Elementarzelle angeboten. Mit den Vektoren $\mathbf{a}_1/3$, $\mathbf{a}_2/3$, $2\mathbf{a}_1/9+\mathbf{a}_2/9+\mathbf{c}/9$ baut man eine $B1$-Fundamentalkonfiguration mit 81 Plätzen je Atomgitterzelle auf. Für idealkubische Fundamentalkonfiguration folgt ein Achsverhältnis von 1,2 während das beobachtete 1,1 beträgt. Legt man nur 8 äquidistante Elektronenplatzebenen senkrecht zur $c$-Achse in die Zelle, so bekommt man einerseits eine bessere Übereinstimmung des Achsverhältnisses und der Elektronenzahl, dafür aber andererseits die Phasenwechselerscheinung. Die angegebene Ortskorrelation gestattet einige Züge der Struktur des Quarzes besser zu verstehen.

Die Berücksichtigung einer kristallinen Ortskorrelation die verschiedene Gruppen von Elektronen erfasst, bildet nicht nur ein neues Einteilungsprinzip der Kristallstrukturen, sondern gestattet auch, wie anderweitig dargelegt werden soll, eine Erklärung spezieller Eigenschaften der Kristallstrukturen.

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## Crystal data for spurrite, $5CaO \cdot 2SiO_2 \cdot CO_2$.

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The minerals spurrite, tilleyite and scawtite together comprise the calcium carbonate–silicate group. All three members are the product of thermal metamorphism in contact zones between hot acid magmas and rocks bearing calcium carbonate. The crystal structure of tilleyite has been determined by Smith (1953). The lattice parameters and other crystal data for scawtite have been measured by McConnell (1955).

Spurrite was first described by Wright (1908) and was later recognized by Tilley (1929) in the well-known contact zone at Scawt Hill, Northern Ireland. The crystals used in the present X-ray investigation were kindly provided by Prof. C. E. Tilley and the optical and physical data are taken from his paper. Results are shown in Table 1.

Table 1. *Crystallographic data for spurrite*

Lattice parameters

$a=10{\cdot}46\pm0{\cdot}05$, $b=6{\cdot}70\pm0{\cdot}03$, $c=14{\cdot}28\pm0{\cdot}07$ Å, $\beta=101\pm1°$

Space group

$P2_1/a$

Composition

4 (calc. 4·03) units of $5CaO.2SiO_2.CO_2$ in the above unit cell

Optical data

$\alpha = 1{\cdot}640\pm0{\cdot}003$, $\beta = 1{\cdot}674\pm0{\cdot}003$, $\gamma = 1{\cdot}679\pm0{\cdot}003$
$y = X$, $z : Z = 33°$, $2V = 39\frac{1}{2}°$, negative

Physical data

Specific gravity: 3·01
Cleavages: (001) perfect, (100) poor
Twinning: (*a*) parallel to (001), polysynthetic
(*b*) rare, simple, almost parallel to optic axial plane

The author has measured the intensities of 1300 *hkl* reflexions from oscillation photographs taken with Mo$K\alpha$ radiation. Five bounded projections of the Patterson synthesis were calculated, the plane of projection being parallel to (010).

Attempts to solve the crystal structure of spurrite have so far been unsuccessful. The chemical formula may be rewritten $Ca_5.2SiO_4.CO_3$, which is consistent with the presence of isolated silicon tetrahedra and planar $CO_3$ groups linked together by Ca ions. The orientation of the tetrahedra is revealed by the direction of the short vectors in the Patterson maps. The bases of the tetrahedra are nearly parallel to (010) and the projection of one of the Si–O vectors on this plane is parallel to the $x$ axis. The bulk of the vector density is contained in an array of peaks which lie close to the pseudo-hexagonal lattice points defined by the intersections of the plane (040) with the lines formed by the mutual intersections of the planes (204), (20$\bar{5}$) and (40$\bar{1}$). The spacing of the (040) planes is 1·7 Å and the planes (204), (20$\bar{5}$) and (40$\bar{1}$) form an hexagonal array of side 3·1 Å. There are planes of pseudo-symmetry along the mutually perpendicular planes (40$\bar{1}$) and (001). As the (001) plane is also the preferred twin-plane the crystal structure should have a high pseudo-symmetry across (001). There should also be a plane parallel to (001) which cuts only weak bonds, for this direction is a plane of perfect cleavage. The calcium atoms must form a pseudo-hexagonal array and the oxygen atoms probably fall on a similar hexagonal array which is a sub-multiple of the calcium array. The $CO_3$ group is probably parallel or sub-parallel to (010), since spurrite is optically negative and the $y$ axis is the acute bisectrix.

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