pendent reflections, 104 parameters refined. Maximum and minimum peak heights in difference Fourier map were 0·92 and $-1·94$ e Å^{-3}, ratio of max. (shift/σ) = 0·35. Atomic scattering factors and anomalous-scattering corrections from *International Tables for X-ray Crystallography* (1974). All the calculations were made by *UNICS*III (Sakurai & Kobayashi, 1979) and *ORTEP* (Johnson, 1965). Deviations from the least-squares plane and their e.s.d.'s were calculated by the procedure proposed by Ito (1981).

Atomic parameters are given in Table 1.* Relevant interatomic distances and angles and hydrogen-bond distances are presented in Table 2. Fig. 1 shows the linear-chain structure and the atomic numbering scheme. A stereoscopic view of the crystal structure is shown in Fig. 2.

Related literature. This compound is one of a series of one-dimensional halogen-bridged mixed valence compounds which are of interest due to the strong electron–lattice interaction. Crystal structures and solid state properties of the related compounds, $K_4[Pt_2(P_2O_5H_2)_4X].nH_2O$ (X = Cl, Br and I), were reported (Butler *et al.*, 1988; Clark, Kurmoo, Dawes & Hursthouse, 1986; Che, Herbstein, Schaefer, Marsh & Gray, 1983). The Pt—Pt distance of 2·830 (1) Å is intermediate between the Pt^{II}—Pt^{II} distance [2·925 (1) Å] observed for $K_4[Pt_2(P_2O_5H_2)_4].2H_2O$ (Marsh & Herbstein, 1983; Che *et al.*, 1983) and the Pt^{III}—Pt^{III} distance [2·695 (1) Å] for $K_4[Pt_2(P_2O_5H_2)Cl_2].2H_2O$ (Che *et al.*, 1983).

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* Lists of structure factors, anisotropic thermal parameters, and positional and isotropic thermal parameters of H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51917 (6 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 of $NaVP_2O_7$

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(*Received* 27 *December* 1988; *accepted* 13 *March* 1989)

Abstract. Sodium vanadium pyrophosphate, M_r = 247·874, monoclinic, $P2_1/c$, a = 7·324 (5), b = 7·930 (4), c = 9·586 (6) Å, β = 111·96 (4)°, V = 516·3 (5) Å^3, Z = 4, D_x = 3·189 g cm^{-3}, Mo $K\alpha$, λ = 0·71073 Å, μ = 2·53 mm^{-1}, $F(000)$ = 480, T = 296 K, R = 0·020, wR = 0·022 for 793 reflections with $I > 3·0\sigma(I)$. The compound, which forms a tunnel structure along the [101] direction, is isostructural with $NaMoP_2O_7$ [Leclaire, Borel, Grandin & Raveau (1988). *J. Solid State Chem.* **76**, 131–135]. The Na^+ cations are located in the tunnels formed by pyrophosphate groups and $V^{3+}O_6$ octahedra.

Experimental. The title compound $NaVP_2O_7$ was obtained as yellowish green crystals in an attempt to prepare a sodium analogue of $Cs_2V_3P_4O_{17}$ (Lii, Wang & Wang, 1989) by heating a mixture of $Na_4V_2O_7$, V, VO_2 and P_2O_5 at 1170 K in a sealed quartz tube. Nicolet $R3/V$ diffractometer, graphite-monochromated Mo $K\alpha$ radiation; ω–2θ scan technique. Cell parameters on crystal 0·18 × 0·10 × 0·10 mm from least-squares procedure on 10 reflec-

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0108-2701/89/091417-02$03.00

Table 1. *Positional parameters and equivalent isotropic thermal parameters*

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

	x	y	z	$U_{\rm eq}$(Å^2)
V	0·23917 (6)	0·50786 (5)	0·25143 (5)	0·0056 (2)
P(1)	0·1732 (1)	0·21095 (9)	0·45535 (7)	0·0064 (2)
P(2)	0·5738 (1)	0·25532 (9)	0·45573 (7)	0·0058 (2)
Na	0·2131 (2)	−0·0229 (2)	0·2065 (2)	0·0234 (5)
O(1)	0·5108 (3)	0·0843 (2)	0·8618 (2)	0·0095 (7)
O(2)	0·1926 (3)	0·1982 (2)	0·6183 (2)	0·0097 (7)
O(3)	0·3140 (3)	−0·2119 (2)	0·8780 (2)	0·0105 (7)
O(4)	0·3775 (3)	0·1550 (2)	0·4416 (2)	0·0095 (7)
O(5)	0·0334 (3)	0·0862 (2)	0·3489 (2)	0·0099 (7)
O(6)	0·1347 (3)	0·3921 (2)	0·4010 (2)	0·0097 (7)
O(7)	0·6850 (3)	0·1376 (2)	0·3958 (2)	0·0117 (7)

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

V—O(6)	2·074 (3)	P(2)—O(7)	1·488 (3)
V—O(1$^{\rm i}$)	2·009 (2)	P(2)—O(1$^{\rm i}$)	1·526 (2)
V—O(2$^{\rm i}$)	2·022 (2)	P(2)—O(3$^{\rm iv}$)	1·518 (2)
V—O(3$^{\rm i}$)	1·973 (2)	Na—O(5)	2·385 (3)
V—O(5$^{\rm ii}$)	1·964 (2)	Na—O(1$^{\rm v}$)	2·397 (3)
V—O(7$^{\rm iii}$)	1·986 (3)	Na—O(2$^{\rm i}$)	2·697 (3)
P(1)—O(4)	1·612 (3)	Na—O(3$^{\rm vi}$)	2·600 (3)
P(1)—O(5)	1·513 (2)	Na—O(6$^{\rm vii}$)	2·458 (3)
P(1)—O(6)	1·518 (2)	Na—O(6$^{\rm i}$)	2·954 (3)
P(1)—O(2)	1·518 (2)	Na—O(7$^{\rm viii}$)	3·052 (3)
P(2)—O(4)	1·604 (2)	Na—O(4)	2·547 (3)
O(1$^{\rm i}$)—V—O(6)	91·4 (1)	O(7$^{\rm iii}$)—V—O(5$^{\rm ii}$)	89·5 (1)
O(2$^{\rm i}$)—V—O(6)	93·4 (1)	O(4)—P(1)—O(2)	109·5 (1)
O(2$^{\rm i}$)—V—O(1$^{\rm i}$)	86·5 (1)	O(5)—P(1)—O(2)	115·4 (1)
O(3$^{\rm i}$)—V—O(6)	91·6 (1)	O(5)—P(1)—O(4)	100·4 (1)
O(3$^{\rm i}$)—V—O(1$^{\rm i}$)	89·0 (1)	O(6)—P(1)—O(2)	110·5 (1)
O(3$^{\rm i}$)—V—O(2$^{\rm i}$)	173·3 (1)	O(6)—P(1)—O(4)	106·9 (1)
O(5$^{\rm ii}$)—V—O(6)	84·7 (1)	O(6)—P(1)—O(5)	113·3 (1)
O(5$^{\rm ii}$)—V—O(1$^{\rm i}$)	175·9 (1)	O(7)—P(2)—O(4)	105·0 (1)
O(5$^{\rm ii}$)—V—O(2$^{\rm i}$)	92·6 (1)	O(1$^{\rm i}$)—P(2)—O(4)	107·4 (1)
O(5$^{\rm ii}$)—V—O(3$^{\rm i}$)	92·3 (1)	O(1$^{\rm i}$)—P(2)—O(7)	112·5 (1)
O(7$^{\rm iii}$)—V—O(6)	173·5 (1)	O(3$^{\rm iv}$)—P(2)—O(4)	106·8 (1)
O(7$^{\rm iii}$)—V—O(1$^{\rm i}$)	94·5 (1)	O(3$^{\rm iv}$)—P(2)—O(7)	110·7 (1)
O(7$^{\rm iii}$)—V—O(2$^{\rm i}$)	89·8 (1)	O(3$^{\rm iv}$)—P(2)—O(1$^{\rm i}$)	113·7 (1)
O(7$^{\rm iii}$)—V—O(3$^{\rm i}$)	85·7 (1)	P(1)—O(4)—P(2)	133·3 (1)

Symmetry codes: (i) x, $0·5-y$, $-0·5+z$; (ii) $-x$, $0·5+y$, $0·5-z$; (iii) $1-x$, $0·5+y$, $0·5-z$; (iv) $1-x$, $0·5+y$, $1·5-z$; (v) $1-x$, $-y$, $1-z$; (vi) x, $-0·5-y$, $-0·5+z$; (vii) $-x$, $-0·5+y$, $0·5-z$; (viii) $1-x$, $-0·5+y$, $0·5-z$.

tions ($16 < 2\theta < 29°$). Corrections for absorption effects were based on ψ scans of a few suitable reflections with χ values close to 90°. Max./min. transmission factors: 0·918/0·857. Systematic absences: $0k0$, $k = 2n+1$; $h0l$, $l = 2n+1$. Total of 1073 reflections measured with $(\sin\theta/\lambda)_{\max} = 0·595$ Å^{-1} and in the range $-8 \le h \le 8$, $0 \le k \le 9$, $0 \le l \le 11$. No significant variation in intensities of three standards monitored every 50 reflections. Scan width of $1·0 + K\alpha_1,\alpha_2$ separation and scan speed 2·93–14·95° min^{-1}. 793 unique structure amplitudes with $I > 3·0\sigma(I)$. The structure was solved by direct methods and refined by full-matrix least squares based on F values. All of the atoms were refined with anisotropic temperature factors. At convergence $R = 0·020$, $wR = 0·022$, $w = [\sigma^2(F) + 0·000403F^2]^{-1}$, $\sigma^2(F)$ based on counting statistics, $(\Delta/\sigma)_{\max} = 0·004$, $S = 1·10$, $(\Delta\rho)_{\max} = 0·38$, $(\Delta\rho)_{\min} = -0·32$ e Å^{-3}. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974). All calculations were performed on a DEC MicroVAX II computer system using the *SHELXTL-Plus* programs (Sheldrick, 1987). Atomic parameters are given in Table 1, selected bond distances and angles in Table 2.* A view of the structure of $NaVP_2O_7$ along [101] is shown in Fig. 1.

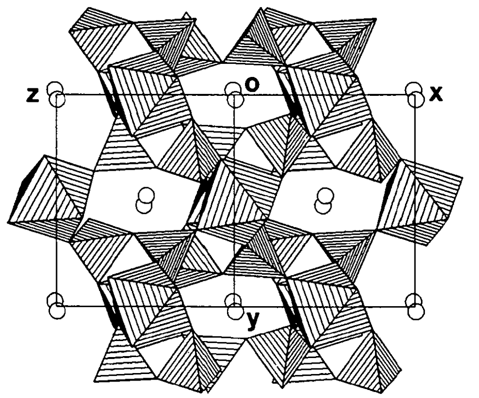

Fig. 1. *STRUPLO*84 drawing (Fischer, 1985) in a direction parallel to [101] displaying the framework of $NaVP_2O_7$ and the tunnels occupied by Na^+ ions. In this polyhedral representation of the structure, the corners of the octahedra and tetrahedra are O^{2-} ions, the V and P ions are at the center of each octahedron and tetrahedron respectively, and the circles represent the Na^+ ions.

Related literature. $NaVP_2O_7$ is isostructural with $NaMoP_2O_7$ (Leclaire, Borel, Grandin & Raveau, 1988).

Support of this study by the National Science Council and the Institute of Chemistry, Academia Sinica, is gratefully acknowledged.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51820 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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