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catena-Poly[trimethylphenylammonium [[bromidocadmate(II)]-μ-bromido-μ-chlorido]]

Kong Mun Lo and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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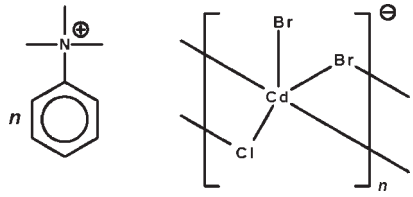
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(N–C) = 0.006 Å; disorder in main residue; R factor = 0.027; wR factor = 0.070; data-to-parameter ratio = 24.7.

In the title salt, $(C_9H_{14}N)[CdBr_2Cl]$, the Cd^{II} atom is five-coordinated in a trigonal-bipyramidal coordination environment. All three of the halogen sites show disorder as a result of substitution of Cl for Br or Br for Cl. Two of the three halogen atoms are involved in bridging a pair of Cd^{II} atoms, generating a linear polyanionic chain motif.

Related literature

For the crystal structure of bis[4-(dimethylamino)pyridinium]-tetrabromidocadmate monohydrate, see: Lo & Ng (2009).



Experimental

Crystal data

$(C_9H_{14}N)[CdBr_2Cl]$
M_r = 443.88
Monoclinic, *Cc*
a = 12.9403 (2) Å
b = 14.7059 (2) Å
c = 7.3866 (1) Å
β = 95.1590 (8)°
V = 1399.97 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 7.43 mm^{-1}
T = 293 K
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.378, T_{max} = 0.746
6431 measured reflections
3068 independent reflections
2966 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.070
S = 1.06
3068 reflections
124 parameters
10 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}
Absolute structure: Flack (1983), 1451 Friedel pairs
Flack parameter: 0.021 (9)

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5034).

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supporting information

Acta Cryst. (2010). E**66**, m308 [doi:10.1107/S1600536810005817]

catena-Poly[trimethylphenylammonium [[bromidocadmate(II)]-μ-bromido-μ-chlorido]]

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S1. Experimental

Cadmium chloride hemipentahydrate (0.45 g , 2 mmol) and trimethylphenylammonium tribromide (0.76 g, 2mmol) were heated in ethanol for 1 h. After filtering of the reaction mixture, colourless crystals were obtained upon slow evaporation of the yellow filtrate.

S2. Refinement

The aromatic ring was refined as a rigid hexagon (C—C = 1.39 Å). The N—C_{methyl} distances were restrained to 1.50 (1) Å. H atoms were placed at calculated positions (C–H = 0.93–0.96 Å) and were treated as riding on their parent atoms, with U(H) set to 1.2–1.5 times U_{eq}(C).

Each of the three halogen sites are occupied by Cl or Br atoms. The total site occupancy of the Cl atoms refined to nearly 1 and that of Br atoms to nearly 2. Hence, the total site occupancy was fixed as 1.0 for Cl and 2.0 for Br atoms. The same U^{ij} parameters were used for Br and Cl atoms occupying the same site.

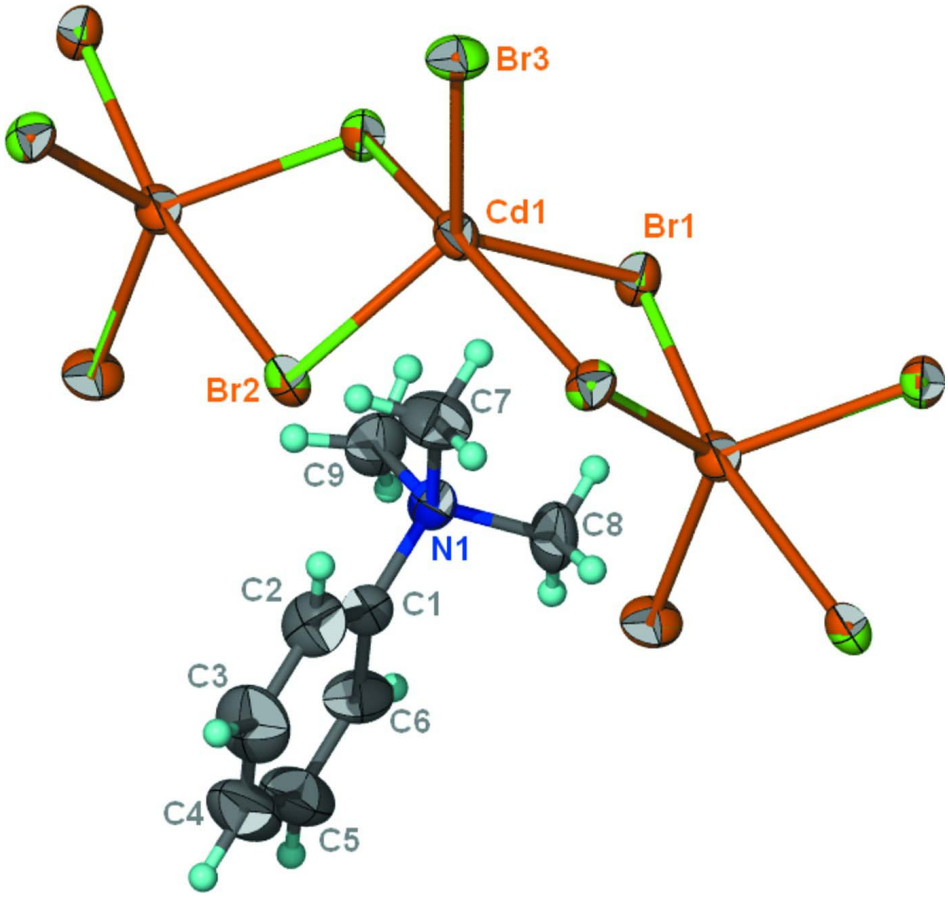

Figure 1

Displacement ellipsoid plot (Barbour, 2001) of a portion of polymeric $C_9H_{14}N^+$ $[CdBr_2Cl]^-$ at the 50% probability level. H are drawn as spheres of arbitrary radius. The disorder in the halogen sites not shown.

catena-Poly[trimethylphenylammonium [[bromidocadmate(II)]-μ-bromido-μ-chlorido]]

Crystal data

$(C_9H_{14}N)[CdBr_2Cl]$
$M_r = 443.88$
Monoclinic, *Cc*
Hall symbol: C -2yc
$a = 12.9403$ (2) Å
$b = 14.7059$ (2) Å
$c = 7.3866$ (1) Å
$\beta = 95.1590$ (8)°
$V = 1399.97$ (3) Å^3
$Z = 4$
$F(000) = 840$
$D_x = 2.106$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5267 reflections
$\theta = 2.7$–28.3°
$\mu = 7.43$ mm^{-1}
$T = 293$ K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.378$, $T_{max} = 0.746$
6431 measured reflections
3068 independent reflections
2966 reflections with $I > 2\sigma(I)$

R_{int} = 0.026
θ_{max} = 27.5°, θ_{min} = 2.1°
h = −16→16
k = −19→19
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.070
S = 1.06
3068 reflections
124 parameters
10 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
$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 0.0436P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}
Absolute structure: Flack (1983), 1451 Friedel pairs
Absolute structure parameter: 0.021 (9)

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cd1	0.50000 (2)	0.451513 (19)	0.50000 (3)	0.04131 (10)	
Br1	0.63269 (6)	0.51023 (6)	0.29653 (9)	0.04153 (19)	0.302 (2)
Br2	0.36460 (4)	0.55946 (3)	0.61951 (6)	0.04104 (14)	0.861 (2)
Br3	0.48809 (5)	0.28104 (3)	0.54560 (8)	0.05001 (16)	0.837 (2)
Cl1	0.63269 (6)	0.51023 (6)	0.29653 (9)	0.04153 (19)	0.698 (2)
Cl2	0.36460 (4)	0.55946 (3)	0.61951 (6)	0.04104 (14)	0.139 (2)
Cl3	0.48809 (5)	0.28104 (3)	0.54560 (8)	0.05001 (16)	0.163 (2)
N1	0.6446 (3)	0.8091 (3)	0.5732 (4)	0.0399 (8)	
C1	0.5525 (2)	0.8692 (2)	0.5708 (5)	0.0405 (9)	
C2	0.4530 (3)	0.8337 (2)	0.5711 (6)	0.0623 (14)	
H2	0.4432	0.7710	0.5716	0.075*	
C3	0.3682 (2)	0.8917 (3)	0.5705 (8)	0.089 (2)	
H3	0.3017	0.8679	0.5706	0.106*	
C4	0.3830 (3)	0.9854 (3)	0.5696 (8)	0.091 (3)	
H4	0.3262	1.0242	0.5692	0.109*	
C5	0.4825 (4)	1.02091 (19)	0.5694 (7)	0.082 (2)	
H5	0.4923	1.0835	0.5688	0.098*	
C6	0.5673 (3)	0.9628 (2)	0.5700 (6)	0.0594 (14)	
H6	0.6339	0.9866	0.5698	0.071*	
C7	0.6156 (6)	0.7104 (3)	0.5704 (10)	0.0697 (16)	
H7A	0.5714	0.6975	0.4620	0.104*	
H7B	0.5796	0.6966	0.6751	0.104*	
H7C	0.6773	0.6740	0.5722	0.104*	
C8	0.7023 (4)	0.8299 (5)	0.4097 (7)	0.0624 (14)	
H8A	0.6595	0.8148	0.3009	0.094*	
H8B	0.7650	0.7946	0.4153	0.094*	
H8C	0.7193	0.8934	0.4086	0.094*	
C9	0.7151 (4)	0.8261 (5)	0.7446 (7)	0.0623 (15)	
H9A	0.7481	0.8843	0.7365	0.093*	

H9B	0.7670	0.7794	0.7583	0.093*
H9C	0.6749	0.8255	0.8476	0.093*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.04678 (18)	0.03161 (15)	0.04784 (18)	0.00106 (13)	0.01690 (13)	−0.00100 (13)
Br1	0.0383 (4)	0.0526 (5)	0.0341 (3)	−0.0033 (3)	0.0054 (3)	0.0011 (3)
Br2	0.0381 (3)	0.0426 (3)	0.0431 (3)	0.00585 (18)	0.00755 (18)	−0.00786 (17)
Br3	0.0605 (3)	0.0296 (2)	0.0590 (3)	0.0028 (2)	0.0003 (2)	0.00449 (19)
Cl1	0.0383 (4)	0.0526 (5)	0.0341 (3)	−0.0033 (3)	0.0054 (3)	0.0011 (3)
Cl2	0.0381 (3)	0.0426 (3)	0.0431 (3)	0.00585 (18)	0.00755 (18)	−0.00786 (17)
Cl3	0.0605 (3)	0.0296 (2)	0.0590 (3)	0.0028 (2)	0.0003 (2)	0.00449 (19)
N1	0.0381 (19)	0.042 (2)	0.0400 (18)	−0.0041 (15)	0.0046 (14)	0.0012 (14)
C1	0.040 (2)	0.040 (2)	0.041 (2)	−0.0041 (17)	0.0006 (17)	−0.0010 (16)
C2	0.047 (3)	0.068 (4)	0.072 (4)	−0.014 (3)	0.005 (2)	0.005 (3)
C3	0.046 (3)	0.120 (7)	0.098 (5)	0.005 (4)	0.001 (3)	−0.006 (5)
C4	0.084 (5)	0.103 (6)	0.082 (5)	0.047 (5)	−0.013 (4)	−0.011 (4)
C5	0.091 (5)	0.064 (4)	0.089 (5)	0.025 (4)	−0.003 (4)	−0.008 (4)
C6	0.065 (4)	0.040 (3)	0.071 (3)	−0.004 (2)	−0.004 (3)	0.005 (2)
C7	0.082 (4)	0.038 (3)	0.090 (5)	−0.001 (3)	0.007 (3)	−0.002 (3)
C8	0.046 (3)	0.093 (5)	0.050 (3)	0.001 (3)	0.017 (2)	−0.001 (3)
C9	0.051 (3)	0.085 (4)	0.048 (3)	0.002 (3)	−0.008 (2)	0.001 (3)

Geometric parameters (Å, º)

Cd1—Br1	2.5332 (8)	C3—H3	0.93
Cd1—Br3	2.5361 (6)	C4—C5	1.39
Cd1—Br2	2.5782 (5)	C4—H4	0.93
Cd1—Cl1^{i}	2.7178 (8)	C5—C6	1.39
Cd1—Br1^{i}	2.7178 (8)	C5—H5	0.93
Cd1—Br2^{ii}	3.1795 (5)	C6—H6	0.93
Br1—Cd1^{ii}	2.7178 (8)	C7—H7A	0.96
N1—C1	1.483 (4)	C7—H7B	0.96
N1—C7	1.499 (6)	C7—H7C	0.96
N1—C8	1.507 (5)	C8—H8A	0.96
N1—C9	1.513 (5)	C8—H8B	0.96
C1—C2	1.39	C8—H8C	0.96
C1—C6	1.39	C9—H9A	0.96
C2—C3	1.39	C9—H9B	0.96
C2—H2	0.93	C9—H9C	0.96
C3—C4	1.39		
Br1—Cd1—Br3	117.92 (3)	C4—C3—H3	120.0
Br1—Cd1—Br2	120.74 (3)	C2—C3—H3	120.0
Br3—Cd1—Br2	120.79 (2)	C3—C4—C5	120.0
Br1—Cd1—Cl1^{i}	89.70 (2)	C3—C4—H4	120.0
Br3—Cd1—Cl1^{i}	98.00 (2)	C5—C4—H4	120.0

Br2—Cd1—Cl1^{i}	89.78 (2)	C6—C5—C4	120.0
Br1—Cd1—Br1^{i}	89.70 (2)	C6—C5—H5	120.0
Br3—Cd1—Br1^{i}	98.00 (2)	C4—C5—H5	120.0
Br2—Cd1—Br1^{i}	89.78 (2)	C5—C6—C1	120.0
Cl1^{i}—Cd1—Br1^{i}	0.00 (4)	C5—C6—H6	120.0
Br1—Cd1—Br2^{ii}	80.904 (19)	C1—C6—H6	120.0
Br3—Cd1—Br2^{ii}	91.835 (17)	N1—C7—H7A	109.5
Br2—Cd1—Br2^{ii}	89.796 (16)	N1—C7—H7B	109.5
Cl1^{i}—Cd1—Br2^{ii}	168.79 (2)	H7A—C7—H7B	109.5
Br1^{i}—Cd1—Br2^{ii}	168.79 (2)	N1—C7—H7C	109.5
Cd1—Br1—Cd1^{ii}	97.81 (3)	H7A—C7—H7C	109.5
C1—N1—C7	112.1 (4)	H7B—C7—H7C	109.5
C1—N1—C8	109.0 (4)	N1—C8—H8A	109.5
C7—N1—C8	109.1 (5)	N1—C8—H8B	109.5
C1—N1—C9	109.5 (4)	H8A—C8—H8B	109.5
C7—N1—C9	107.6 (4)	N1—C8—H8C	109.5
C8—N1—C9	109.4 (4)	H8A—C8—H8C	109.5
C2—C1—C6	120.0	H8B—C8—H8C	109.5
C2—C1—N1	121.3 (3)	N1—C9—H9A	109.5
C6—C1—N1	118.7 (3)	N1—C9—H9B	109.5
C3—C2—C1	120.0	H9A—C9—H9B	109.5
C3—C2—H2	120.0	N1—C9—H9C	109.5
C1—C2—H2	120.0	H9A—C9—H9C	109.5
C4—C3—C2	120.0	H9B—C9—H9C	109.5

Br3—Cd1—Br1—Cd1^{ii}	103.65 (3)	C9—N1—C1—C2	−117.8 (4)
Br2—Cd1—Br1—Cd1^{ii}	−67.89 (3)	C7—N1—C1—C6	−179.0 (4)
Cl1^{i}—Cd1—Br1—Cd1^{ii}	−157.45 (4)	C8—N1—C1—C6	−58.1 (4)
Br1^{i}—Cd1—Br1—Cd1^{ii}	−157.45 (4)	C9—N1—C1—C6	61.6 (4)
Br2^{ii}—Cd1—Br1—Cd1^{ii}	16.407 (19)	N1—C1—C2—C3	179.4 (4)
C7—N1—C1—C2	1.6 (5)	N1—C1—C6—C5	−179.5 (3)
C8—N1—C1—C2	122.5 (4)		

Symmetry codes: (i) x, $-y+1$, $z+1/2$; (ii) x, $-y+1$, $z-1/2$.