American Mineralogist, Volume 88, pages 653–666, 2003

Model pyroxenes I: Ideal pyroxene topologies

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ABSTRACT

Ideal pyroxenes are hypothetical structures based on ideal closest-packed arrangements of O anions. They are modeled after observed pyroxene structures and have the general formula $M2M1T_2O_6$, where M2 and M1 represent octahedrally coordinated cations, and T represents tetrahedrally coordinated cations. An algorithm has been created to construct all possible ideal pyroxenes based on closest-packed stacking sequences of length 12 or less. These structures are reported.

The only significant structural parameters that vary between different ideal pyroxenes are the M1-T and M2-T distances. We show that the repulsive forces between these pairs of cations distinguishes the energetics of the ideal pyroxenes and may be important in determining the topologies of observed pyroxenes.