Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# *catena*-Poly[trimethylphenylammonium [[bromidocadmate(II)]-$\mu$-bromido-$\mu$-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

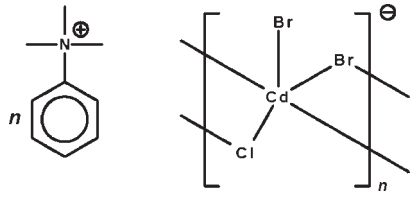
Received 10 February 2010; accepted 12 February 2010

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(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
$\beta$ = 95.1590 (8)°
$V$ = 1399.97 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 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).

The authors thank the University of Malaya (RG020/09AFR) for supporting this study.

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

## References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Lo, K. M. & Ng, S. W. (2009). *Acta Cryst.* E**65**, m560.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *publCIF*. In preparation.

# supplementary materials

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

# *catena*-Poly[trimethylphenylammonium [[bromidocadmate(II)]-$\mu$-bromido-$\mu$-chlorido]]

**K. M. Lo and S. W. Ng**

## 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.

## 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.

## Figures

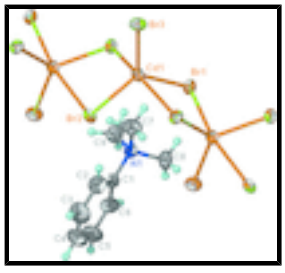


Fig. 1. Displacement ellipsoid plot (Barbour, 2001) of a portion of polymeric $C_9H_{14}N^+$ $[CdBr_2Cl]^-$ at the 50% probability level. H are drawn as spheres of arbitrary radius. The disorder in the halogen sites not shown.

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

*Crystal data*

| | |
|---|---|
| $(C_9H_{14}N)[CdBr_2Cl]$ | $F(000)$ = 840 |
| $M_r$ = 443.88 | $D_x$ = 2.106 Mg m$^{-3}$ |
| Monoclinic, *Cc* | Mo *K*α radiation, λ = 0.71073 Å |
| Hall symbol: C -2yc | Cell parameters from 5267 reflections |
| *a* = 12.9403 (2) Å | θ = 2.7–28.3° |
| *b* = 14.7059 (2) Å | μ = 7.43 mm$^{-1}$ |
| *c* = 7.3866 (1) Å | *T* = 293 K |
| β = 95.1590 (8)° | Block, colourless |

| | |
|---|---|
| $V$ = 1399.97 (3) Å$^3$ | 0.30 × 0.25 × 0.20 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX diffractometer | 3068 independent reflections |
| Radiation source: fine-focus sealed tube | 2966 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int}$ = 0.026 |
| ω scans | $\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.1° |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −16→16 |
| $T_{min}$ = 0.378, $T_{max}$ = 0.746 | $k$ = −19→19 |
| 6431 measured reflections | $l$ = −9→9 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.027 | H-atom parameters constrained |
| $wR(F^2)$ = 0.070 | $w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 0.0436P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.06 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 3068 reflections | $\Delta\rho_{max}$ = 0.67 e Å$^{-3}$ |
| 124 parameters | $\Delta\rho_{min}$ = −0.68 e Å$^{-3}$ |
| 10 restraints | Absolute structure: Flack (1983), 1451 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.021 (9) |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | 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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, °)*

| | | | |
|---|---|---|---|
| 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.

**Fig. 1**