Graph Theory, Symmetry and Inorganic Solids

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The Principle of Maximum Symmetry states that a structure adopts the highest symmetry consistent with the constraints acting on it.

Chemical constraints are determined by the properties of the bond graph, which for molecular compounds is the same as the bond diagram. Inorganic solids have infinite bond graphs, but a finite graph that retains all the essential nearest neighbour properties can be created by extracting one formula unit from the infinite graph. The lengths of the bonds can be predicted from this graph using the bond valence model and the principle of maximum symmetry. They necessarily have the symmetry of the graph.

Steric constraints are introduced when the bond graph is mapped into three dimensional space. The ideal space group adopted by the crystal must be a subgroup of the symmetry group of the graph, but the steric constraints may further lower the symmetry by distorting the structure along one or more of its normal coordinates.

Examples will illustrate this approach.

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