	0.496 (3)	0.1779 (11)	0.695 (5)	0.102 (12)
H15A	0.448471	0.159821	0.778411	0.153*
H15B	0.575688	0.163174	0.690046	0.153*
H15C	0.458851	0.175336	0.583038	0.153*
C16	0.540 (3)	0.3897 (10)	0.913 (3)	0.070 (8)
H16A	0.468909	0.398740	0.978443	0.084*
H16B	0.608749	0.390979	0.991197	0.084*
N1	0.6051 (15)	0.0563 (6)	0.373 (2)	0.044 (4)
H1A	0.619536	0.063181	0.483461	0.066*
H1B	0.600284	0.022474	0.357929	0.066*
H1C	0.535699	0.070774	0.341058	0.066*
N2	0.558 (2)	0.4277 (8)	0.780 (4)	0.091 (9)

H2A	0.636714	0.431734	0.760790	0.136*
H2B	0.526185	0.457349	0.814056	0.136*
H2C	0.522054	0.417394	0.683012	0.136*
Zn1	0.74939 (18)	0.47543 (8)	0.3213 (3)	0.0353 (5)
Br1	0.7646 (2)	0.56660 (8)	0.2732 (3)	0.0568 (7)
Br2	0.8370 (2)	0.44791 (8)	0.5903 (3)	0.0473 (5)
Br3	0.53762 (18)	0.45225 (9)	0.3424 (4)	0.0561 (6)
Br4	0.8535 (2)	0.43435 (8)	0.0869 (3)	0.0480 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.069 (16)	0.056 (14)	0.046 (13)	0.003 (12)	0.001 (12)	0.008 (12)
C2	0.059 (16)	0.079 (19)	0.047 (14)	0.010 (14)	−0.011 (12)	0.017 (13)
C3	0.051 (14)	0.081 (19)	0.036 (12)	−0.014 (13)	−0.004 (11)	−0.011 (13)
C4	0.031 (10)	0.049 (12)	0.048 (12)	−0.003 (9)	0.010 (9)	−0.008 (11)
C5	0.036 (10)	0.072 (16)	0.029 (12)	0.008 (10)	−0.009 (9)	−0.004 (11)
C6	0.049 (12)	0.058 (15)	0.041 (13)	−0.014 (10)	0.010 (11)	−0.008 (11)
C7	0.16 (3)	0.032 (14)	0.12 (3)	−0.010 (18)	−0.01 (3)	0.023 (18)
C8	0.046 (13)	0.063 (16)	0.082 (18)	−0.003 (11)	0.019 (13)	0.008 (15)
C9	0.032 (10)	0.051 (12)	0.046 (12)	−0.004 (9)	−0.012 (11)	0.004 (11)
C10	0.049 (14)	0.071 (18)	0.09 (2)	−0.004 (13)	0.016 (14)	−0.025 (16)
C11	0.052 (16)	0.10 (2)	0.067 (18)	0.026 (16)	0.008 (14)	−0.021 (16)
C12	0.072 (16)	0.044 (13)	0.042 (13)	0.011 (12)	−0.019 (12)	−0.008 (10)
C13	0.048 (12)	0.068 (16)	0.063 (14)	−0.013 (11)	−0.011 (15)	−0.005 (15)
C14	0.021 (10)	0.082 (17)	0.036 (12)	0.000 (10)	0.006 (8)	0.007 (11)
C15	0.13 (3)	0.056 (18)	0.12 (3)	0.014 (19)	−0.04 (2)	−0.020 (19)
C16	0.082 (19)	0.073 (18)	0.055 (15)	−0.012 (16)	−0.020 (15)	0.013 (15)
N1	0.055 (11)	0.044 (11)	0.033 (11)	0.006 (8)	−0.001 (8)	0.008 (8)
N2	0.11 (2)	0.046 (13)	0.11 (2)	0.011 (12)	0.059 (17)	−0.013 (14)
Zn1	0.0342 (10)	0.0417 (12)	0.0299 (10)	−0.0021 (9)	0.0006 (11)	0.0021 (10)
Br1	0.0774 (17)	0.0412 (12)	0.0519 (13)	−0.0059 (11)	0.0131 (12)	0.0037 (10)
Br2	0.0508 (12)	0.0592 (13)	0.0319 (10)	0.0072 (10)	−0.0009 (11)	0.0076 (13)
Br3	0.0352 (10)	0.0574 (14)	0.0757 (15)	−0.0107 (9)	0.0000 (13)	−0.0002 (14)
Br4	0.0532 (13)	0.0552 (13)	0.0355 (11)	0.0062 (10)	0.0054 (11)	−0.0036 (14)

Geometric parameters (Å, º)

C1—C6	1.37 (3)	C11—C12	1.37 (4)
C1—C2	1.38 (3)	C11—H11	0.9300
C1—C7	1.51 (3)	C12—C13	1.36 (3)
C2—C3	1.38 (4)	C12—C15	1.54 (3)
C2—H2	0.9300	C13—C14	1.39 (3)
C3—C4	1.39 (3)	C13—H13	0.9300
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.41 (3)	C15—H15A	0.9600
C4—C8	1.52 (3)	C15—H15B	0.9600
C5—C6	1.38 (3)	C15—H15C	0.9600

C5—H5	0.9300	C16—N2	1.44 (3)
C6—H6	0.9300	C16—H16A	0.9700
C7—H7A	0.9600	C16—H16B	0.9700
C7—H7B	0.9600	N1—H1A	0.8900
C7—H7C	0.9600	N1—H1B	0.8900
C8—N1	1.49 (3)	N1—H1C	0.8900
C8—H8A	0.9700	N2—H2A	0.8900
C8—H8B	0.9700	N2—H2B	0.8900
C9—C14	1.37 (3)	N2—H2C	0.8900
C9—C10	1.37 (3)	Zn1—Br4	2.399 (3)
C9—C16	1.47 (3)	Zn1—Br2	2.404 (3)
C10—C11	1.38 (4)	Zn1—Br1	2.411 (3)
C10—H10	0.9300	Zn1—Br3	2.426 (3)

C6—C1—C2	120 (2)	C13—C12—C11	117 (2)
C6—C1—C7	122 (3)	C13—C12—C15	122 (3)
C2—C1—C7	118 (3)	C11—C12—C15	121 (3)
C3—C2—C1	119 (2)	C12—C13—C14	122 (2)
C3—C2—H2	120.5	C12—C13—H13	118.8
C1—C2—H2	120.5	C14—C13—H13	118.8
C2—C3—C4	122 (2)	C9—C14—C13	119 (2)
C2—C3—H3	118.9	C9—C14—H14	120.3
C4—C3—H3	118.9	C13—C14—H14	120.3
C3—C4—C5	117 (2)	C12—C15—H15A	109.5
C3—C4—C8	123 (2)	C12—C15—H15B	109.5
C5—C4—C8	120 (2)	H15A—C15—H15B	109.5
C6—C5—C4	120 (2)	C12—C15—H15C	109.5
C6—C5—H5	120.0	H15A—C15—H15C	109.5
C4—C5—H5	120.0	H15B—C15—H15C	109.5
C1—C6—C5	121 (2)	N2—C16—C9	115 (2)
C1—C6—H6	119.3	N2—C16—H16A	108.4
C5—C6—H6	119.3	C9—C16—H16A	108.4
C1—C7—H7A	109.5	N2—C16—H16B	108.4
C1—C7—H7B	109.5	C9—C16—H16B	108.4
H7A—C7—H7B	109.5	H16A—C16—H16B	107.5
C1—C7—H7C	109.5	C8—N1—H1A	109.5
H7A—C7—H7C	109.5	C8—N1—H1B	109.5
H7B—C7—H7C	109.5	H1A—N1—H1B	109.5
N1—C8—C4	111.0 (19)	C8—N1—H1C	109.5
N1—C8—H8A	109.4	H1A—N1—H1C	109.5
C4—C8—H8A	109.4	H1B—N1—H1C	109.5
N1—C8—H8B	109.4	C16—N2—H2A	109.5
C4—C8—H8B	109.4	C16—N2—H2B	109.5
H8A—C8—H8B	108.0	H2A—N2—H2B	109.5
C14—C9—C10	120 (2)	C16—N2—H2C	109.5
C14—C9—C16	120 (2)	H2A—N2—H2C	109.5
C10—C9—C16	120 (2)	H2B—N2—H2C	109.5
C9—C10—C11	119 (2)	Br4—Zn1—Br2	109.05 (11)

C9—C10—H10	120.3	Br4—Zn1—Br1	106.84 (11)
C11—C10—H10	120.3	Br2—Zn1—Br1	113.53 (12)
C12—C11—C10	122 (2)	Br4—Zn1—Br3	113.82 (13)
C12—C11—H11	119.0	Br2—Zn1—Br3	104.90 (12)
C10—C11—H11	119.0	Br1—Zn1—Br3	108.86 (11)
C6—C1—C2—C3	−2 (4)	C14—C9—C10—C11	1 (4)
C7—C1—C2—C3	178 (3)	C16—C9—C10—C11	178 (2)
C1—C2—C3—C4	3 (4)	C9—C10—C11—C12	−2 (5)
C2—C3—C4—C5	−1 (3)	C10—C11—C12—C13	2 (4)
C2—C3—C4—C8	−177 (2)	C10—C11—C12—C15	−177 (3)
C3—C4—C5—C6	−1 (3)	C11—C12—C13—C14	−1 (4)
C8—C4—C5—C6	174 (2)	C15—C12—C13—C14	178 (3)
C2—C1—C6—C5	0 (4)	C10—C9—C14—C13	1 (4)
C7—C1—C6—C5	180 (2)	C16—C9—C14—C13	−177 (2)
C4—C5—C6—C1	2 (3)	C12—C13—C14—C9	0 (4)
C3—C4—C8—N1	−76 (3)	C14—C9—C16—N2	−124 (3)
C5—C4—C8—N1	109 (2)	C10—C9—C16—N2	59 (4)

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C9–C14 benzene rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···*Cg*2^{i}	0.93	2.94	3.73 (3)	143
C14—H14···*Cg*1^{ii}	0.93	2.94	3.72 (2)	143
C8—H8*B*···Br3^{iii}	0.97	2.88	3.81 (2)	161
C8—H8*A*···Br1^{iv}	0.97	2.91	3.82 (3)	157
C16—H16*B*···Br4^{v}	0.97	3.03	3.90 (3)	150
N1—H1*A*···Br1^{vi}	0.89	2.58	3.427 (17)	159
N1—H1*B*···Br2^{iv}	0.89	2.92	3.626 (17)	137
N1—H1*B*···Br4^{vi}	0.89	2.94	3.613 (16)	133
N1—H1*C*···Br2^{vii}	0.89	2.96	3.414 (17)	113
N1—H1*C*···Br4^{vii}	0.89	2.82	3.563 (17)	142
N2—H2*A*···Br2	0.89	2.61	3.46 (2)	159
N2—H2*B*···Br3^{viii}	0.89	2.47	3.34 (2)	166
N2—H2*C*···Br3	0.89	2.79	3.45 (3)	132

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) *x*−1/2, −*y*+1/2, *z*+1; (iii) *x*+1/2, −*y*+1/2, *z*; (iv) −*x*+3/2, *y*−1/2, *z*−1/2; (v) *x*, *y*, *z*+1; (vi) −*x*+3/2, *y*−1/2, *z*+1/2; (vii) *x*−1/2, −*y*+1/2, *z*; (viii) −*x*+1, −*y*+1, *z*+1/2.