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Model pyroxenes II: Structural variation as a function of tetrahedral rotation

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ABSTRACT

Model pyroxenes with regular tetrahedral and M1 octahedral coordination polyhedra have been derived. The M2 polyhedron is not constrained to be regular. These models are parameterized in terms of the O3-O3-O3 angle, θ, and the model O atom radius, *r*. Crystallographic parameters such as interatomic distances, unit cell volume, and packing distortion are determined as a function of the O3-O3-O3 angle. Results are compared with observed pyroxenes, providing insight into which interatomic interactions are important in determining pyroxene topology and behavior. Temperature is shown to favor polyhedral regularity in orthopyroxene and protopyroxene. Compression and expansion strain ellipsoids for observed and model pyroxenes are compared, demonstrating that a combination of tetrahedral rotation and isotropic compression approximately reproduces the compression ellipsoids of pyroxenes, but not the expansion ellipsoids.