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Bis(pyridinium) tetrabromocadmate(II) monohydrate

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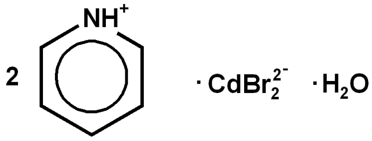
The title compound, $(C_5H_6N)_2[CdBr_4]\cdot H_2O$, consists of discrete anions, cations and solvent water molecules. Both pyridinium cations and the tetrabromocadmate anion possess a crystallographically imposed mirror symmetry. The solvent water molecule and one pyridinium cation form intermolecular N—H···O and O—H···Br hydrogen bonds, giving a three-dimensional hydrogen-bonded structure.

Key indicators

Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.007 Å
R factor = 0.030
wR factor = 0.077
Data-to-parameter ratio = 23.0

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



(I)

Experimental

Pyridine (0.010 mol, 0.791 g) and $CdBr_2$ (0.005 mol, 1.3601 g) were dissolved in dilute HBr (10 ml, 1 *M*) and the resultant solution was evaporated slowly at *ca* 323 K. The title compound was obtained as prismatic colourless crystals after several days.

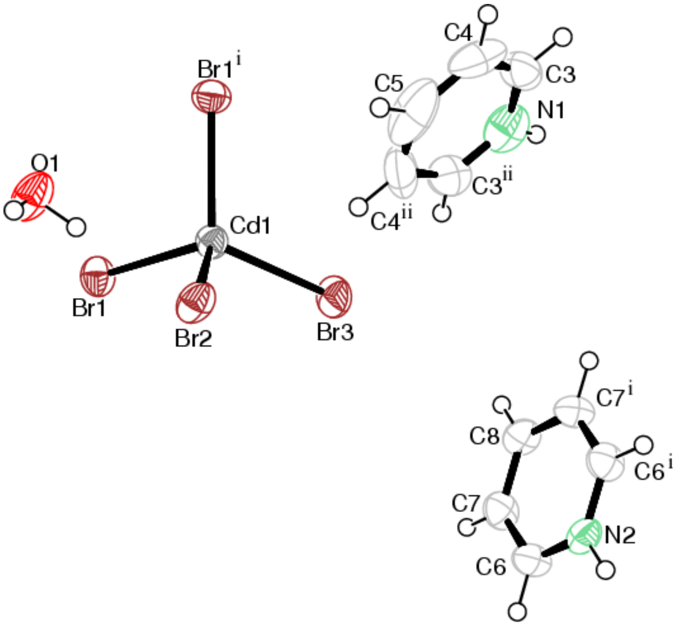


Figure 1
ORTEP-3 drawing (Farrugia, 1997) of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been assigned arbitrary radii. [Symmetry codes: (i) $x, \frac{1}{2} - y, z$; ii) $x, \frac{3}{2} - y, z$.]

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Crystal data

$(C_5H_6N)_2[CdBr_4]\cdot H_2O$
$M_r = 610.27$
Orthorhombic, *Pnma*
$a = 14.951$ (2) Å
$b = 9.1564$ (15) Å
$c = 12.815$ (2) Å
$V = 1754.3$ (5) Å^3
$Z = 4$
$D_x = 2.311$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2299 reflections
$\theta = 2.1$–$28.3°$
$\mu = 10.35$ mm^{-1}
$T = 223$ (2) K
Prism, colourless
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.234$, $T_{\max} = 0.355$
22963 measured reflections
2299 independent reflections
1776 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.060$
$\theta_{\max} = 28.3°$
$h = -19 \rightarrow 19$
$k = -12 \rightarrow 12$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.077$
$S = 1.10$
2299 reflections
100 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2 + 2.3887P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.66$ e Å^{-3}
$\Delta\rho_{\min} = -0.66$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—Br1	2.5736 (6)	Cd1—Br2	2.5983 (9)
Cd1—Br3	2.5838 (9)		
Br1$^{\rm i}$—Cd1—Br1	106.84 (3)	Br1—Cd1—Br2	108.188 (18)
Br1—Cd1—Br3	114.474 (19)	Br3—Cd1—Br2	104.38 (3)

Symmetry code: (i) $x, \frac{1}{2} - y, z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2$\cdots$O1$^{\rm ii}$	0.87	1.80	2.669 (7)	176
O1—H9$\cdots$Br3$^{\rm iii}$	0.86 (8)	2.50 (8)	3.365 (6)	175 (7)
O1—H10$\cdots$Br2	0.90 (9)	2.36 (9)	3.263 (6)	174 (8)

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

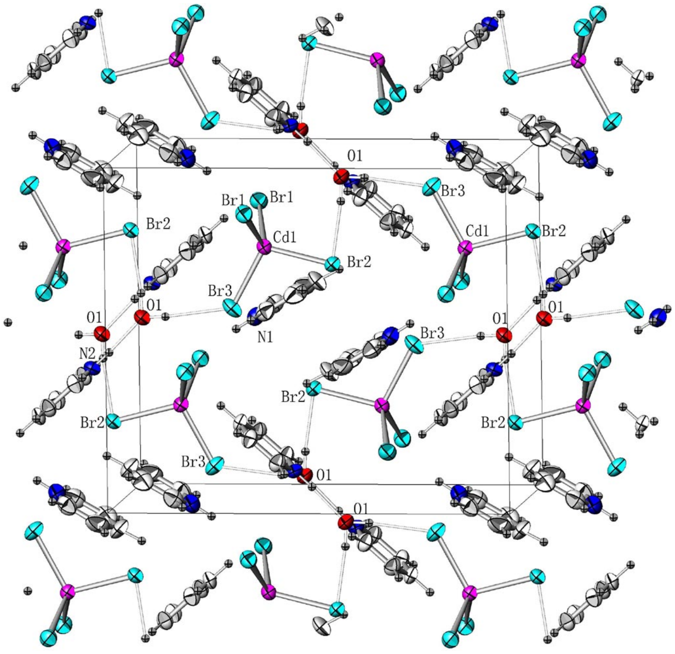

Figure 2
Fig. 2. The crystal packing, viewed approximately down the *b* axis, showing the hydrogen-bonded network (dashed lines) formed by atom O1 associated with N2, Br2 and Br3.

H atoms attached to C and N were constrained to an ideal geometry, with C—H and N—H distances of 0.94 and 0.87 Å, respectively, and refined as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. Water H atoms were initially located in a difference Fourier map and their positions were refined freely along with an isotropic displacement parameter.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXTL*.

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