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Bis(4-methoxybenzylammonium) tetrabromidocadmate(II)

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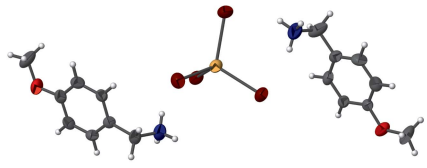
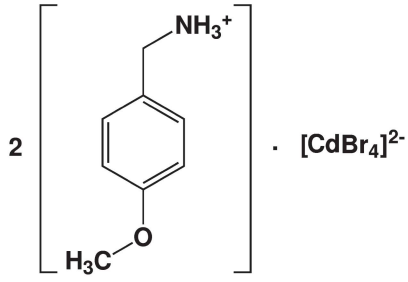
The asymmetric unit of the organic–inorganic hybrid salt, $(C_8H_{12}NO)_2[CdBr_4]$, consists of two 4-methoxybenzylammonium cations and one $[CdBr_4]^{2-}$ anion. The cations and anions are connected by a complex series of N—H···Br and C—H···Br hydrogen bonds. No π–π stacking interactions occur between the benzene rings but two C—H···π interactions are observed.

3D view



Chemical scheme



Structure description

Work on non-linear optical (NLO) crystals is an attractive field of interest in current research into applications of laser technology, optical data storage, optical communication, optical switching, optical signal processing, and optical power-limiting processes (Umarani *et al.*, 2017; Mageshwari *et al.*, 2016). Recently, researchers have concentrated on the design of new metal–organic NLO crystals. These materials enhance the desirable NLO response of organic crystals with the high thermal and mechanical properties of inorganic crystals. This new class of materials with remarkable properties are ideal for device fabrication. Incorporating transition metal ions such as Cd^{2+}, Zn^{2+}, Hg^{2+} with filled electron *d* shells into organic materials creates more energy sublevels and enhances the optical non-linearity through a charge-transfer mechanism (Yang *et al.*, 2013).

As a part of a continuation of our research work on 4-methoxybenzylamine-based crystals, we report here the synthesis and crystal structure of the metal–organic title structure, bis(4-methoxybenzylammonium) tetrabromidocadmate(II). As the crystal belongs to the centrosymmetric monoclinic space group $P2_1/n$, it can be used in third-harmonic generation for a Nd:YAG laser at a wavelength of 1064 nm (Mageshwari *et al.*, 2016).

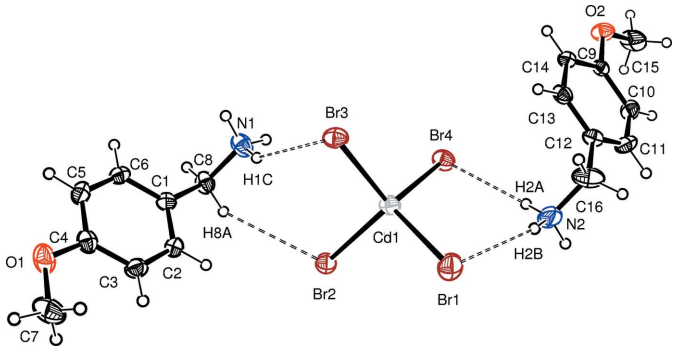


Figure 1
A view of the asymmetric unit of the title compound showing the atom numbering with displacement ellipsoids drawn at the 30% probability level. Dashed lines indicate hydrogen-bonding interactions.

The asymmetric unit of the the title compound consists of one tetrabromidocadmate anion, $[CdBr_4]^{2-}$, and two 4-methoxybenzylammonium cations, $(C_8H_{12}NO)^+$, as shown in Fig. 1. The cadmium cation coordination environment is distorted tetrahedral. The 4-methoxybenzylammonium cations are sandwiched between the tetrabromidocadmate layers (Fig. 2). The crystal packing is stabilized by a complex hydrogen-bonding system, involving the N—H bonds of the positively charged ammonium groups and, to a minor extent, the methylene group as donors, with the bromide ligands of the anions as acceptors (Table 1). The benzene rings of the cations are also linked by weak C—H$\cdots\pi$ interactions (Fig. 3, Table 1).

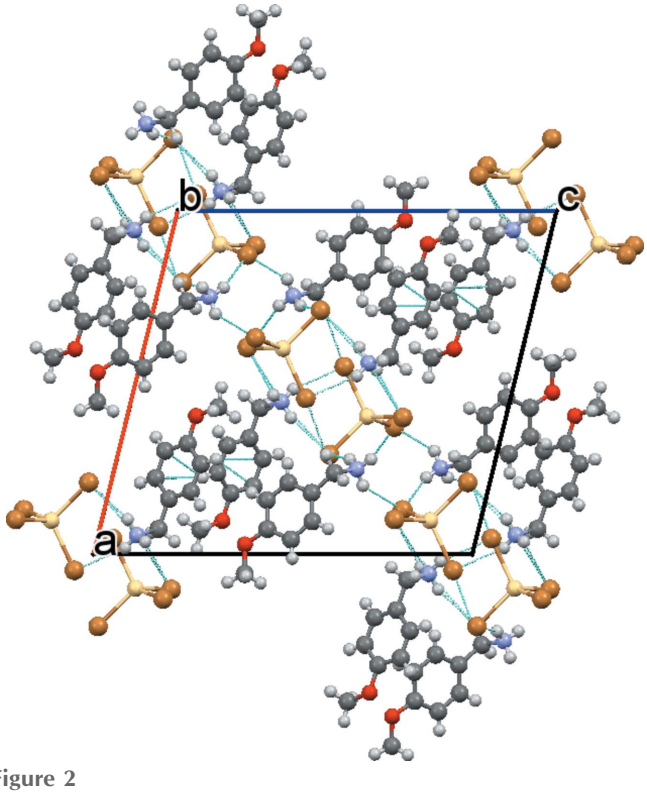


Figure 2
Packing diagram of the title compound viewed along the *b* axis, showing the alternate stacking of the organic and inorganic layers. Dashed lines indicate hydrogen bonds.

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$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
C8—H8*A*$\cdots$Br2	0.97	3.10	3.822 (8)	133
C8—H8*B*$\cdots$Br1^{i}	0.97	2.98	3.846 (9)	150
N1—H1*A*$\cdots$Br4^{ii}	0.89	2.62	3.439 (7)	154
N1—H1*B*$\cdots$Br3^{iii}	0.89	2.63	3.450 (7)	154
N1—H1*C*$\cdots$Br3	0.89	2.67	3.418 (7)	142
N2—H2*A*$\cdots$Br4	0.89	2.54	3.380 (8)	157
N2—H2*B*$\cdots$Br1	0.89	2.64	3.446 (8)	152
N2—H2*C*$\cdots$Br1^{iv}	0.89	3.13	3.651 (10)	119
N2—H2*C*$\cdots$Br2^{iv}	0.89	2.67	3.377 (7)	137
C10—H10$\cdots$*Cg*2^{v}	0.93	2.88	3.682 (9)	145
C14—H14$\cdots$*Cg*1^{ii}	0.93	2.82	3.621 (8)	146

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

Synthesis and crystallization

20 mmol (2.74 g) of 4-methoxybenzylamine (Sigma Aldrich 98%), 20 mmol of aqueous hydrobromic acid (Merck 48%), and 10 mmol (2.72 g) of cadmium (II) bromide (Sigma Aldrich 98%) were mixed in 50 ml of water. The solution was stirred at room temperature for more than 3 h and was then set aside to allow slow evaporation. Transparent crystals suitable for single-crystal X-ray diffraction were collected after two weeks.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

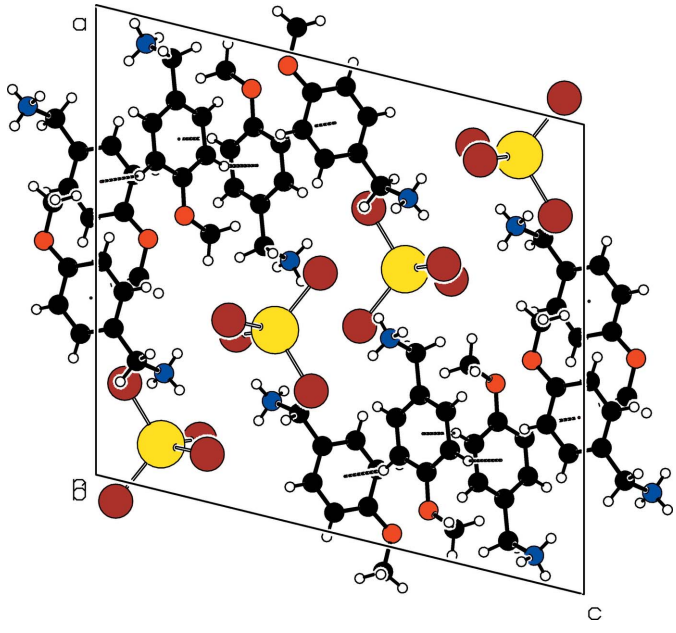


Figure 3
A partial packing diagram showing the C—H$\cdots\pi$ interactions (details in Table 1).

Table 2
Experimental details.

Crystal data	
Chemical formula	$(C_8H_{12}NO)_2[CdBr_4]$
M_r	708.41
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	16.7564 (13), 7.9403 (6), 17.9303 (13)
β (°)	103.777 (3)
V (Å^3)	2317.0 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	7.85
Crystal size (mm)	0.38 × 0.22 × 0.05
Data collection	
Diffractometer	Bruker Kappa APEXII CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.11, 0.67
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	54597, 4087, 2873
R_{int}	0.151
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.123, 1.06
No. of reflections	4087
No. of parameters	231
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.96, −0.67

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2018). **3**, x180795 [https://doi.org/10.1107/S2414314618007952]

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Crystal data

$(C_8H_{12}NO)_2[CdBr_4]$
M_r = 708.41
Monoclinic, $P2_1/n$
a = 16.7564 (13) Å
b = 7.9403 (6) Å
c = 17.9303 (13) Å
β = 103.777 (3)°
V = 2317.0 (3) Å^3
Z = 4
$F(000)$ = 1352
D_x = 2.031 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8254 reflections
θ = 3.0–28.3°
μ = 7.85 mm^{-1}
T = 296 K
Block, colourless
0.38 × 0.22 × 0.05 mm

Data collection

Bruker Kappa APEXII CMOS diffractometer
Radiation source: Sealed tube
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.11, T_{max} = 0.67
54597 measured reflections
4087 independent reflections
2873 reflections with $I > 2\sigma(I)$
R_{int} = 0.151
θ_{max} = 25.0°, θ_{min} = 3.0°
h = −19→19
k = −9→9
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.123
S = 1.06
4087 reflections
231 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 2.4383P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0028 (2)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3209 (5)	0.7778 (8)	0.0360 (4)	0.0328 (18)
C2	0.4039 (5)	0.8134 (10)	0.0565 (4)	0.0369 (19)
H2	0.424975	0.869023	0.102633	0.044*
C3	0.4564 (5)	0.7701 (10)	0.0117 (5)	0.043 (2)
H3	0.511854	0.797298	0.027182	0.052*
C4	0.4263 (5)	0.6851 (10)	−0.0572 (4)	0.041 (2)
C5	0.3421 (5)	0.6441 (10)	−0.0770 (4)	0.041 (2)
H5	0.320654	0.584154	−0.121905	0.049*
C6	0.2918 (5)	0.6909 (10)	−0.0316 (4)	0.0368 (19)
H6	0.236312	0.663756	−0.046372	0.044*
C7	0.5570 (6)	0.6793 (14)	−0.0882 (7)	0.075 (3)
H7A	0.563794	0.799177	−0.083723	0.112*
H7B	0.581299	0.638488	−0.128077	0.112*
H7C	0.583353	0.627100	−0.040354	0.112*
C8	0.2633 (5)	0.8351 (10)	0.0836 (5)	0.043 (2)
H8A	0.284919	0.937115	0.110847	0.052*
H8B	0.210510	0.862030	0.049830	0.052*
C9	0.1778 (5)	0.7024 (9)	0.6772 (4)	0.0312 (17)
C10	0.2372 (5)	0.7994 (10)	0.7252 (5)	0.043 (2)
H10	0.223555	0.867941	0.762396	0.052*
C11	0.3170 (5)	0.7928 (10)	0.7170 (5)	0.045 (2)
H11	0.357070	0.857191	0.749481	0.054*
C12	0.3383 (5)	0.6958 (10)	0.6635 (5)	0.0368 (19)
C13	0.2779 (5)	0.6029 (10)	0.6151 (4)	0.0390 (19)
H13	0.291633	0.537914	0.576832	0.047*
C14	0.1987 (5)	0.6038 (9)	0.6218 (4)	0.0351 (18)
H14	0.159200	0.538303	0.589320	0.042*
C15	0.0719 (6)	0.7992 (14)	0.7341 (6)	0.070 (3)
H15A	0.101521	0.771306	0.785338	0.105*
H15B	0.014064	0.784414	0.729689	0.105*
H15C	0.082611	0.914238	0.723309	0.105*
C16	0.4257 (5)	0.6896 (13)	0.6554 (7)	0.066 (3)
H16A	0.462467	0.706797	0.705434	0.079*
H16B	0.436524	0.578452	0.637616	0.079*
Br1	0.54615 (6)	0.74974 (14)	0.45961 (6)	0.0640 (3)
Br2	0.39836 (6)	0.99964 (10)	0.27210 (5)	0.0474 (3)
Br3	0.37040 (5)	0.48202 (10)	0.28754 (5)	0.0444 (3)
Br4	0.29050 (5)	0.81457 (11)	0.44107 (5)	0.0475 (3)
Cd1	0.40127 (4)	0.75364 (7)	0.36670 (3)	0.0405 (2)
N1	0.2515 (5)	0.7073 (8)	0.1396 (4)	0.0504 (19)
H1A	0.223587	0.620510	0.114873	0.076*
H1B	0.223546	0.752231	0.171145	0.076*
H1C	0.300243	0.672039	0.166698	0.076*
N2	0.4437 (5)	0.8145 (12)	0.6025 (5)	0.075 (3)
H2A	0.397883	0.839279	0.567472	0.112*

H2B	0.480916	0.773609	0.579280	0.112*
H2C	0.463229	0.907295	0.628329	0.112*
O1	0.4710 (4)	0.6390 (8)	−0.1067 (3)	0.0615 (18)
O2	0.0975 (3)	0.6926 (7)	0.6813 (3)	0.0493 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.036 (4)	0.023 (4)	0.040 (4)	0.003 (3)	0.009 (4)	0.001 (3)
C2	0.038 (5)	0.041 (4)	0.031 (4)	−0.004 (4)	0.006 (4)	−0.001 (4)
C3	0.037 (5)	0.045 (5)	0.045 (5)	−0.007 (4)	0.002 (4)	0.003 (4)
C4	0.051 (5)	0.035 (4)	0.037 (5)	0.008 (4)	0.012 (4)	0.009 (4)
C5	0.050 (5)	0.037 (5)	0.033 (4)	0.002 (4)	0.004 (4)	−0.003 (4)
C6	0.032 (4)	0.035 (4)	0.040 (5)	−0.004 (3)	0.003 (4)	−0.001 (4)
C7	0.053 (7)	0.086 (8)	0.099 (9)	0.002 (6)	0.046 (6)	0.003 (7)
C8	0.053 (5)	0.039 (5)	0.042 (5)	0.008 (4)	0.019 (4)	0.000 (4)
C9	0.034 (4)	0.028 (4)	0.032 (4)	0.000 (3)	0.009 (3)	0.006 (3)
C10	0.054 (6)	0.037 (5)	0.039 (5)	−0.001 (4)	0.012 (4)	−0.008 (4)
C11	0.037 (5)	0.039 (5)	0.051 (5)	−0.008 (4)	−0.002 (4)	−0.005 (4)
C12	0.033 (4)	0.032 (4)	0.047 (5)	0.000 (3)	0.012 (4)	0.007 (4)
C13	0.046 (5)	0.037 (5)	0.040 (5)	0.000 (4)	0.022 (4)	−0.001 (4)
C14	0.034 (4)	0.038 (5)	0.036 (4)	−0.008 (3)	0.011 (4)	0.000 (4)
C15	0.060 (7)	0.081 (8)	0.087 (8)	−0.012 (6)	0.051 (6)	−0.017 (6)
C16	0.039 (6)	0.054 (6)	0.110 (9)	0.001 (4)	0.030 (6)	0.003 (6)
Br1	0.0371 (5)	0.0957 (8)	0.0570 (6)	0.0043 (5)	0.0072 (4)	−0.0010 (5)
Br2	0.0576 (5)	0.0397 (5)	0.0452 (5)	−0.0055 (4)	0.0127 (4)	0.0002 (4)
Br3	0.0452 (5)	0.0311 (4)	0.0594 (6)	−0.0011 (4)	0.0175 (4)	−0.0045 (4)
Br4	0.0446 (5)	0.0487 (5)	0.0548 (5)	0.0017 (4)	0.0229 (4)	−0.0016 (4)
Cd1	0.0388 (4)	0.0391 (4)	0.0457 (4)	−0.0014 (3)	0.0145 (3)	−0.0048 (3)
N1	0.063 (5)	0.043 (4)	0.052 (4)	0.006 (4)	0.027 (4)	0.003 (3)
N2	0.050 (5)	0.119 (7)	0.059 (5)	−0.036 (5)	0.022 (4)	−0.021 (5)
O1	0.061 (4)	0.081 (5)	0.050 (4)	0.011 (4)	0.028 (3)	−0.006 (3)
O2	0.038 (3)	0.049 (3)	0.065 (4)	−0.007 (3)	0.022 (3)	−0.011 (3)

Geometric parameters (Å, º)

C1—C6	1.379 (11)	C11—C12	1.344 (12)
C1—C2	1.380 (10)	C11—H11	0.9300
C1—C8	1.503 (11)	C12—C13	1.380 (10)
C2—C3	1.369 (12)	C12—C16	1.507 (12)
C2—H2	0.9300	C13—C14	1.360 (10)
C3—C4	1.392 (11)	C13—H13	0.9300
C3—H3	0.9300	C14—H14	0.9300
C4—O1	1.342 (10)	C15—O2	1.412 (11)
C4—C5	1.409 (11)	C15—H15A	0.9600
C5—C6	1.356 (11)	C15—H15B	0.9600
C5—H5	0.9300	C15—H15C	0.9600
C6—H6	0.9300	C16—N2	1.452 (13)

C7—O1	1.435 (11)	C16—H16A	0.9700
C7—H7A	0.9600	C16—H16B	0.9700
C7—H7B	0.9600	Br1—Cd1	2.5968 (11)
C7—H7C	0.9600	Br2—Cd1	2.5798 (10)
C8—N1	1.474 (10)	Br3—Cd1	2.5659 (10)
C8—H8A	0.9700	Br4—Cd1	2.5761 (11)
C8—H8B	0.9700	N1—H1A	0.8900
C9—O2	1.367 (9)	N1—H1B	0.8900
C9—C14	1.374 (10)	N1—H1C	0.8900
C9—C10	1.385 (11)	N2—H2A	0.8900
C10—C11	1.380 (12)	N2—H2B	0.8900
C10—H10	0.9300	N2—H2C	0.8900

C6—C1—C2	117.4 (7)	C11—C12—C16	121.2 (8)
C6—C1—C8	120.7 (7)	C13—C12—C16	120.4 (8)
C2—C1—C8	121.9 (7)	C14—C13—C12	121.7 (8)
C3—C2—C1	122.7 (7)	C14—C13—H13	119.1
C3—C2—H2	118.7	C12—C13—H13	119.1
C1—C2—H2	118.7	C13—C14—C9	119.3 (7)
C2—C3—C4	119.6 (8)	C13—C14—H14	120.3
C2—C3—H3	120.2	C9—C14—H14	120.3
C4—C3—H3	120.2	O2—C15—H15A	109.5
O1—C4—C3	125.3 (8)	O2—C15—H15B	109.5
O1—C4—C5	117.0 (7)	H15A—C15—H15B	109.5
C3—C4—C5	117.8 (8)	O2—C15—H15C	109.5
C6—C5—C4	120.8 (7)	H15A—C15—H15C	109.5
C6—C5—H5	119.6	H15B—C15—H15C	109.5
C4—C5—H5	119.6	N2—C16—C12	113.5 (8)
C5—C6—C1	121.7 (7)	N2—C16—H16A	108.9
C5—C6—H6	119.1	C12—C16—H16A	108.9
C1—C6—H6	119.1	N2—C16—H16B	108.9
O1—C7—H7A	109.5	C12—C16—H16B	108.9
O1—C7—H7B	109.5	H16A—C16—H16B	107.7
H7A—C7—H7B	109.5	Br3—Cd1—Br4	111.65 (4)
O1—C7—H7C	109.5	Br3—Cd1—Br2	107.64 (4)
H7A—C7—H7C	109.5	Br4—Cd1—Br2	107.16 (4)
H7B—C7—H7C	109.5	Br3—Cd1—Br1	112.30 (4)
N1—C8—C1	112.8 (6)	Br4—Cd1—Br1	110.42 (4)
N1—C8—H8A	109.0	Br2—Cd1—Br1	107.41 (4)
C1—C8—H8A	109.0	C8—N1—H1A	109.5
N1—C8—H8B	109.0	C8—N1—H1B	109.5
C1—C8—H8B	109.0	H1A—N1—H1B	109.5
H8A—C8—H8B	107.8	C8—N1—H1C	109.5
O2—C9—C14	115.5 (7)	H1A—N1—H1C	109.5
O2—C9—C10	124.7 (7)	H1B—N1—H1C	109.5
C14—C9—C10	119.8 (7)	C16—N2—H2A	109.5
C11—C10—C9	118.9 (8)	C16—N2—H2B	109.5
C11—C10—H10	120.5	H2A—N2—H2B	109.5

C9—C10—H10	120.5	C16—N2—H2C	109.5
C12—C11—C10	121.8 (7)	H2A—N2—H2C	109.5
C12—C11—H11	119.1	H2B—N2—H2C	109.5
C10—C11—H11	119.1	C4—O1—C7	118.3 (7)
C11—C12—C13	118.4 (7)	C9—O2—C15	117.5 (6)
C6—C1—C2—C3	1.8 (11)	C9—C10—C11—C12	0.5 (13)
C8—C1—C2—C3	−176.3 (7)	C10—C11—C12—C13	0.9 (12)
C1—C2—C3—C4	−0.7 (12)	C10—C11—C12—C16	−179.9 (8)
C2—C3—C4—O1	178.6 (7)	C11—C12—C13—C14	−1.9 (12)
C2—C3—C4—C5	−1.3 (11)	C16—C12—C13—C14	178.9 (8)
O1—C4—C5—C6	−177.8 (7)	C12—C13—C14—C9	1.4 (12)
C3—C4—C5—C6	2.1 (12)	O2—C9—C14—C13	−178.5 (7)
C4—C5—C6—C1	−1.0 (12)	C10—C9—C14—C13	0.1 (11)
C2—C1—C6—C5	−1.0 (11)	C11—C12—C16—N2	−90.0 (11)
C8—C1—C6—C5	177.2 (7)	C13—C12—C16—N2	89.2 (10)
C6—C1—C8—N1	88.6 (9)	C3—C4—O1—C7	0.0 (13)
C2—C1—C8—N1	−93.3 (9)	C5—C4—O1—C7	179.9 (8)
O2—C9—C10—C11	177.4 (7)	C14—C9—O2—C15	−176.3 (8)
C14—C9—C10—C11	−1.0 (12)	C10—C9—O2—C15	5.3 (12)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 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*
C8—H8*A*···Br2	0.97	3.10	3.822 (8)	133
C8—H8*B*···Br1^{i}	0.97	2.98	3.846 (9)	150
N1—H1*A*···Br4^{ii}	0.89	2.62	3.439 (7)	154
N1—H1*B*···Br3^{iii}	0.89	2.63	3.450 (7)	154
N1—H1*C*···Br3	0.89	2.67	3.418 (7)	142
N2—H2*A*···Br4	0.89	2.54	3.380 (8)	157
N2—H2*B*···Br1	0.89	2.64	3.446 (8)	152
N2—H2*C*···Br1^{iv}	0.89	3.13	3.651 (10)	119
N2—H2*C*···Br2^{iv}	0.89	2.67	3.377 (7)	137
C10—H10···*Cg*2^{v}	0.93	2.88	3.682 (9)	145
C14—H14···*Cg*1^{ii}	0.93	2.82	3.621 (8)	146

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