ically. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). $(\Delta/\sigma)_{max} = 0.0$, $\Delta\rho < 1.61$ e Å^{-3}, $R = 0.041$, $wR = 0.048$, $w = 1$, $S = 3.0$. Atomic parameters are given in Table 1.* Bond distances and angles are given in Table 2. A view of the structure of $SrCoP_2O_7$ along the b axis is given in Fig. 1.

Related literature. $SrCoP_2O_7$ is isostructural with $CaCuP_2O_7$ (Riou & Goreaud, 1990) and derives from α-$Ca_2P_2O_7$ (Calvo, 1968). It is worth pointing out that cobalt atoms tend to be located close to the centre of the $[CoO_5]$ pyramid, unlike copper atoms which are located close to the square basal plane leading to a long Cu—O apical distance [2·201 (2) Å], in agreement with the Jahn–Teller effect of the Cu^{2+} cation.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53924 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
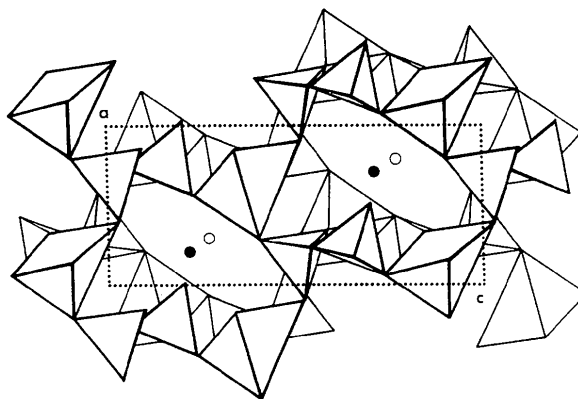

Fig. 1. $SrCoP_2O_7$: polyhedron representation of the structure viewed along [010]. Full circle for Sr at $x = 0.66$ and $x = 0.84$. Open circle for Sr at $x = 0.16$ and $x = 0.34$.

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Structure of Vanadyl(IV) Dihydrogenarsenate

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Abstract. Vanadyl(IV) dihydrogenarsenate, $VO(H_2AsO_4)_2$, $M_r = 348.8$, tetragonal, $P4/ncc$, $a = 9.131$ (1), $c = 8.146$ (3) Å, $V = 679.1$ (4) Å^3, $Z = 4$, $D_x = 3.412$ Mg m^{-3}, $\lambda = 0.71073$ Å, $\mu = 11.089$ mm^{-1}, $F(000) = 660$, $T = 297$ K, $R = 0.0255$, $wR = 0.0260$ for 248 unique reflections with $I > 3.0\sigma(I)$. The compound, which is composed of chains of VO_6 octahedra and $AsO_2(OH)_2$ tetrahedra, is isostructural with $VO(H_2PO_4)_2$ [Linde, Gorbunova, Lavrov & Kuznetsov (1979). *Dokl. Akad. Nauk SSSR*, **244**, 1411–1414]. The coordination environment of the V atom is distorted octahedral. Four O atoms in the equatorial plane of the octahedron are from different As tetrahedra and the two axial O atoms are from different VO^{2+} groups. The V atom is displaced from the plane of four equatorial O atoms towards one of the apical O atoms, giving rise to $\cdots V{=}O\cdots V{=}O\cdots$ chains.

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Experimental. Blue-green crystals of $VO(H_2AsO_4)_2$ were obtained in an attempt to prepare the arsenic analog of $K_2V_3P_4O_{17}$ (Lii, Tsai & Wang, 1990; Leclaire, Chahboun, Groult & Raveau, 1988) by heating a reaction mixture of $K_4V_2O_7$, V_2O_3, VO_2 and 12 ml 40% H_3AsO_4(aq) in a 23 ml teflon-lined autoclave at 503 K for 3 d followed by slow cooling at 10 K h^{-1}. The structure was determined from single-crystal X-ray diffraction. Peak profile analysis (ω scan) on the rod-like crystals using a Nicolet R3m/V diffractometer with Mo $K\alpha$ radiation ($\lambda = 0.71073$ Å) indicated that most reflections were not suitable for indexing and intensity data collection. Many had to be selected from the reaction product before a satisfactory crystal was obtained. Finally a piece of dimensions $0.05 \times 0.05 \times 0.12$ mm was selected for X-ray analysis. The unit-cell parameters were determined by a least-squares fit of 16 reflections with 2θ ranging from 9 to 30°. The intensity data were collected up to $2\theta = 55°$ ($\sin\theta_{max}/\lambda = $

Table 1. *Atomic coordinates and equivalent isotropic displacement coefficients* ($\AA^2$)

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
As(1)	0·4668 (1)	0·5332 (1)	0·2500	0·008 (1)
V(1)	0·2500	0·2500	0·1952 (3)	0·008 (1)
O(1)	0·3886 (6)	0·6123 (5)	0·0793 (6)	0·018 (1)
O(2)	0·4345 (4)	0·3549 (5)	0·2435 (6)	0·012 (1)
O(3)	0·2500	0·2500	−0·0008 (9)	0·015 (2)
H(1)*	0·4436	0·6853	0·0463	0·05

* The position of H(1) was derived from a difference map.

Table 2. *Selected bond lengths* ($\AA$) *and angles* (°)

V(1)—O(2)	1·977 (4)	As(1)—O(1)	1·722 (5)
V(1)—O(3)	1·597 (8)	As(1)—O(2)	1·655 (4)
V(1)—O(2A)	1·977 (4)	As(1)—O(1D)	1·722 (5)
V(1)—O(2B)	1·977 (4)	As(1)—O(2D)	1·655 (4)
V(1)—O(2C)	1·977 (4)	O(1)—H(1)	0·877
V(1)—O(3E)	2·476 (8)		

O(2)—V(1)—O(3)	101·5 (2)	O(1)—As(1)—O(2)	108·2 (2)
O(2)—V(1)—O(2A)	157·1 (3)	O(1)—As(1)—O(1D)	107·7 (3)
O(3)—V(1)—O(2A)	101·5 (2)	O(1)—As(1)—O(2D)	111·0 (2)
O(2)—V(1)—O(2B)	87·7 (1)	O(2)—As(1)—O(2D)	110·6 (3)
O(3)—V(1)—O(2B)	101·5 (2)	O(1D)—As(1)—O(2D)	108·2 (2)
O(2A)—V(1)—O(2B)	87·7 (1)	As(1)—O(1)—H(1)	109·2
O(2)—V(1)—O(2C)	87·7 (1)		
O(3)—V(1)—O(2C)	101·5 (2)		
O(2A)—V(1)—O(2C)	87·7 (1)		
O(2B)—V(1)—O(2C)	157·1 (3)		
O(2)—V(1)—O(3E)	78·5 (2)		
O(3)—V(1)—O(3E)	180·0 (1)		
O(2A)—V(1)—O(3E)	78·5 (2)		
O(2B)—V(1)—O(3E)	78·5 (2)		
O(2C)—V(1)—O(3E)	78·5 (2)		

Symmetry codes: (A) $\frac{1}{2} - x, \frac{1}{2} - y, z$; (B) $\frac{1}{2} - y, x, z$; (C) $y, \frac{1}{2} - x, z$; (D) $1 - y, 1 - x, \frac{1}{2} - z$; (E) $y, x, \frac{1}{2} + z$.

0·650 $\AA^{-1}$) with $\theta/2\theta$ scans. A periodic check of three standard reflections did not reveal any significant variation in intensity. A total of 530 reflections were measured in the range $0 \le h \le 8$, $0 \le k \le 11$, $0 \le l \le 10$. Scan width of 1·02° plus $K\alpha$ separation and scan speed 2·44–14·95° min^{-1}. The space group $P4/ncc$ (No. 130) was determined from the systematic absences $hk0$, $h + k = 2n + 1$; $0kl$, $l = 2n + 1$; hhl, $l = 2n + 1$. No absorption correction was applied ($T_{min}/T_{max} = 0·918/0·940$). After corrections for Lorentz and polarization effects, 248 unique structure amplitudes with $I > 3\sigma(I)$ were obtained ($R_{int} = 0·015$). The structure was solved by direct methods and refined by full-matrix least squares based on F values. All of the non-H atoms were refined with anisotropic temperature factors. At convergence $R = 0·0255$, $wR = 0·0260$, $w = [\sigma^2(F) + 0·0007F^2]^{-1}$, $\sigma^2(F)$ based on counting statistics, $(\Delta/\sigma)_{max} = 0·004$, $S = 1·01$, $(\Delta\rho)_{max} = 1·03$, $(\Delta\rho)_{min} = -1·02$ e $\AA^{-3}$. As(1) lies on a twofold axis of rotation running parallel to the *ab* diagonal. V(1) and O(3) lie on a

fourfold axis of rotation parallel to the *c*-axis direction. The other atoms lie in general positions. The position of H(1) was located on a difference map. Its coordinates with a fixed U (0·05 $\AA^2$) were included in the final structure-factor calculation. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). All calculations were performed on a DEC MicroVAX II computer system using *SHELXTL-Plus* (Sheldrick, 1990). Atomic parameters are given in Table 1, and selected bond distances and angles in Table 2.* A view of the structure of VO(H$_2$AsO$_4$)$_2$ along [001] is shown in Fig. 1. There is no hydrogen bond in the structure.

Related literature. VO(H$_2$AsO$_4$)$_2$ is isostructural with VO(H$_2$PO$_4$)$_2$ (Linde, Gorbunova, Lavrov & Kuznetsov, 1979). This compound was first synthesized and its thermal decomposition products were studied by Chernorukov, Korshunov & Egorov (1978).
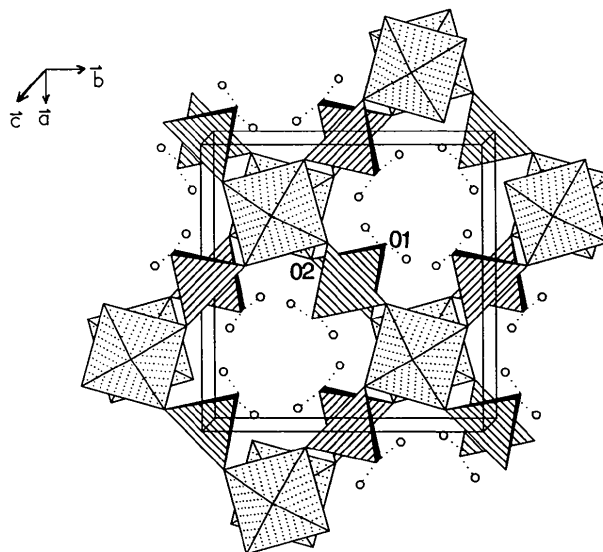
Fig. 1. Polyhedral representation of VO(H$_2$AsO$_4$)$_2$ projected approximately along the *c* axis. The corners of the octahedra and the tetrahedra are O atoms. The V and As atoms are at the center of each octahedron and tetrahedron, respectively. H atoms, which are bonded to the two O(1) atoms forming one edge of the AsO$_4$ tetradron, are represented by small circles.

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Structure of Decastrontium Hexachromate(V) Difluoride

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Abstract. $Sr_{10}(CrO_4)_6F_2$, $M_r = 1610.1$, hexagonal, $P6_3/m$, $a = 9.956$ (1), $c = 7.437$ (1) Å, $V = 638.4$ Å^3, $Z = 1$, $D_x = 4.188$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 22.89$ mm^{-1}, $F(000) = 734$, $T = 296$ K. The structure was refined to $R = 0.029$, $wR = 0.035$ for 564 reflections. The title compound has an apatite-type structure with slightly distorted chromate tetrahedra (Cr—O = 1.693–1.698 Å, O—Cr—O = 106.9–114.9°).

Experimental. $Sr_{10}(CrO_4)_6F_2$ was prepared by the high-temperature reaction of a stoichiometric mixture of $SrCO_3$, SrF_2 and Cr_2O_3 at 1400 K in a corundum crucible. To avoid hydrolysis all experiments were carried out in a dry N_2 atmosphere. After slowly cooling (50 K h^{-1}), dark bluish-green needles were obtained. A crystal fragment (approximately $0.10 \times 0.10 \times 0.60$ mm) was used for data collection on an Enraf–Nonius CAD-4 diffractometer (Mo $K\alpha$, $\lambda = 0.71073$ Å, graphite monochromator, $T = 296$ K). Lattice parameters were refined using 2θ values of 98 reflections taken from a powder diffraction pattern (Cu $K\alpha_1$, $\lambda = 1.54051$ Å, $10.2 \le 2\theta \le 114.4°$, Si as internal standard). Intensities measured for $3 \le \theta \le 30°$; ω–2θ-scan technique, scan width $(0.70 + 0.60\tan\theta)°$. Three standard reflections indicated no decay throughout data collection. An experimental correction for absorption and decay was not applied. After Lp corrections (program *CADLP*; Müller, Schmidt & Massa, 1979), merging 637 data with $I > 1.0\sigma(I)$ out of 769 collected intensities ($0 \le h \le 14$, $0 \le k \le 14$, $0 \le l \le 10$) yielded 564 unique reflections ($R_{int} = 0.029$) which were used for all calculations (*SHELX*76; Sheldrick, 1976).

The systematic absences (00l: $l = 2n + 1$) indicated the space groups $P6_3$ or $P6_3/m$. The results of the refinement confirmed the latter space group. The atomic positions of Sr were derived from a Patterson map; the remaining atoms were found in successive difference Fourier maps. Final $R = 0.029$, $wR = 0.035$, $w = 1.62/\sigma^2(F_o)$, $(\Delta/\sigma)_{max} < 0.01$ for 40 variables (all atoms had anisotropic temperature factors). Maximum and minimum features in the final difference Fourier map were $+0.97$, -2.85 e Å^{-3}. Atomic scattering factors, f' and f'' values were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). Bond distances and angles were calculated using the program *SADIAN* (Baur & Wenninger, 1969).

Final atomic coordinates and equivalent isotropic temperature factors are given in Table 1, derived interatomic distances and angles are in Table 2.* The structure, well known as an apatite-type structure, contains Jahn–Teller-distorted (d^1)-CrO_4^{3-} tetrahedra (Fig. 1). The F atom is located in the channel position $2(a)$ $\{0,0,\frac{1}{4}\}$.

Related literature. Isomorphic replacements in compounds of the general formula $A_{10}(BO_4)_6X_2$ provide an immense variety of apatite-type and apatite-like structures. Many apatites, both natural and synthetic, contain a high proportion of carbonate; others show cation or anion deficiency (Wyckoff, 1965). Single-crystal data, only available for a small number of these compounds, often proved a lower symmetry than indicated by powder data. A typical example is the doubling of the c axis in oxipyromorphite $Pb_{10}(PO_4)_6O$ (Fischer, 1988). Finally, the relationship of all these different