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N-Methylethylenediammonium tetraiodocadmium(II)

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Key indicators

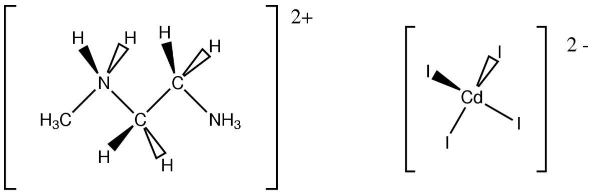
Single-crystal X-ray study
T = 83 K
Mean σ(C–C) = 0.006 Å
R factor = 0.019
wR factor = 0.045
Data-to-parameter ratio = 26.6

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

The title compound, $(C_3H_{12}N_2)[CdI_4]$ [abbreviated (MEDA)-CdI_4], contains isolated *N*-methylethylenediammonium cations and tetrahedral tetraiodidecadmate(II) anions, forming segregated layers. Hydrogen bonding between cations and anions provides three-dimensional stability to the crystal structure.

Comment

The (MEDA)CdI_4 structure, (I), is composed of isolated tetrahedral $[CdI_4]^{2-}$ monomeric anions and individual *N*-methylethylenediammonium (MEDA) cations, as displayed in Fig. 1. There does not appear to be any unusual distortion in the metal–halide structure due to the presence of the MEDA cation. The cadmium coordination involves Cd—I bond distances of 2.7958 (8), 2.7857 (7), 2.7736 (7), and 2.7683 (7) Å, with bond angles ranging between 104.82 (3) and 113.023 (13)°. The average Cd—I distance for isolated $[CdI_4]^{2-}$ anions from the Cambridge Structural Database (Version 5.24 of November 2002; Allen, 2002) is 2.778 (8)° [Cd—I range 2.728–2.813 Å and I—Cd—I bond angle range 101.98–118.46°].



(I)

Both the CdI_4 anions and the MEDA cations form individual layers that run parallel to the *ab* plane (Fig. 2). Three-dimensional stability is achieved through hydrogen bonding between these layers by the NH_3^+ groups on one side and the NH_2^+ groups on the other side of each cation layer (Fig. 2). Table 1 lists the various hydrogen-bond contacts.

The secondary ammonium group of the MEDA cation has one normal and one bifurcated hydrogen bond, resulting in asymmetrical H···I contacts. The primary ammonium group has two bifurcated hydrogen bonds (see Table 1). This unique arrangement of hydrogen bonding forces the *trans,gauche* conformation of the MEDA cations (Fig. 2).

Experimental

Crystals were prepared by the slow evaporation of a solution containing (MEDA)I_2 (0.655 g, 2 mmol) and CdI_2 (1.465 g, 4 mmol) dissolved in 20 ml of deionized water and acidified by 10 drops of 1 *M* HI. The resulting crystals were fragile colorless parallelepipeds.

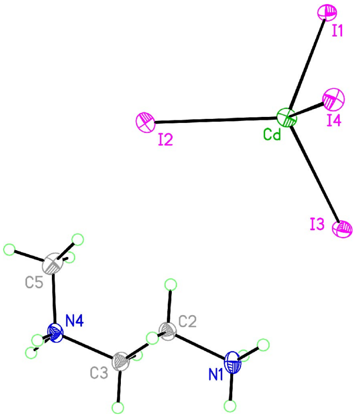


Figure 1
The asymmetric unit of the structure. Displacement ellipsoids are drawn at the 50% probability level.

Crystal data

$(C_3H_{12}N_2)[CdI_4]$
$M_r = 696.15$
Monoclinic, $P2_1/c$
$a = 8.4114\ (17)$ Å
$b = 10.891\ (2)$ Å
$c = 15.245\ (3)$ Å
$\beta = 100.55\ (3)^\circ$
$V = 1372.9\ (5)$ Å^3
$Z = 4$
$D_x = 3.368$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7493 reflections
$\theta = 2.5$–30.0°
$\mu = 10.54$ mm^{-1}
$T = 83\ (2)$ K
Parallelepiped, colorless
0.20 × 0.10 × 0.10 mm

Data collection

Bruker/Siemens SMART APEX diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.189$, $T_{max} = 0.349$
17982 measured reflections
2418 independent reflections
2320 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.0^\circ$
$h = -10 \rightarrow 10$
$k = -12 \rightarrow 12$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.045$
$S = 1.16$
2418 reflections
91 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0117P)^2 + 1.6835P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···I4^{i}	0.92	3.01	3.652 (4)	129
N4—H4A···I2^{i}	0.92	3.15	3.695 (4)	120
N4—H4B···I1^{ii}	0.92	2.76	3.565 (4)	147
N1—H1A···I3	0.91	2.81	3.526 (4)	136
N1—H1A···I4^{iii}	0.91	3.27	3.779 (4)	118
N1—H1B···I1^{iv}	0.91	3.07	3.691 (4)	127
N1—H1B···I3^{iv}	0.91	3.27	3.945 (4)	133
N1—H1C···I2^{v}	0.91	2.70	3.607 (4)	177

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

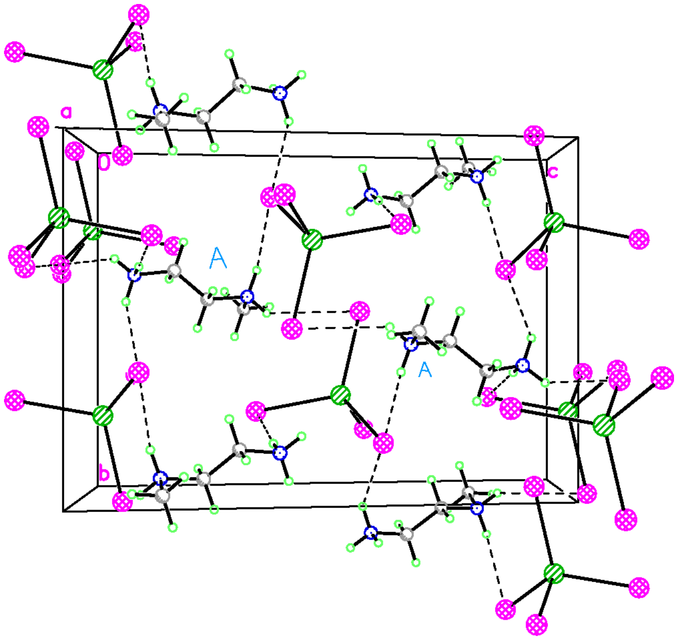


Figure 2
Illustration of the MEDA cation and the CdI_4 anion layers parallel to the *ab* plane. The dashed lines represent hydrogen bonds. Only the two central cations (labeled *A*) show all of the H···I interactions.

H atoms were positioned geometrically and refined using a riding model, with U_{iso} for the secondary C—H and N—H groups constrained to be $1.2U_{eq}$ of the carrier atom, while those of the primary C—H and N—H protons were set at $1.5U_{eq}$. There is a residual of 0.727 e Å^{-3} *ca* 0.703 Å from Cd1.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bruker (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SAINT-Plus*. Version 6.22. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2002). *SMART*. Version 5.626. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

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