

Infrared optical properties and vibrational studies of barium nitroprusside trihydrate are reported by Piro, González, Aymonino & Castellano (1987) and similar studies of sodium nitroprusside dihydrate by Piro, Castellano, Guida & Aymonino (1989). The attenuated total reflectance infrared spectrum of the latter compound is reported by Guida, Piro, Castellano & Aymonino (1989).

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References

- AMALVY, J. I., VARETTI, E. L. & AYMONINO, P. J. (1985). *J. Phys. Chem. Solids*, **46**, 1153–1161.
 AMALVY, J. I., VARETTI, E. L., AYMONINO, P. J., CASTELLANO, E. E., PIRO, O. E. & PUNTE, G. (1986). *J. Crystallogr. Spectrosc. Res.* **16**, 537–555.
 GUIDA, J. A., PIRO, O. E., CASTELLANO, E. E. & AYMONINO, P. J. (1989). *J. Chem. Phys.* In the press.
 HAMILTON, W. C. (1959). *Acta Cryst.* **12**, 609–610.
 JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.
 PIRO, O. E., CASTELLANO, E. E., GUIDA, J. A. & AYMONINO, P. J. (1989). *Phys. Rev. B*, **39**, 1919–1926.
 PIRO, O. E., GONZÁLEZ, S. R., AYMONINO, P. J. & CASTELLANO, E. E. (1987). *Phys. Rev. B*, **36**, 3125–3134.
 SHELDRICK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.

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Structure of CsVP₂O₇

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Abstract. Caesium vanadium pyrophosphate, $M_r = 357.790$, monoclinic, $P2_1/c$, $a = 7.701$ (3), $b = 9.997$ (2), $c = 8.341$ (4) Å, $\beta = 104.82$ (4)°, $V = 620.8$ (2) Å³, $Z = 4$, $D_x = 3.828$ g cm⁻³, $Mo K\alpha$, $\lambda = 0.7093$ Å, $\mu = 77.9$ cm⁻¹, $F(000) = 656$, $T = 296$ K, $R = 0.029$, $wR = 0.038$ for 1241 reflections with $I > 2.5\sigma(I)$. The title compound is isostructural with CsMoP₂O₇ [Lii & Haushalter (1987). *Acta Cryst.* **C43**, 2036–2038]. The Cs⁺ ions are located in tunnels formed by pyrophosphate groups and V³⁺O₆ octahedra and are each coordinated by ten O atoms.

Experimental. Yellow crystals of CsVP₂O₇ crystallized as a minor product in an attempt to prepare 'CsV₃P₄O₁₇' by heating a mixture of Cs₄V₂O₇, V, V₂O₅ and P₂O₅ at 1423 K in a sealed silica tube. Enraf-Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation; $\theta/2\theta$ scan technique. Cell parameters on crystal 0.08 × 0.11 × 0.16 mm from least-squares procedure on 25 reflections ($21 < 2\theta < 30^\circ$). Corrections for absorption effects were based on ψ scans of a few suitable reflections with χ values close to 90°. Max./min. transmission factors: 1.000/0.870. Systematic absences: $0k0$, $k = 2n$; $h0l$, $l = 2n$. Total of 1413 reflections measured with $(\sin\theta/\lambda)_{\max} = 0.595$ Å⁻¹ ($-9 \leq h \leq 9$, $0 \leq k \leq 12$, $0 \leq l \leq 10$). No significant variation in intensities of three standards monitored

every 300 reflections. Scan width of $(0.70 + 0.35\tan\theta)^\circ$ and scan speed $5.5^\circ \text{ min}^{-1}$. 1241 unique structure amplitudes with $I > 2.5\sigma(I)$. The structure was solved by direct methods and refined by full-matrix least squares based on F values. All of the atoms were refined anisotropically. At convergence $R = 0.029$, $wR = 0.038$, $w = 1/\sigma^2(F)$, $\sigma^2(F)$ based on counting statistics, $(\Delta/\sigma)_{\max} = 0.001$, $S = 0.779$, $(\Delta\rho)_{\max} = 1.15$, $(\Delta\rho)_{\min} = -1.34$ e Å⁻³. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974). All calculations were performed on a VAX 11/780 computer system using the NRC VAX program (Larson, Lee, Le Page & Gabe, 1986). Atomic parameters are given in Table 1, bond distances and

Table 1. Positional parameters and equivalent isotropic thermal parameters

$$B_{\text{eq}} = \frac{1}{3} \sum_i \sum_j \beta_{ij} a_i \cdot a_j$$

	x	y	z	B _{eq} (Å ²)
Cs	0.80211 (6)	0.20510 (5)	0.96096 (6)	1.112 (17)
V	0.75946 (14)	-0.39878 (11)	0.74130 (13)	0.28 (4)
P(1)	0.86838 (21)	-0.09430 (18)	0.66697 (20)	0.33 (6)
P(2)	0.57426 (22)	-0.37300 (17)	0.31783 (20)	0.31 (6)
O(1)	0.9052 (6)	-0.2372 (5)	0.7296 (6)	0.59 (17)
O(2)	0.6777 (7)	-0.3974 (6)	0.4931 (6)	1.05 (19)
O(3)	0.6119 (6)	-0.5660 (5)	0.7280 (6)	0.62 (18)
O(4)	0.8423 (7)	-0.4163 (5)	0.9841 (6)	0.84 (19)
O(5)	0.5639 (6)	-0.2725 (5)	0.7673 (6)	0.67 (18)
O(6)	0.9882 (6)	-0.5031 (5)	0.7336 (6)	0.55 (16)
O(7)	0.6817 (6)	-0.4513 (5)	0.2033 (6)	0.54 (17)

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Table 2. Selected bond lengths (Å) and bond angles (°)

V—O(1)	1.984 (5)	P(2)—O(5 ^{III})	1.511 (5)
V—O(2)	2.004 (5)	P(2)—O(7)	1.617 (5)
V—O(3)	2.009 (5)	Cs—O(1 ^I)	2.978 (5)
V—O(4)	1.969 (5)	Cs—O(1 ^{II})	3.126 (5)
V—O(5)	2.019 (5)	Cs—O(2 ^{IV})	3.253 (6)
V—O(6)	2.062 (5)	Cs—O(3 ^{VI})	3.114 (5)
P(1)—O(1)	1.522 (5)	Cs—O(3 ^V)	3.273 (5)
P(1)—O(4 ^{III})	1.491 (5)	Cs—O(4 ^I)	3.395 (5)
P(1)—O(6 ^V)	1.507 (5)	Cs—O(5 ^{VII})	2.979 (5)
P(1)—O(7 ^{VI})	1.610 (5)	Cs—O(6 ^V)	3.304 (5)
P(2)—O(2)	1.495 (5)	Cs—O(6 ^{VI})	3.104 (5)
P(2)—O(3 ^{II})	1.514 (5)	Cs—O(7 ^{VI})	3.301 (5)
O(1)—V—O(2)	88.62 (22)	O(5)—V—O(6)	170.5 (2)
O(1)—V—O(3)	173.93 (21)	O(1)—P(1)—O(4 ^{III})	112.5 (3)
O(1)—V—O(4)	94.85 (21)	O(1)—P(1)—O(6 ^V)	109.4 (3)
O(1)—V—O(5)	86.73 (20)	O(1)—P(1)—O(7 ^{VI})	107.3 (3)
O(1)—V—O(6)	84.94 (20)	O(4 ^{III})—P(1)—O(6 ^V)	114.1 (3)
O(2)—V—O(3)	85.69 (22)	O(4 ^{III})—P(1)—O(7 ^{VI})	106.2 (3)
O(2)—V—O(4)	175.23 (23)	O(6 ^V)—P(1)—O(7 ^{VI})	106.8 (3)
O(2)—V—O(5)	93.50 (21)	O(2)—P(2)—O(3 ^{II})	114.5 (3)
O(2)—V—O(6)	90.94 (21)	O(2)—P(2)—O(5 ^{III})	114.0 (3)
O(3)—V—O(4)	90.71 (22)	O(2)—P(2)—O(7)	105.9 (3)
O(3)—V—O(5)	95.71 (20)	O(3 ^{II})—P(2)—O(5 ^{III})	109.8 (3)
O(3)—V—O(6)	93.03 (20)	O(3 ^{II})—P(2)—O(7)	104.5 (3)
O(4)—V—O(5)	89.97 (21)	O(5 ^{III})—P(2)—O(7)	107.5 (3)
O(4)—V—O(6)	86.12 (20)	P(1 ^{III})—O(7)—P(2)	126.2 (3)

Symmetry codes: (i) $2.0-x, -y, 2.0-z$; (ii) $1.0-x, -1-y, 1-z$; (iii) $x, -0.5-y, -0.5+z$; (iv) $x, -0.5-y, 0.5+z$; (v) $2.0-x, 0.5+y, 1.5-z$; (vi) $x, 1.0+y, z$; (vii) $1.0-x, 0.5+y, 1.5-z$.

angles in Table 2.* A view of the structure of CsVP_2O_7 along the c axis is shown in Fig. 1.

Related literature. CsVP_2O_7 is isostructural with CsMoP_2O_7 (Lii & Haushalter, 1987).

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51798 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure Cristalline des Bis(dichromate) de Bismuth et de Thallium et Bis(dichromate) d'Ammonium et de Bismuth

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Abstract. $\text{BiTl}(\text{Cr}_2\text{O}_7)_2$, $M_r = 845.3$, monoclinic, $P2_1/a$, $a = 8.310$ (11), $b = 17.092$ (7), $c = 8.645$ (7) Å, $\beta = 91.65$ (4)°, $V = 1227.3$ Å³, $Z = 4$, $D_m = 4.52$ (1), $D_x = 4.574$ (12) Mg m⁻³, Mo $K\alpha$, $\lambda = 0.71069$ Å, $\mu = 30.44$ mm⁻¹, $F(000) = 1488$, room temperature, $R = 0.07$ for 1680 reflections. $\text{Bi}(\text{NH}_4)(\text{Cr}_2\text{O}_7)_2$, M_r

0108-2701/89/081211-03\$03.00

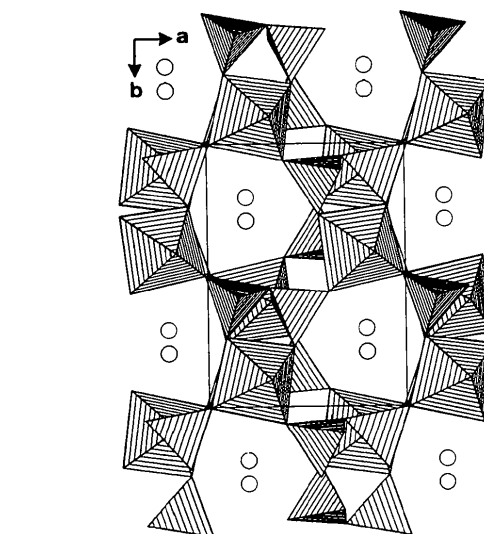


Fig. 1. STRUPL084 drawing (Fischer, 1985) displaying the framework of CsVP_2O_7 , and the tunnels occupied by Cs^+ ions. The c axis is perpendicular to this plane. In this polyhedral representation of the structure, the corners of the octahedra and tetrahedra are O^{2-} ions, the V and P ions are at the center of each octahedron and tetrahedron, respectively, and the circles represent the Cs^+ ions.

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References

- FISCHER, R. X. (1985). *J. Appl. Cryst.* **18**, 258–262.
International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
 LARSON, A. C., LEE, F. L., LE PAGE, Y. & GABE, E. J. (1986). *The NRC VAX Crystal Structure System*. National Research Council of Canada, Ottawa, Canada.
 LII, K. H. & HAUSHALTER, R. C. (1987). *Acta Cryst.* **C43**, 2036–2038.

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