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Using vertex symbols and coordination sequences to analyze beryllosilicate crystal structures

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The vertex symbol (VS) (O'Keefe & Hyde 1997) numerically describes a circuit. For each tetrahedral site (usually Be or Si in beryllosilicates), a node is assigned. If the tetrahedral node is connected via an O atom to the next tetrahedral node they are joined by a line. If the path continues until the original node is rejoined, then a 'circuit' is formed. The number of lines in the circuit is described as a net or ring. For each vertex, usually tetrahedrally connected, there are six possible angles, each of which will describe at least one circuit. The sum of all circuits, taken at each unique node, describes a vertex symbol. The VS numerically describes the net topology of the structure.

The concept of the coordination sequence (CS) was first introduced by Brunner & Laves (1971) and initially was called, 'growth series', which emphasizes its close relationship to the process of crystal growth. The CS is a number sequence that tallies atoms bonded in each subsequent shell of a defined diameter. In this study I chose the tetrahedral atoms that are coordinated to next-nearest tetrahedrally coordinated neighbours i.e. the topology nodes. For tetrahedral sites to be considered as part of the same CS, they must share a common oxygen atom. These sites are in consecutive spheres of approximately 3.0 to 3.3 Å. The CS integer string quantifies the degree of polymerization and the summation quantifies the framework density.

Vertex symbols and coordination sequences are determined for each unique tetrahedrally coordinated site in every beryllosilicate crystal structure (Grice 2010). The number sets, VS and CS, identify structural similarities in beryllosilicates and in natural and synthetic zeolites. The frequency for of ring-size occurrence varies with Be content in both layered and framework beryllosilicates. Framework density (FD) is derived from structure diagrams and topological density (TD) is derived from CS sums. FD and TD are strongly correlated. TD is controlled by the Be content in tetrahedrally coordinated sites. This structural control could be used to design specific framework arrangements.

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