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CRYSTALLOGRAPHY

Crystal Structure of Lamprophyllite

A specimen of the mineral lamprophyllite (from Kola, the U.S.S.R.) at present being investigated is monoclinic, space group $C2/m$, with unit cell dimensions: $a = 19{\cdot}76$ Å, $b = 7{\cdot}06$ Å, $c = 5{\cdot}40$ Å, $\beta = 96{\cdot}5°$. The unit cell formula is: $4 \times (Ba,Sr,K)Na(Ti,Fe)TiSi_2(O,OH,F)_9$.

Using 174 $hk0$ reflexions, the structure has been determined in projection along the z-axis. The atom positions found are given in Table 1 and the projection along the z-axis is shown in Fig. 1. The short repeat distance of the z-axis enables the main features of the structure in three dimensions to be determined unambiguously.

The structure is closely related to those of the minerals seidozerite[1], rosenbuschite[2] and bafertisite[3]. The basic unit is an infinite sheet of cations, chiefly sodium and titanium, in octahedral co-ordination. To either side of this are attached sheets of silicon–oxygen tetrahedra and titanium–oxygen polyhedra arranged as shown in Fig. 2.

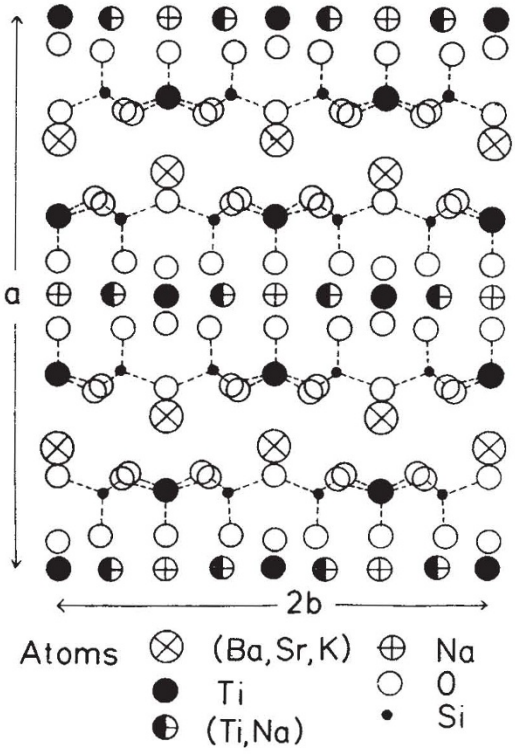

Fig. 1. Lamprophyllite projection along z-axis

Table 1. Atom Co-ordinates

Atom	x	y
(Ba, Sr, K)	0·217	0·000
Si	0·140	0·217
Ti	0·000	0·000
(Ti, Na)	0·000	0·239
Na	0·000	0·500
Ti	0·146	0·500
O	0·056	0·000
O	0·059	0·205
O	0·062	0·500
O	0·165	0·310
O	0·173	0·312
O	0·174	0·000

These composite sheets are separated by barium atoms. The titanium–oxygen polyhedra shown in Fig. 2 are square pyramids, the titanium being in five-fold co-ordination. In this respect lamprophyllite differs from the minerals mentioned above, in which the titanium, or zirconium in some cases, is in six-fold, octahedral, co-ordination.

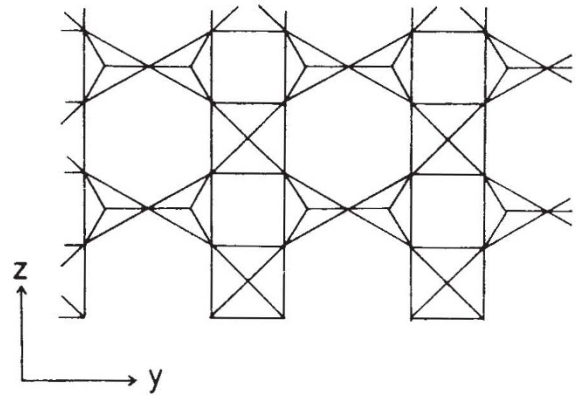

Fig. 2. Arrangement of SiO_4 and TiO_5 polyhedra

Work is in progress to determine directly a second projection of the structure.

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CHEMISTRY

Aluminium Oxyfluoride and the Polymerized Species in AlOCl Solutions

Although the crystalline aluminium oxyhalides AlOCl, AlOBr and AlOI are known[1–3], the corresponding AlOF is not. We have tried to prepare AlOF by the procedure which is commonly used to prepare the other AlOX compounds, namely, the reaction of 3 AlF_3 with As_2O_3 in sealed evacuated glass ampoules at elevated temperatures. However, AlOF was not formed at temperatures up to 480° C, although reaction between AlF_3 and As_2O_3 did occur. Details of these experiments will be published elsewhere. Whereas AlOCl can be prepared by the reaction of steam and $AlCl_3$ (ref. 4), it does not appear that AlOF can be prepared by a comparable reaction with AlF_3. Schober and Thilo[5] found that AlF_3 reacts with steam at temperatures up to 600° C to form a product with a 5·2 per cent fluorine content, and lower fluorine contents at higher temperatures. They formulated their product as $Al_7O_{10}F$. Locsei[6] obtained similar results but preferred to formulate the product as a mixture of Al_2O_3 and AlOF. No reason