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Singularities of the atomic arrays in beryllium tellurate as compared with spinel.

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Abstract

In spite of entirely different symmetry descriptions, the structure types of beryllium tellurate, $Be_4^tTe^o[O_7\square]^c$, and spinel, $Al_2^oMg^t[O_4]^c$, present similar arrays of positively charged positions when the packing vacancies of the tellurate are taken into account: the Al and Mg atoms in spinel form a $[T' + D]$ connection pattern, which is also the point array of the Be and Te atoms plus vacant packing positions in beryllium tellurate.

The crystal structure of Be_4TeO_7 was recently determined by neutron diffraction and a relationship with the sphalerite structure was then mentioned: TeO_6 and Be_4O groups are arranged like the Zn and S atoms in the cubic sulfide (Trömel, Maetz & Müllner, 1977). However, a certain similarity with the spinel structure was remarked on when the condensed model (Lima-de-Faria, 1965) of this novel structure type was compared with that of spinel.

The spinel structure type, which has the symbol $Al_2^oMg^t[O_4]^c$ (Lima-de-Faria & Figueiredo, 1976), is based on a cubic closest packing of oxygens where the octahedral interstices are half filled by Al according to a T' lattice complex, and where Mg occupies part of the available tetrahedral sites forming a D lattice complex (Hellner, 1965). Such a structural arrangement is described by the invariant equipoints 16(*d*) for Al and 8(*a*) for Mg, and by the monovariant set of equivalent positions 32(*e*) for O, with x close to $\frac{3}{8}$, in space group $Fd3m$. The oxygen atoms therefore correspond to a 32-pointer cell within the cubic closest packing.

Beryllium tellurate is also cubic, but the different symmetry description masks any structural relationship with spinel: the space group is $F\bar{4}3m$, and the occupied equivalent positions are 16(*e*) for Be, 4(*a*) for Te, and 4(*d*) plus 24(*f*) for O. Nevertheless, the oxygen atoms are also arranged according to a cubic closest packing, with a unit cell covering 32 packing positions, out of which four are vacant. The main dissimilarity to spinel lies in a different occupancy of the available interstices: $\frac{1}{8}$ of the octahedral sites are filled by Te and $\frac{1}{4}$ of the tetrahedral positions are occupied by Be. The corresponding structure-type symbol should then be $Be_4^tTe^o[O_7\square]^c$, the symbol $\square$ standing for closest-packed vacant positions.

It was noticed through the condensed models of both structures that, if the packing vacancies in beryllium tellurate were considered together with the point array of cations, the resulting connection pattern would become analogous to the cationic array in spinel. This is also apparent from the symmetry description if the symbolism of the lattice complexes is used (Table 1): (1) The occupied octahedral positions in the spinel structure are described by a T' lattice complex, and the point array of the tetrahedrally coordinated Be atoms in the tellurate, corresponding to the mono-variant set of equivalent positions 16(*e*), is also very close to this lattice complex; in fact, it would coincide with a T' complex if the positional parameter x, which actually has the value 0·6270, was 0·6250, that is, precisely $\frac{5}{8}$. (2) The occupied tetrahedral sites in spinel correspond to a D lattice complex, which is also the point array formed by the assemblage of the octahedrally coordinated Te atoms plus the packing vacancies in the tellurate.

This formal analogy between spinel and beryllium tellurate suggests that vacancies in a close-packed array of anions may behave as positions with a positive character. Accordingly, the crystal structure of beryllium tellurate provides further evidence of the structural stability associated with the assemblage of $[T' + D]$ lattice complexes, possibly as a consequence of its homogeneous spatial arrangement. Such a point array can be found under various cubic space groups (Hellner, 1976), and occurs in highly populated structure types, ranging from intermetallic phases like the $MgCu_2$ structure type, through ionic compounds, up to covalent linkages such as the high-cristobalite structure type.

Table 1. *Crystallographic and structural data for spinel and beryllium tellurate*

Structure type symbol	Space group	Atoms, equipoints, values of parameters	Lattice complexes
$Al_2^oMg^t[O_4]^c$	$Fd3m$	Al (16*d*) Mg (8*a*) O (32*e*) $x=0.387$	T' D $F_2'''x$ $(x=3/8)$
$Be_4^tTe^o[O_7\square]^c$	$F\bar{4}3m$	Be (16*e*) $x=0.6270$ Te (4*a*) $\square$ (4*c*) O (4*d*) (24*f*) $x=0.2532$	$T'x$ $(x=5/8)$ F F'' } D F''' $J_2'x$ $(x=1/4)$

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