Table 1. *Atomic parameters*

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}(Å^2)
Yb(1)	0	0	0·2742 (1)	0·30 (1)
Yb(2)	$\frac{1}{3}$	$\frac{2}{3}$	0·2330 (1)	0·37 (1)
Mn	0·3269 (5)	0	0	0·30 (2)
O(1)	0·3040 (17)	0	0·1610 (9)	0·5 (1)
O(2)	0·6436 (23)	0	0·3343 (8)	0·6 (2)
O(3)	0	0	0·4779 (15)	0·3 (1)
O(4)	$\frac{1}{3}$	$\frac{2}{3}$	0·0136 (13)	1·4 (2)

Table 2. *Bond lengths* (Å) *and angles* (°)

Yb(1)—O(1)	(3×)	2·255 (10)	O(2^i)—O(2^v)	(3×)	3·731 (17)
Yb(1)—O(2^i)	(3×)	2·263 (13)	O(1)—O(2^i)	(6×)	2·841 (12)
Yb(1)—O(3)		2·354 (17)	O(1^i)—O(1^{ii})	(3×)	3·652 (9)
Yb(1)—O(3^{iii})		3·425 (17)	O(2^i)—O(2^{ii})	(3×)	3·375 (11)
Yb(2)—O(1^i)	(3×)	2·267 (7)	O(1^i)—O(2^i)	(3×)	2·868 (16)
Yb(2)—O(2^i)	(3×)	2·273 (7)	O(1^{ii})—O(2^i)	(3×)	2·841 (12)
Yb(2)—O(4)		2·536 (15)	O(2^{iv})—O(3^{iii})		2·719 (16)
Yb(2)—O(4^{vii})		3·243 (15)	O(2^{iv})—O(4^{ii})	(2×)	2·844 (13)
Mn—O(3^{iii})		1·992 (4)	O(3^{iii})—O(4^{ii})	(2×)	3·513 (3)
Mn—O(4^{ii})	(2×)	2·040 (2)	O(4^{ii})—O(4^{vi})		3·489 (1)
Mn—O(1)		1·866 (11)	O(1)—O(3^{iii})		2·803 (17)
Mn—O(2^{iv})		1·924 (9)	O(1)—O(4^{ii})	(2×)	2·711 (12)
O(1)—O(1^{ii})	(3×)	3·182 (12)			

O(1)—Yb(1)—O(1^{ii})	(3×)	89·7 (3)	O(3^{iii})—Mn—O(4^{ii})	(2×)	121·2 (1)
O(2^i)—Yb(1)—O(2^v)	(3×)	111·0 (2)	O(4^{ii})—Mn—O(4^{vi})		117·5 (2)
O(1)—Yb(1)—O(2^i)	(6×)	77·9 (2)	O(1)—Mn—O(3^{iii})		93·1 (6)
O(1^i)—Yb(2)—O(1^{ii})	(3×)	107·3 (3)	O(1)—Mn—O(4^{ii})	(2×)	87·8 (5)
O(2^i)—Yb(2)—O(2^{ii})	(3×)	95·9 (4)	O(2^{iv})—Mn—O(3^{iii})		87·9 (6)
O(1^i)—Yb(2)—O(2^i)	(3×)	78·3 (3)	O(2^{iv})—Mn—O(4^{ii})	(2×)	91·7 (5)
O(1^{ii})—Yb(2)—O(2^i)	(3×)	77·5 (4)			

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

parameter g to $0{\cdot}45\,(1)\times10^{-6}$. A final difference electron density map exhibited no peaks higher than 8·7 and lower than $-10{\cdot}9$ e Å^{-3}, all in the vicinity of the Yb atom. The final atomic parameters are given in Table 1.* Selected bond lengths and angles are listed in Table 2 together with their estimated standard deviations. All of the calculations were performed with the *SDP* program system (B. A. Frenz & Associates, Inc., 1985).

Related literature. The structure of $LuMnO_3$ which is isostructural with $YbMnO_3$ was first determined by Yakel *et al.* (1963), and its structure is related to that of $YAlO_3$ (Bertaut & Mareschal, 1963) and $InGaO_3$ (II) (Shannon & Prewitt, 1968).

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53397 (10 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of KVP_2O_7

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Abstract. Potassium vanadium diphosphate, KVP_2O_7, $M_r = 263{\cdot}98$, monoclinic, $P2_1/c$, $a = 7{\cdot}3686\,(3)$, $b = 10{\cdot}0527\,(5)$, $c = 8{\cdot}1874\,(4)$ Å, $\beta = 106{\cdot}580\,(3)°$, $V = 581{\cdot}3\,(7)$ Å^3, $Z = 4$, $D_x = 3{\cdot}02$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 2{\cdot}9$ mm^{-1}, $F(000) = 512$, $T = 294$ K, $R = 0{\cdot}027$, $wR = 0{\cdot}030$ for 2710 independent reflections with $I > 3\sigma(I)$. The title compound is isostructural with $KMoP_2O_7$. The framework is built up from corner-sharing VP_2O_{11} units which delimit cages where K atoms are located. These cavities are interconnected leading to an intersecting tunnel structure.

Experimental. Green crystals of KVP_2O_7 crystallized as a minor product in an attempt to prepare $KV_2P_3O_{12}$: first a mixture of $H(NH_4)_2PO_4$, V_2O_5 and K_2CO_3 in appropriate ratios was heated in a platinum crucible for two hours at 553K to decompose the phosphate and carbonate; in a second step, the appropriate amount of vanadium was added, the

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Table 1. *Positional parameters and their e.s.d.'s*

$B_{eq} = (4/3)[a^2\beta_{11} + b^2\beta_{22} + c^2\beta_{33} + (2ab\cos\gamma)\beta_{12} + (2ac\cos\beta)\beta_{13} + (2bc\cos\alpha)\beta_{23}]$.

	x	y	z	B_{eq}(Å^2)
V	0·23510 (3)	0·10036 (2)	0·26134 (3)	0·364 (2)
P(1)	0·13510 (5)	0·40356 (4)	0·33024 (4)	0·415 (4)
P(2)	0·44366 (5)	0·36225 (4)	0·19165 (5)	0·417 (4)
K	0·82177 (6)	0·17838 (5)	0·44649 (6)	1·406 (5)
O(1)	0·1445 (2)	0·0908 (2)	0·0151 (1)	1·03 (2)
O(2)	0·3213 (2)	0·1077 (2)	0·5136 (2)	1·09 (2)
O(3)	−0·0025 (2)	0·0050 (1)	0·2788 (1)	0·65 (1)
O(4)	0·4554 (2)	0·2162 (1)	0·2413 (2)	0·76 (1)
O(5)	0·3591 (2)	−0·0792 (1)	0·2689 (2)	0·80 (1)
O(6)	0·0831 (2)	0·2650 (1)	0·2556 (2)	0·73 (1)
O(7)	0·3425 (2)	0·4385 (1)	0·3158 (2)	0·72 (1)

product was ground up and placed in an evacuated silica ampoule for 7 days at 1173 K. Crystal 0·072 × 0·072 × 0·132 mm. Enraf–Nonius CAD-4 diffractometer. Unit cell: least squares on 25 reflections, $\pm 2\theta$, $36 < 2\theta < 44°$. Intensity measurement by ω–θ scan of width $(0{\cdot}85 + 0{\cdot}35\tan\theta)°$ and a counter slit aperture of $(1 + \tan\theta)$ mm, values determined by a study of some reflections in the ω–θ plane. Scanning speed adjusted to obtain $\sigma(I)/I < 0{\cdot}018$ or to approach it in a time limited to 60 s. Three standards for count every 7000 s; no appreciable trends. 5188 reflections measured ($h = 14$, $k = 20$, $l = 16$, $\theta < 45°$), 2711 with $I/\sigma(I) \geq 3$ used to solve and refine the structure. No correction made for extinction and absorption. All subsequent calculations on a MicroVAX II with the *SDP* system (B. A. Frenz & Associates, Inc., 1982). All atoms refined anisotropically. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). $(\Delta/\sigma)_{max} = 0{\cdot}004$, $\Delta\rho < 0{\cdot}7$ e Å^{-3}, $R = 0{\cdot}027$, $wR = 0{\cdot}030$, $w = f(\sin\theta/\lambda)$, $S = 1{\cdot}001$. Atomic parameters in Table 1, bond distances and angles in Table 2.*

A view of the structure of KVP_2O_7 projected onto the *ab* plane is shown in Fig. 1.

Related literature. The investigation of the systems *A*–V–P–O (*A* = Na, K, Cs) allowed several alkaline vanadium diphosphates AVP_2O_7 to be isolated in which vanadium exhibits the trivalent oxidation state. The diphosphates $NaVP_2O_7$ (Wang, Lii & Wang, 1989) and $CsVP_2O_7$ (Wang & Lii, 1989) are isotypic with $NaMoP_2O_7$ (Leclaire, Borel, Grandin & Raveau, 1988) and with $CsMoP_2O_7$ (Lii & Haushalter, 1987) respectively. KVP_2O_7 is isostructural with $KMoP_2O_7$ (Leclaire, Borel, Grandin & Raveau, 1989).

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53092 (19 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond lengths* (Å) *and angles* (°) *in* PO_4 *tetrahedra*

P(1)	O(1^{i})	O(3^{ii})	O(6)	O(7)
O(1^{i})	1·496 (1)	2·525 (2)	2·505 (2)	2·498 (2)
O(3^{ii})	113·99 (7)	1·514 (1)	2·481 (2)	2·493 (2)
O(6)	111·96 (9)	109·43 (7)	1·525 (1)	2·530 (2)
O(7)	107·22 (8)	106·07 (7)	107·80 (7)	1·605 (1)

P(2)	O(2^{iii})	O(4)	O(5^{iv})	O(7)
O(2^{iii})	1·510 (1)	2·557 (2)	2·531 (2)	2·478 (2)
O(4)	115·12 (8)	1·520 (1)	2·484 (2)	2·520 (2)
O(5^{iv})	113·59 (8)	109·90 (7)	1·515 (1)	2·493 (2)
O(7)	104·90 (8)	106·96 (7)	105·56 (7)	1·615 (1)

VO_6 octahedron

V	O(1)	O(2)	O(3)	O(4)	O(5)	O(6)
O(1)	1·937 (1)	3·917 (3)	2·813 (3)	2·801 (2)	2·804 (2)	2·767 (2)
O(2)	178·43 (6)	1·981 (1)	2·800 (2)	2·897 (2)	2·818 (2)	2·816 (2)
O(3)	90·10 (5)	88·33 (6)	2·037 (1)	4·072 (3)	2·819 (2)	2·708 (2)
O(4)	89·45 (6)	92·10 (6)	173·27 (5)	2·042 (1)	3·076 (2)	2·822 (2)
O(5)	90·35 (7)	89·64 (6)	88·14 (5)	98·57 (5)	2·016 (1)	3·999 (3)
O(6)	89·54 (6)	90·27 (6)	84·49 (5)	88·79 (5)	172·63 (5)	1·991 (1)

KO_{10} polyhedron

K—O(3^{v})	2·759 (1)	K—O(5^{iv})	3·080 (1)
K—O(6^{vi})	2·766 (1)	K(1)—O(2^{vii})	3·112 (2)
K—O(4)	2·768 (1)	K—O(5^{viii})	3·158 (1)
K—O(3^{viii})	2·919 (1)	K—O(7^{viii})	3·226 (1)
K—O(6^{v})	2·937 (1)	K—O(1^{vi})	3·255 (2)

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

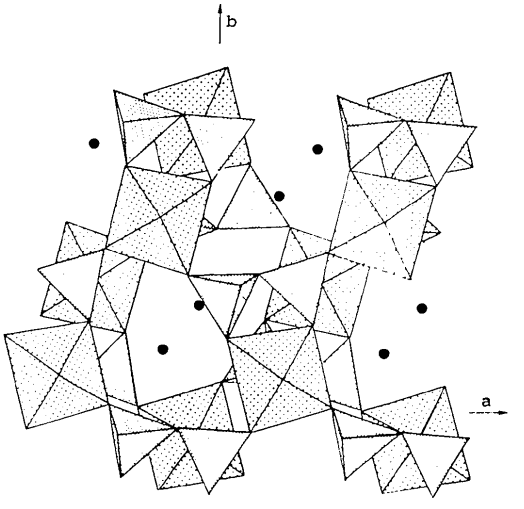

Fig. 1. Projection of the structure of KVP_2O_7 onto the (001) plane.

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