positions about the $M(1)$ centre is 1.59 Å for CuTi$_2$(PO$_4$)$_3$ and 2.18 (neutron), 2.25 Å (X-ray) for CuZr$_2$(PO$_4$)$_3$. The small discrepancy between these last values is probably a result of the experimental conditions. In both cases the refinement procedures were complete and it would not be meaningfull to try to refine more detailed structural models. Actually, the least-squares deviations are usually an underestimation of the real e.s.d. and the Cu positions within $M(1)$ are probably subjected to greater uncertainties than the non-Cu atoms.

At first sight coexistence of two Cu atoms within the same $M(1)$ site seems to be unrealistic. Nevertheless, the two reported fluorescence bands of CuZr$_2$(PO$_4$)$_3$ arise clearly from two distinct excitation centres (Le Polles *et al.*, 1988). The present investigation, however, cannot relate these emissions to the existence of two crystallographic sites of the Cu ion.

As was described in detail by Rath, Holt & Tanimura (1985) various fluorescent Cu$^{\mathrm{I}}$ complexes show low-energy emissions with their maximum located between 550 and 628 nm as Cu$^{\mathrm{I}}$—Cu$^{\mathrm{I}}$ distances are less than 2.8 Å. The question of interaction between metal–metal centres in d^{10} systems is then raised. Previous calculations of Mehotra & Hoffmann (1978) do not exclude soft attractive Cu$^{\mathrm{I}}$—Cu$^{\mathrm{I}}$ interactions and the creation of such pairs could explain the room-temperature luminescence of CuZr$_2$(PO$_4$)$_3$. The occurrence of such pairs with a more precise determination of the Cu$^{\mathrm{I}}$—Cu$^{\mathrm{I}}$ nearest neighbours is presently under examination by an EXAFS investigation.

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A Niobium Silicophosphate Belonging to the Niobium Phosphate Bronze Series: K$_4$Nb$_8$P$_4$SiO$_{34}$

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(*Received* 8 *July* 1991; *accepted* 13 *February* 1992)

Abstract. Niobium potassium silicophosphate, K$_4$Nb$_8$P$_4$SiO$_{34}$, $M_r = 1595.6$, tetragonal $P\bar{4}m2$, $a = 10.6050\,(9)$, $c = 6.4099\,(5)$ Å, $V = 720.9\,(1)$ Å^3, $Z = 1$, $D_x = 3.67$ Mg m^{-3}, $\lambda(\mathrm{Mo}\ K\alpha) = 0.71073$ Å, $\mu = 3.90$ mm^{-1}, $F(000) = 750$, $T = 294$ K, $R = 0.030$, $wR = 0.028$ for 793 reflections with $I > 3\sigma(I)$ out of 3355 unique reflections measured. This oxide is isotypic with Na$_{2-x}$K$_2$Nb$_8$P$_5$O$_{34}$, *i.e.* its structure consists of similar [Nb$_6$P$_4$O$_{26}$]$_\infty$ double layers related to the hexagonal tungsten bronzes which are linked through [Nb$_2$SiO$_8$]$_\infty$ chains instead of [Nb$_2$PO$_8$]$_\infty$ chains. It represents the first member of the niobium phosphate bronze series (K$_3$Nb$_6$P$_4$O$_{26}$)$_n$(KNb$_2M$O$_8$) with M = P, Si. The stability of the structure is discussed in terms of the size of the cages where K atoms are located.

0108-2701/92/101744-04$06.00

Introduction. The different studies of niobium phosphate bronzes (Borel, Goreaud, Grandin, Labbé, Leclaire & Raveau, 1991; Benabbas, Borel, Grandin, Leclaire & Raveau, 1991; Costentin, Borel, Grandin, Leclaire & Raveau, 1991) on the one hand and of niobium silicates (Shanon & Katz, 1970; Choisnet, Nguyen, Groult & Raveau, 1976; Crosnier, Guyomard, Verbaere & Piffard, 1990) on the other, have shown the existence of original frameworks closely related to the tunnel structures of pure octahedral oxygen bronzes. However, silicates and phosphates always exhibit different structures in spite of the similar tetrahedral coordination of Si and P atoms. Moreover, the existence of niobium silicophosphates corresponding to substitution of Si for P in one of these structures has not been observed owing to the different size of these elements and to the great rigidity of the PO_4 and SiO_4 tetrahedra. During the investigation of the K–Nb–P–O system, in evacuated silica ampoules we have isolated a new silicophosphate $K_4Nb_8P_4SiO_{34}$. We report here the structure of this phase which is isotypic with β-$Na_{2-x}K_2Nb_8P_5O_{34}$ (Benabbas, Borel, Grandin, Chardon, Leclaire & Raveau, 1991) and can be considered as a substituted bronzoid of the series $(K_3Nb_6P_4O_{26})_nKNb_2PO_8$.

Experimental. The growth of single crystals of the bronzoid $K_4Nb_8P_4SiO_{34}$ was performed in two steps. First a stoichiometric mixture of K_2CO_3, $H(NH_4)_2PO_4$ and Nb_2O_5 corresponding to the nominal composition 'KNb_2PO_8' was heated at 673 K to eliminate CO_2, NH_3 and H_2O. In the second step, the resulting finely ground product was sealed in an evacuated silica ampoule. This sample was then heated to 1273 K during two months and quenched at room temperature. In this mixture, two sorts of colourless crystals have been isolated. One sort is isotypic with $K_7Nb_{14}P_9O_{60}$, and the other with β-$Na_{2-x}K_2Nb_8P_5O_{34}$. The composition of the second type of crystal '$K_4Nb_8P_4SiO_{34}$' was initially determined by microprobe analysis and then with precision by the structure refinement of the selected crystal.

Subsequently, a reaction to prepare pure compound $K_4Nb_8P_4SiO_{34}$ was performed but synthesis of the pure phase proved unsuccessful.

A crystal of dimensions 0.103 × 0.026 × 0.026 mm was used for data collection on an Enraf–Nonius diffractometer. Unit-cell dimensions were determined by least squares on 25 reflections, $\pm 2\theta$, $18 \leq \theta \leq 22°$. Intensity measurements were made to $\theta = 45°$ with an ω–$\frac{4}{3}\theta$ scan of width $(1 + 0.35\tan\theta)°$ and a counter slit aperture of $(1 + \tan\theta)$ mm; values determined by a study of reflections in the ω–θ plane [h $-0 \rightarrow 21$, k $-0 \rightarrow 21$, l $-0 \rightarrow 12$]. Scanning speed was adjusted to obtain $\sigma(I)/I < 0.018$ or to approach it in 60 s. Three standards (605, 006, 353), monitored for counting every 3600 s and for orientation every 600 reflections, showed no significant trends. No corrections were made for extinction or absorption. The structure was solved by the heavy-atom method. Full-matrix least-squares refinement was based on F. Usual f' and f'' values were obtained from *International Tables for X-ray Crystallography* (1974, Vol. IV). 70 parameters were refined, yielding $R = 0.030$, $wR = 0.028$ [$w = 1/\sigma^2(F)$], $S = 0.999$. $\Delta/\sigma < 0.005$, $\Delta\rho < 1.3$ e Å^{-3}. Calculations were performed on a MicroVAX II computer with the *SDP* system (B. A. Frenz & Associates, Inc., 1982). Atomic parameters are given in Table 1.*

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$$B_{eq} = (4/3)\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Nb(1)	0.500	0.1847 (1)	0.2035 (1)	1.04 (1)
Nb(2)	0.17750 (5)	0.178	0.000	0.910 (6)
Si	0.500	0.500	0.000	0.37 (5)
P	0.2397 (1)	0.240	0.500	0.52 (2)
K(1)	0.000	0.000	0.500	2.20 (7)
K(2)	0.000	0.500	0.2923 (8)	4.0 (1)
K(3)	0.500	0.500	0.500	3.95 (8)
O(1)	0.500	0.000	0.261 (2)	1.3 (2)
O(2)	0.3638 (4)	0.1747 (5)	0.0215 (8)	1.07 (8)
O(3)	0.3790 (4)	0.2154 (5)	0.4530 (7)	1.33 (9)
O(4)	0.500	0.3819 (7)	0.145 (1)	1.4 (1)
O(5)	0.1756 (8)	0.000	0.032 (1)	1.6 (1)
O(6)	0.1586 (4)	0.1982 (4)	0.3115 (6)	0.74 (7)

Discussion. This new bronzoid is closely related to the niobium phosphate bronzes $(K_3Nb_6P_4O_{26})_n$-(KNb_2PO_8). Like the different members of this series, α-$K_4Nb_8P_5O_{34}$ (Benabbas, Borel, Grandin, Leclaire & Raveau, 1990*b*), β-$Na_{2-x}K_2Nb_8P_5O_{34}$ (Benabbas *et al.*, 1991), $K_7Nb_{14}P_9O_{60}$ (Leclaire, Benabbas, Borel, Grandin & Raveau, 1989) and $K_3Nb_6P_4O_{26}$ (Benabbas, Borel, Grandin, Leclaire & Raveau, 1990*a*), its structure consists of $[Nb_3P_2O_{13}]_\infty$ layers derived from the hexagonal tungsten bronze (HTB) (Magneli, 1953) by replacing NbO_6 octahedra by PO_4 tetrahedra (Fig. 1). In fact, this oxide is isotypic with β-$Na_{2-x}K_2Nb_8P_5O_{34}$, *i.e.* it contains similar double $[Nb_6P_4O_{26}]_\infty$ layers which are linked along **a** by $[Nb_2SiO_8]_\infty$ chains, instead of $[Nb_2PO_8]_\infty$ chains in the pure phosphate compound as shown from the projection into the (001) plane (Fig. 2). This ordered replacement of phosphorus by silicon in the niobium phosphate bronze β-$Na_{2-x}K_2Nb_8P_5O_{34}$ suggests the possible existence of the series of bronzoids $(K_3Nb_6P_4O_{26})_n(KNb_2SiO_8)$ in which $K_4Nb_8P_4SiO_{34}$ represents the first member.

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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 55193 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: DU0309]

Table 2. *Distances* (Å) *and angles* (°) *in the* NbO_6, PO_4 *and* SiO_4 *polyhedra and main* K—O *distances* (Å)

The Nb—O(*i*) or P—O(*i*) or Si—O(*i*) are on the diagonal, above it are the O(*i*)—O(*j*) distances and under it are O(*i*)—Nb—O(*j*) or O(*i*)—P—O(*j*) or O(*i*)—Si—O(*j*) angles.

Nb(1)	O(1)	O(2)	O(2^i)	O(3)	O(3^i)	O(4)
O(1)	1.993 (3)	2.808 (9)	2.808 (9)	2.893 (8)	2.893 (8)	4.12 (1)
O(2)	93.5 (3)	1.859 (5)	2.888 (9)	2.804 (9)	3.91 (1)	2.75 (1)
O(2^i)	93.5 (3)	101.9 (4)	1.859 (5)	3.91 (1)	2.804 (9)	2.75 (1)
O(3)	90.6 (3)	90.7 (3)	166.5 (2)	2.076 (5)	2.57 (1)	2.94 (1)
O(3^i)	90.6 (3)	166.5 (2)	90.7 (3)	76.4 (3)	2.076 (5)	2.94 (1)
O(4)	179.4 (5)	86.9 (3)	86.9 (3)	88.9 (3)	88.9 (3)	2.124 (9)

Nb(2)	O(2)	O(2^{ii})	O(5)	O(5^{ii})	O(6)	O(6^{ii})
O(2)	1.981 (5)	2.85 (1)	2.72 (1)	3.87 (1)	2.873 (8)	2.770 (7)
O(2^{ii})	92.0 (4)	1.981 (5)	3.87 (1)	2.72 (1)	2.770 (7)	2.873 (8)
O(5)	89.3 (4)	177.3 (4)	1.894 (1)	2.67 (1)	2.768 (8)	2.782 (9)
O(5^{ii})	177.3 (4)	89.3 (4)	89.5 (6)	1.894 (1)	2.782 (9)	2.768 (8)
O(6)	91.8 (2)	87.6 (2)	90.0 (3)	90.6 (3)	2.019 (5)	4.04 (1)
O(6^{ii})	87.6 (2)	91.8 (2)	90.6 (3)	90.0 (3)	179.2 (3)	2.019 (5)

Si	O(4)	O(4^{ii})	O(4^{iii})	O(4^{iv})
O(4)	1.561 (9)	2.57 (2)	2.51 (2)	2.57 (2)
O(4^{ii})	110.9 (4)	1.561 (9)	2.57 (2)	2.51 (2)
O(4^{iii})	106.7 (7)	110.9 (4)	1.561 (9)	2.57 (2)
O(4^{iv})	110.9 (4)	106.7 (7)	110.9 (4)	1.561 (9)

P	O(3)	O(3^v)	O(6)	O(6^v)
O(3)	1.530 (5)	2.53 (1)	2.513 (7)	2.513 (7)
O(3^v)	111.4 (5)	1.530 (5)	2.513 (7)	2.513 (7)
O(6)	109.6 (3)	109.6 (3)	1.546 (5)	2.488 (9)
O(6^v)	109.6 (3)	109.6 (3)	107.1 (4)	1.546 (5)

K(1)—O(6)	2.951 (5) × 8	K(2)—O(1^{vi})	2.86 (1)
		K(2)—O(2)	3.092 (8) × 4
K(3)—O(3)	3.294 (6) × 8	K(2)—O(3)	3.087 (7) × 3
K(3)—O(4)	2.60 (1) × 4		

Symmetry code: (i) $1-x, y, z$; (ii) $y, x, -z$; (iii) $1-x, 1-y, z$; (iv) $1-y, x, -z$; (v) $y, x, 1-z$; (vi) $-y, x, 1-z$.

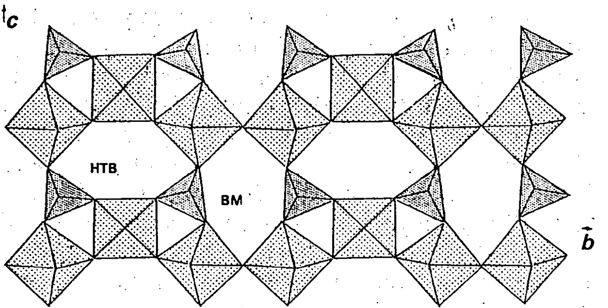

Fig. 1. $[Nb_3P_2O_{13}]_\infty$ layers in $Na_{2-x}K_2Nb_8P_5O_{34}$.

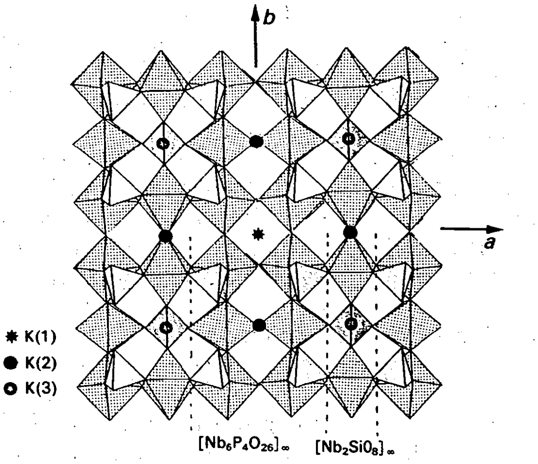

Fig. 2. Projection of $K_4Nb_8P_4SiO_{34}$ onto (001).

The geometry of the polyhedra NbO_6 and PO_4 in $K_4Nb_8P_4SiO_{34}$ (Table 2) is quite similar to that of their equivalent polyhedra in the phosphate bronze β-$Na_{1.73}K_2Nb_8P_5O_{34}$. The Nb(1) octahedron which forms the $[Nb_2SiO_8]_\infty$ chains is more distorted than the Nb(2) one. The PO_4 tetrahedron has P—O bonds and O—P—O angles characteristic of an almost regular monophosphate group and the SiO_4 tetrahedron is also almost regular (Table 2).

For the K cations, one observes three sorts of sites. K(1) is located in a site only formed of NbO_6 octahedra and PO_4 tetrahedra, as in β-$Na_{2-x}K_2Nb_8P_5O_{34}$; consequently, K(1) exhibits the same eightfold coordination as in the latter pure phosphate bronze, with Nb—O distances of 2.951 Å (Table 2). The second type of site in which the Nb_2SiO_8 are involved is located at the intersection of BM and HTB tunnels; in this site K(2) is characterized by a ninefold coordination with distances ranging from 2.860 to 3.092 Å very similar to those shown for (K,Na) in β-$Na_{1.73}K_2Nb_8P_5O_{34}$. In the third site, K(3) exhibits a 12-fold coordination with four short K—O bonds of 2.60 Å and eight long distances of 3.294 Å. This site, surrounded by NbO_6 octahedra, PO_4 tetrahedra and SiO_4 tetrahedra, corresponds to that which is only occupied by Na in $Na_{2-x}K_2Nb_8P_5O_{34}$, with four Na—O distances of 2.54 Å. From the comparison of K(3)—O and Na—O distances it is clear that the replacement of P by a larger element like Si is absolutely necessary to form larger cages allowing a pure K phase to be synthesized. Nevertheless, the rather small K(3)—O distances (2.598 Å) observed for the silicophosphate $K_4Nb_8P_4SiO_{34}$ explain the difficulty in synthesizing such a compound.

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Acta Cryst. (1992). **C48**, 1747–1749

Structure Refinement of the Semi-Metallic Oxide $SrTl_2O_4$: a Neutron Diffraction Study

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(*Received* 12 *September* 1991; *accepted* 11 *February* 1992)

Abstract. Strontium thallium oxide, $SrTl_2O_4$, M_r = 559.4, orthorhombic, *Pnam*, a = 10.0451 (2), b = 11.6905 (2), c = 3.40860 (4) Å, V = 400.28 (2) Å^3, Z = 4, D_x = 9.28 Mg m^{-3}, powder neutron diffraction data, λ = 1.594 Å, T = 293 K, 457 reflections, R_p = 0.048, R_{wp} = 0.064, R_i = 0.046. The lattice belongs to the $CaFe_2O_4$-type structure; it is built up from double ribbons of edge-sharing TlO_6 octahedra, linked through their corners. Comparison is made with Tl—O distances in other oxides and especially with high T_c superconductors. The JCPDS File No. for $SrTl_2O_4$ is 43-1497.

Introduction. Recent developments of the high T_c thallium cuprates suggest that the thallium–oxygen layers are not inert for superconductivity (Raveau, Michel & Hervieu, 1989) but that they can play the role of hole reservoirs for the superconductive copper–oxygen layers. This viewpoint is supported by electronic structure calculations (Yu, Massida & Freeman, 1988; Kasowksi, Hsu & Herman, 1988; Hamann & Mattheiss, 1988; Jung, Whangbo, Herron & Torardi, 1989). Consequently, it appears that the knowledge of the chemical bond and also of the electronic properties of pure thallium(III) oxides, without copper, is important for the understanding of the role of thallium in superconductivity. Recently, a new phase, $SrTl_2O_4$, with semi-metallic properties, was isolated (Michel, Hervieu, Raveau, Greaney, Fine, Potenza & Greenblatt, 1991). It was shown to be isotypic with the $CaFe_2O_4$ structure (Hill, Peiser & Rait, 1956). Although the structure was correctly established from X-ray data, it did not allow the oxygen positions to be determined with accuracy. We report here on the refinement of the structure of this phase from neutron diffraction data.

Experimental. About 10 g of $SrTl_2O_4$ were synthesized from mixtures of Tl_2O_3 and SrO_2 in the ratio 1/1. The mixed powders were divided in five parts. Each part was pressed in the form of bars which were heated in evacuated silica ampoules at 1173 K for 6 h. After thermal treatment, the bars were crushed and the purity of the preparation was checked by X-ray diffraction.

Symmetry was established with systematic reflections: $0kl$, $k + l = 2n$; $h0l$, $h = 2n$; space group *Pnam*. Powder neutron diffraction data were collected on a D2B diffractometer [λ = 1.594 Å; Ge monochromator; 64 counters (^{3}He, 506.6 kPa)] at ILL (Grenoble); angular range $10 \leq 2\theta \leq 156°$ with increment of 0.05° (2θ).

Profile refinement used the computer program *DBW*3.2 (Wiles & Young, 1981). Scattering lengths were 0.5805, 0.702, 0.8785 (in 10^{-12} cm) for O, Sr and Tl respectively. Starting parameters were those previously refined from powder X-ray data (Michel *et al.*, 1991). Successive refinements of background, profile and cell parameters and then of positional parameters and isotropic thermal factors were made. Calculations were performed on 457 *hkl*. R_p = 0.048, R_{wp} = 0.064, R_i = 0.046. Further refinement details are given in Table 1. Experimental and calculated diffraction patterns are plotted in Fig. 1. Atomic parameters, compared to those obtained from X-ray diffraction, are given in Table 2.†

Discussion. These results do not differ dramatically from the X-ray data (Table 2) with respect to the positions of the metallic elements, whereas the difference between the O-atom positions is larger.

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† A list of primary diffraction data has been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55180 (11 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

0108-2701/92/101747-03$06.00