Crystal Structure of $Na_2Mg_2Si_6O_{15}$

THE compound $Na_2Mg_2Si_6O_{15}$ has been known since 1937 (ref. 1), but crystal data for it were only determined recently[2]. It is orthorhombic with $a = 10.205$ Å, $b = 17.59$ Å and $c = 14.165$ Å; the space group is $Acam$ or $Aba2$ and $Z = 8$. We have now found the crystal structure, using three-dimensional methods, to be $Acam$. The structure was solved using symbolic addition, and has so far been refined to $R = 0.15$ on 383 observed, independent reflexions. It is interesting because it contains a new type of silicate anion (Fig. 1). This can be described as a corrugated ribbon, two tetrahedra wide, which is made from rings of four tetrahedra fused together, and which repeats at intervals of six pairs of tetrahedra. Each tetrahedron shares three corners with neighbouring ones, thus giving the empirical formula $Si_2O_5^{2-}$. The anions are held together by Mg^{2+} and Na^+ ions. Some of the Mg^{2+} ions are tetrahedrally coordinated and others are octahedrally coordinated, and some of the Na^+ ions have nine oxygen neighbours within 3.1 Å whereas others have ten.
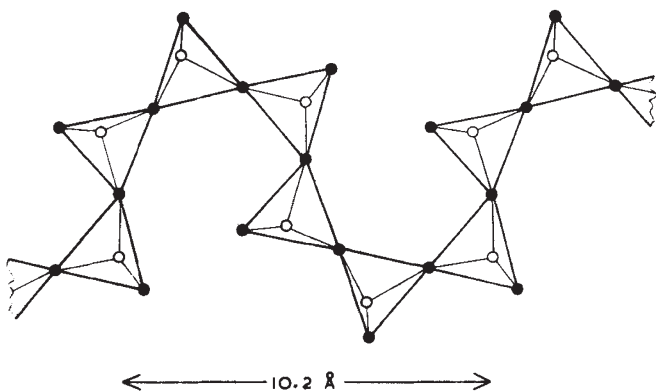

$\longleftarrow$ ———— 10.2 Å ————— $\longrightarrow$

Fig. 1 The silicate anion in $Na_2Mg_2Si_6O_{15}$. Each of the large triangles represents an Si_2O_7 group with its Si–Si direction perpendicular to the plane of the paper, the two tetrahedra in the group coinciding in projection. The oxygen atoms which link the two tetrahedra within these Si_2O_7 groups are shown as open circles, and lie on a plane of symmetry. The Si_2O_7 groups share corners with each other to form a corrugated ribbon, which is seen edge-on in this projection. The repeat distance along the ribbon is shown.

Shahid and Glasser[2] noted that the unit cell is simply related geometrically to that of $Na_2Mg_5Si_{12}O_{30}$, which is hexagonal with $a = 10.16$ Å, $c = 14.24$ Å $(a\sqrt{3} = 17.60$ Å$)^{3,4}$. Comparison of equivalent X-ray photographs shows that the Fourier transforms of the two structures are also similar. This is somewhat remarkable, because the silicate anions in the two structures are apparently entirely different. Schreyer and Schairer[3] suggested that $Na_2Mg_5Si_{12}O_{30}$ had a structure resembling that of osumilite $((K,Na)(Fe,Mg)_2(Al,Fe)_3$-$(Al,Si)_{12}O_{30})$, with double-ring anions of formula $Si_{12}O_{30}^{12-}$, and this hypothesis has recently been confirmed by a structure determination on the isostructural $K_2Mg_5Si_{12}O_{30}$ (ref. 5). Comparison of the structure reported for this compound with that found by us for $Na_2Mg_2Si_6O_{15}$ shows that, in spite of the difference in anion types, many atoms occupy similar relative positions in the two structures. The unit cell relationship and similarity in Fourier transforms may thus be explained.

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Absolute Determination of Particle Size and Shape

THE method suggested by Cheng and Sutton[1] for describing shape and size of a particle by polar coordinates and a subsequent Fourier series is indeed an interesting one and has been proposed and worked out in far greater detail by Schwarcz and Shane[2]. The disadvantage of the method is in locating the centroid of the particle in the first place although Schwarcz and Shane point out that the results are not sensitive to small errors in the location of the centroid.

The difficulties of locating the centroid may be overcome by generating the Fraunhofer diffraction pattern of the shape under analysis and scanning the diffraction pattern with a rotating sector slit[3-5]. The wave form generated is a unique description of the shape under analysis, and the advantage is that the centre of the diffraction pattern is always on the optical axis even if the shape itself is not on the axis. This method of shape analysis for particles has been developed by Kaye and Naylor[6] who are undertaking further work which should result in a relatively simple instrument for shape analysis of any two dimensional object.

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TiO_2 Content and the Shoshonite and Alkaline Associations

THERE are two distinct genetically unrelated "alkaline" magma series. First, there is the alkaline association proper which occurs on oceanic islands, continental margins and continental rift systems. Second, there is the characteristically potassic shoshonite association[1], which typically appears in the later stages of island arc evolution[2]. Basaltic members lie in the alkaline field on the diagram of $Na_2O + K_2O$ against SiO_2, above the Macdonald–Katsura line, but are never strongly nepheline normative.

A comparison of the chemical composition of typical basic rocks ($< 50\%$ SiO_2) in the two associations reveals characteristic chemical differences. Alkali oxides provide a useful discriminant function in most cases. Contrasted with the alkaline association, shoshonites typically have higher K_2O contents and K_2O/Na_2O ratios close to unity, but some overlap—the potassic alkaline lineages[3], for example—has been recognized. A more efficient discriminant is TiO_2, which