Ag2—I^{iv}	2.7885 (10)	Ag5b—O4	2.320 (10)
Ag2—I^{i}	3.1692 (10)	Ag5b—O3^{vi}	2.329 (10)
Ag3—O2^{v}	2.388 (5)	Ag5b—O6	2.373 (7)
Ag3—O4	2.401 (5)	Ag5b—O5^{vi}	2.575 (8)
Ag3—O6^{vi}	2.454 (5)	Ag5b—I^{iv}	3.171 (9)
Ag3—O7^{vii}	2.460 (5)	P1—O3	1.509 (4)
Ag3—I^{iv}	3.0217 (11)	P1—O4	1.511 (5)
Ag4a—O2^{viii}	2.327 (7)	P1—O2	1.519 (5)
Ag4a—O6^{i}	2.429 (7)	P1—O1	1.614 (4)
Ag4a—O5	2.535 (9)	P2—O7	1.512 (5)
Ag4a—O3^{ix}	2.692 (9)	P2—O5	1.521 (5)
Ag4a—I	2.890 (6)	P2—O6	1.522 (5)
Ag4b—O2^{viii}	2.361 (8)	P2—O1	1.633 (5)
P1—O1—P2	133.2 (3)		

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

The data collection included all Friedel pairs in the specified *hkl* range in order to confirm the correctness of the absolute structure. The description of the silver density distribution in a silver-ion conductor by displacement ellipsoids yields only approximate values. Since the quality of the crystals and the data-to-parameter ratio did not allow for a full anharmonic treatment, only the most prominent anharmonicities have been accounted for by the introduction of split positions for Ag4 and Ag5. The occupancies of these split positions were not refined.

Data collection: *DIF*4 (Stoe & Cie, 1992*a*). Cell refinement: *DIF*4. Data reduction: *REDU*4 (Stoe & Cie, 1992*b*). Program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*b*). Program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*). Molecular graphics: *ORTEP*III (Burnett & Johnson, 1996) and *CERIUS*^{2} (Molecular Simulations, 1995).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: BR1248). Services for accessing these data are described at the back of the journal.

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Cadmium sodium trivanadate

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Abstract

The crystal structure of $Cd_{3.23}Na_{1.41}V_{0.36}(VO_4)_3$ has been resolved. This structure is built up of MO_6 (M = Cd, Na and V) octahedral chains linked by VO_4 tetrahedra, and is characterized by cationic disorder and tunnels running along the c axis.

Comment

The orthovanadate formed with cadmium and sodium, $Cd_4Na(VO_4)_3$, was synthesized by Olazcuaga *et al.* (1977) and the crystal structure was later reported in the non-centrosymmetric space group $Pn2_1a$ (Ben Amara, Vlasse *et al.*, 1979). Later still, a new refinement of the same structure was carried out in the centrosymmetric space group $Pnma$ (Abrahams & Marsh, 1983) when non-linear and piezoelectric tests evidenced no asymmetric character of the lattice. In the present work, we report the crystal structure of a new monoclinic cadmium sodium vanadate.

The network is composed of VO_4 tetrahedra [V—O 1.702 (3)–1.734 (3) Å] and MO_6 octahedra (M = Cd, Na and V). Cadmium is encountered in four different sites, three octahedral and one square planar, while sodium is located with cadmium in two mixed sites; however, one of these is almost entirely occupied by sodium, the amount of cadmium being very small but not negligible. The three MO_6 octahedra show various degrees of deformation from idealized geometry. $Cd4O_6$ is regular, $Cd3/V3O_6$ is slightly deformed and $Cd1/Na1O_6$ is quite irregular, with Cd1/Na1—O distances in the range 2.342 (3)–2.709 (3) Å. VO_4 tetrahedra are linked to MO_6 octahedra by the sharing of a corner. $Cd1/Na1O_6$

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octahedra are linked together by the sharing of an edge and form zigzag chains parallel to the *c* axis. Similarly, Cd3/V3O_6 and Cd4O_6 share an edge and are linked in zigzag chains extending in the $[\bar{1}01]$ direction (Fig. 1). The linking of several types of polyhedra forms tunnels parallel to the *c* axis, in which Cd2/Na2 atoms are found. Fig. 2 shows how the polyhedra give rise to the tunnels.

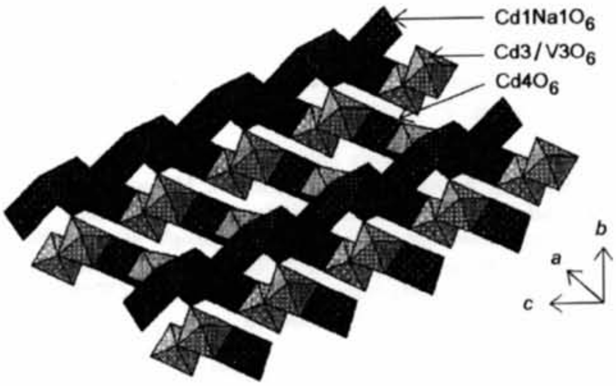

Fig. 1. Perspective view of the $Cd_{3.23}Na_{1.41}V_{0.36}(VO_4)_3$ structure showing the zigzag chains of MO_6 octahedra. V and Cd2/Na2 have been omitted for clarity.

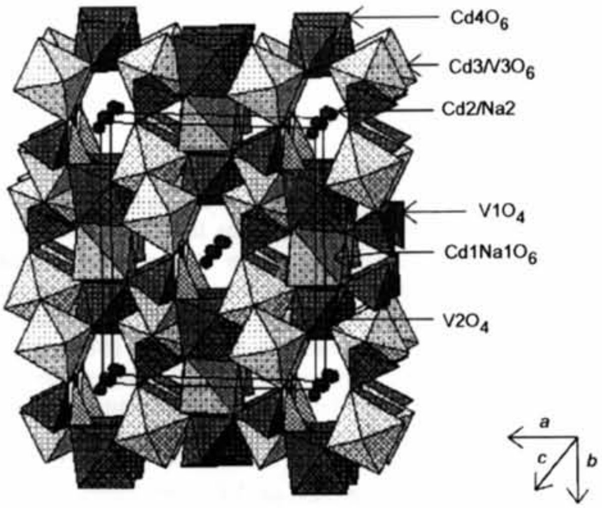

Fig. 2. A three-dimensional view of the crystal structure of $Cd_{3.23}Na_{1.41}V_{0.36}(VO_4)_3$, showing tunnels occupied by Cd2/Na2 running along the *c* axis.

The structure is characterized by cation disorder in three sites, two situated on special positions (4*b* and 4*e*) and the other in the general position 8*f* of space group *C*2/*c*. Refinement of this model without the constraint Cd/Na = 4 leads to the stoichiometry $Cd_{3.23}Na_{1.41}V_{0.36}(VO_4)_3$. This formula is not surprising because vanadium can readily adopt different oxidation states. As a matter of fact, there is a partial reduction of the small quantity of vanadium. A bond-valence analysis based on the empirical formula proposed by Brown & Altermatt (1985) and the electrical neutrality of the molecule confirm the existence of V^{3+} in the Cd3 site and V^{5+} in all other tetrahedral sites.

The cationic distributions obtained in this case are Cd1/Na1 = 55/45%, Cd2/Na2 = 4/96%, Cd3/V3 = 82/18% and Cd4 = 100%; for ease of use, these sites are referred to as *M*1, *M*2, *M*3 and *M*4, respectively. However, the anisotropic atomic displacement parameters in the *M*1 and *M*2 sites are slightly high, as indicated by the ellipsoids represented in Fig. 3. The strong amplitude of thermal vibration of *M*2 is directed perpendicular to the plane of the four short bonds and not along the tunnel as one would expect.

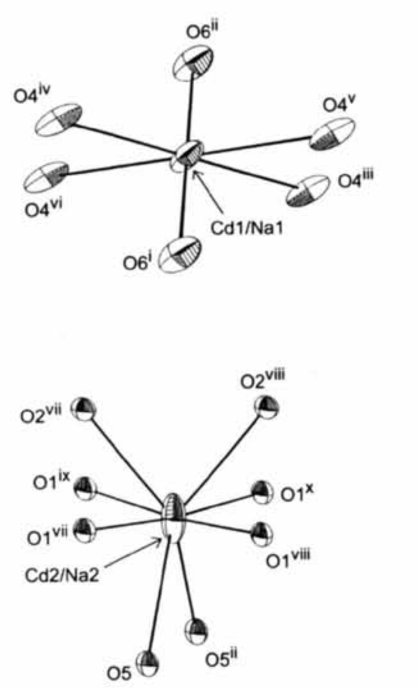

Fig. 3. Atomic displacement ellipsoids of the Cd1/Na1 (*M*1) and Cd2/Na2 (*M*2) sites. The symmetry codes are as in Table 2.

These cationic distributions explain the short Cd3/-V3—O distances for a Cd—O bond length and the distortion of the site around Cd1/Na1 and Cd2/Na2. Therefore, Cd1/Na1O_6 is a lengthened octahedron, whereas the Cd2/Na2 site has square-planar coordination if the distances to O2 [3.085 (4) Å (×2)] and O5 [3.152 (5) Å (×2)] are neglected in favor of the Cd2/Na2—O distances of 2.480 (3) (×2) and 2.534 (3) Å (×2).

The disorder of Cd2/Na2 in the tunnels may presage ionic mobility for this material. The cadmium and sodium cations have approximatly the same ionic radius, which might help ionic migration better than in the isomorphous $Cd_4K(VO_4)_3$ compound. In the monoclinic and orthorhombic varieties of the cadmium sodium vanadate, CdO_6, Cd/VO_6 and Cd/NaO_6 octahedra are arranged so as to build up chains connected by VO_4 tetrahedra. However, the architectures of these chains are totally different in the two phases. In the case of the orthorhombic variety, the chains are linear (Abrahams & Marsh, 1983).

Compounds isotypic with the title monoclinic phase are relatively rare, however, there are three known compounds which adopt this structure, namely $Cu_4Na(AsO_4)_3$, $Mg_2Cu_2K(VO_4)_3$ and $Cd_4K(VO_4)_3$ (Pertlik, 1987; Von Postel & Muller-Buschbaum, 1993; Eddahby *et al.*, 1997; Holt *et al.*, 1977). The homologous monophosphate $Cd_4Na(PO_4)_3$ (Ben Amara, Olazcuaga *et al.*, 1979) has a structure different from that of both $Cd_4Na(VO_4)_3$ and the title compound.

Experimental

Crystals of $Cd_{3.23}Na_{1.41}V_{0.36}(VO_4)_3$ were isolated by slow cooling of the melt (1223 K) obtained from a stoichiometric mixture prepared initially for the synthesis of $CdNaVO_4$. This compound seems to result from the thermal decomposition of $CdNaVO_4$ and partial reduction of a small quantity of vanadium according to the following equilibrium:

$$3.23CdNaVO_4 + 0.065V_2O_5 \rightarrow Cd_{3.23}Na_{1.41}V_{0.36}(VO_4)_3 + 0.91Na_2O + 0.17O_2.$$

Direct preparation of the expected monoclinic phase, $Cd_4Na(VO_4)_3$, always leads to the orthorhombic form, which is apparently the most stable.

Crystal data

$Cd_{3.23}Na_{1.41}V_{0.36}(VO_4)_3$
$M_r = 758.69$
Monoclinic
$C2/c$
$a = 12.564$ (4) Å
$b = 13.452$ (4) Å
$c = 7.021$ (2) Å
$\beta = 113.74$ (3)°
$V = 1086.2$ (6) Å^3
$Z = 4$
$D_x = 4.639$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 12$–30°
$\mu = 9.080$ mm^{-1}
$T = 293$ (2) K
Block
0.12 × 0.11 × 0.06 mm
Colorless, transparent

Data collection

Stoe–Siemens AED-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: ψ scan (Stoe & Cie, 1987)
$T_{min} = 0.350$, $T_{max} = 0.580$
4076 measured reflections
1586 independent reflections

$R_{int} = 0.036$
$\theta_{max} = 30.02°$
$h = -17 \rightarrow 16$
$k = -18 \rightarrow 18$
$l = 0 \rightarrow 9$
3 standard reflections every 100 reflections intensity decay: negligible

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.063$
$S = 1.100$
1586 reflections
101 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 3.0202P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 1.229$ e Å^{-3}
$\Delta\rho_{min} = -1.101$ e Å^{-3}
Extinction correction: *SHELXL*93
Extinction coefficient: 0.00096 (11)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij}a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Cd1†	0	1/2	1/2	0.0421 (3)
Na1‡	0	1/2	1/2	0.0421 (3)
Cd2§	0	0.9859 (3)	3/4	0.0548 (13)
Na2¶	0	0.9859 (3)	3/4	0.0548 (13)
Cd3††	0.71699 (3)	0.65529 (2)	0.63663 (4)	0.01820 (12)
V3‡‡	0.71699 (3)	0.65529 (2)	0.63663 (4)	0.01820 (12)
Cd4	0	0.27268 (3)	3/4	0.01838 (12)
V1	0.72895 (5)	0.60904 (5)	0.12732 (9)	0.01706 (15)
V2	0	0.70621 (6)	3/4	0.0198 (2)
O1	0.6547 (3)	0.5000 (2)	0.1060 (5)	0.0287 (6)
O2	0.6600 (3)	0.6694 (2)	−0.1066 (5)	0.0262 (6)
O3	0.7170 (3)	0.6784 (2)	0.3205 (5)	0.0324 (7)
O4	0.8757 (2)	0.5906 (2)	0.1883 (6)	0.0347 (8)
O5	−0.0422 (3)	0.7771 (2)	0.5282 (5)	0.0257 (6)
O6	−0.1014 (3)	0.6237 (2)	0.7610 (6)	0.0423 (9)

† Site occupancy = 0.550 (3). ‡ Site occupancy = 0.450 (3). § Site occupancy = 0.041 (4). ¶ Site occupancy = 0.959 (4). †† Site occupancy = 0.819 (3). ‡‡ Site occupancy = 0.181 (4).

Table 2. *Selected geometric parameters (Å, °)*

*M*1, *M*2, *M*3 and *M*4 represent the Cd1/Na1, Cd2/Na2, Cd3/V3 and Cd4 sites, respectively.

*M*1—O6^{i}	2.342 (3)	*M*3—O5^{ix}	2.223 (3)
*M*1—O6^{ii}	2.342 (3)	*M*3—O3	2.241 (3)
*M*1—O4^{iii}	2.442 (3)	*M*3—O3^{xiv}	2.363 (3)
*M*1—O4^{iv}	2.442 (3)	*M*4—O2^{xv}	2.314 (3)
*M*1—O4^{v}	2.709 (4)	*M*4—O2^{xvi}	2.314 (3)
*M*1—O4^{vi}	2.709 (4)	*M*4—O5^{xiii}	2.319 (3)
*M*2—O1^{vii}	2.480 (3)	*M*4—O5^{xvii}	2.319 (3)
*M*2—O1^{viii}	2.480 (3)	*M*4—O4^{iii}	2.338 (3)
*M*2—O1^{ix}	2.534 (3)	*M*4—O4^{v}	2.338 (3)
*M*2—O1^{x}	2.534 (3)	V1—O3	1.702 (3)
*M*2—O2^{viii}	3.085 (4)	V1—O1	1.712 (3)
*M*2—O2^{vii}	3.085 (4)	V1—O2	1.721 (3)
*M*2—O5	3.152 (5)	V1—O4	1.734 (3)
*M*2—O5^{ii}	3.152 (5)	V2—O6	1.715 (3)
*M*3—O6^{xi}	2.132 (4)	V2—O6^{ii}	1.715 (3)
*M*3—O2^{xii}	2.200 (3)	V2—O5^{ii}	1.717 (3)
*M*3—O1^{xiii}	2.211 (3)	V2—O5	1.717 (3)
O3—V1—O1	108.6 (2)	O6—V2—O6^{ii}	99.3 (3)
O3—V1—O2	109.25 (15)	O6—V2—O5^{ii}	106.4 (2)
O1—V1—O2	105.9 (2)	O6^{ii}—V2—O5^{ii}	115.9 (2)
O3—V1—O4	107.9 (2)	O6—V2—O5	115.9 (2)
O1—V1—O4	112.75 (14)	O6^{ii}—V2—O5	106.4 (2)
O2—V1—O4	112.3 (2)	O5^{ii}—V2—O5	112.6 (2)

Symmetry codes: (i) $x, 1-y, z-\frac{1}{2}$; (ii) $-x, y, \frac{3}{2}-z$; (iii) $1-x, 1-y, 1-z$; (iv) $x-1, y, z$; (v) $x-1, 1-y, \frac{1}{2}+z$; (vi) $1-x, y, \frac{1}{2}-z$; (vii) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$; (viii) $x-\frac{1}{2}, \frac{1}{2}+y, 1+z$; (ix) $\frac{1}{2}-x, \frac{3}{2}-y, 1-z$; (x) $x-\frac{1}{2}, \frac{3}{2}-y, \frac{1}{2}+z$; (xi) $1+x, y, z$; (xii) $x, y, 1+z$; (xiii) $x, 1-y, \frac{1}{2}+z$; (xiv) $\frac{3}{2}-x, \frac{3}{2}-y, 1-z$; (xv) $\frac{1}{2}-x, y-\frac{1}{2}, \frac{1}{2}-z$; (xvi) $x-\frac{1}{2}, y-\frac{1}{2}, 1+z$; (xvii) $-x, 1-y, 1-z$.

The electron-density peaks $\Delta\rho_{max}$ and $\Delta\rho_{min}$ are at 0.82 and 0.79 Å from Cd4 and Cd3, respectively.

Data collection: *DIF*4 (Stoe & Cie, 1987). Cell refinement: *DIF*4. Data reduction: *REDU*4 (Stoe & Cie, 1987). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ATOMS* (Dowty, 1995).

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fac-Triaquatrichloroindium(III)

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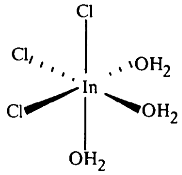
Abstract

The structure of the title compound, $[InCl_3(H_2O)_3]$, features In atoms in a distorted *fac*-octahedral geometry and involves a three-dimensional network of intermolecular hydrogen bonding. It is the first structurally characterized example of a discrete tris-hydrate of a Group 13 M^{III} halide (M = B, Al, Ga or In).

Comment

The title compound, (I), was obtained as a side-product from an anaerobic study of indium trichloride with *n*-butyl acetate (3 equivalents) in hexane. This solution was stored at 278 K for several days, resulting in the slow deposition of colourless block-shaped crystals which were stable within the reaction mixture. On removal, the crystals rapidly decomposed (hydrolysis), even under an atmosphere of dry argon. The crystal for the present X-ray study was obtained by manipulating the crystals under a layer of sodium-dried nujol. The trace of water required in the formation of compound (I) was probably derived from the commercial sample of *n*-butyl acetate.



(I)

Although several stable hydrates of the Group 13 trihalides MX_3 (M = B, Al, Ga or In; X = halogen) are known, structural reports are restricted to anionic forms such as $K[InBr_4(H_2O)_2]$ (Wignacourt *et al.*, 1980) and $Cs_2[InCl_5(H_2O)]$ (Atkinson & Field, 1970). The $InCl_3(H_2O)_3$ moieties in $[fac\text{-}InCl_3(H_2O)_3]\cdot$18-crown-6 (Streltsova *et al.*, 1991) and $[fac\text{-}InCl_3(H_2O)_3]\cdot3$(dioxane) (Whitlow & Gabe, 1975) feature an extensive network of hydrogen bonding between the coordinated water molecules and the organic ligands which serves to stabilize each complex. Similarly, for $InCl_3\cdot4H_2O$, it was concluded that an $[InCl_3(H_2O)_2]$ unit was enmeshed in a network of hydrogen bonding incorporating solvate water molecules (Wignacourt *et al.*, 1982).

In the title compound, which contains two molecules in the asymmetric unit (Fig. 1), each six-coordinate metal centre exhibits a distorted *fac*-octahedral geometry, with interligand angle ranges Cl—In—Cl 95.29 (3)–103.65 (3)° and O—In—O 77.71 (9)–83.96 (10)° (Table 1); these values are consistent with a steric effect opening up the angles between the larger ligand atoms. A survey of complexes of indium(III) halides (Knop *et al.*, 1987) predicts the In—Cl bond distance for an $InCl_3$ fragment in a neutral six-coordinate environment to be 2.432 (17) Å, based upon a linear function of the coordination number and the charge. The observed In—Cl bond lengths in the title com-