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Topology of the pyroxenes as a function of temperature, pressure, and composition as determined from the procrystal electron density

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ABSTRACT

The distribution of bonds associated with the M2 sites in various well-ordered pyroxene minerals is determined using a topological analysis of electron density in the manner proposed by Bader (1998). Each M2 atom is bonded to 2 O1 and to 2 O2 atoms, and to zero, one, two, or four bridging O3 atoms. Each of the symmetries displayed by pyroxenes have their own bonding systematics, and each pyroxene-to-pyroxene phase transition involves a change in bonding to M2. As a function of temperature or pressure, the bonding changes appear as a well-defined sequence of steps that can be related to the degree of distortion from the ideal closest packing of anions. It is proposed that the condition at which an individual phase transition occurs is related to M2-Si repulsion through a shared edge. The bonding analysis should provide a qualitative means to interpret the behavior of all pyroxene structures over *T*, *P*, and *x*, and may guide the interpretation of the changes in properties observed by techniques other than X-ray diffraction, such as Raman spectroscopy.