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Model pyroxenes III: Volume of *C*2/*c* pyroxenes at mantle *P*, *T*, and *x*

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ABSTRACT

Variations in unit-cell volumes of mantle minerals as functions of *P* and *T* are important parameters in the description of the interior of the Earth and the behavior of materials. Recently, Thompson and Downs (2004) presented a model for the crystal structures of pyroxenes parameterized in terms of the O3-O3-O3 angle, θ, and the oxygen radius, *r*. This model has proven useful in the analysis of compression and expansion mechanisms in pyroxenes, providing an understanding of θ and r as functions of *P* and *T*. However, it did not provide a basis for analyzing changes in some properties that are strongly dependent on composition.

In this paper, we show that ambient unit-cell volumes of the *C*2/*c* pyroxenes are correlated with M1 cation radius. This relationship can be used to calculate model ambient unit-cell volumes as a function of chemistry. From this starting point, pyroxene unit-cell volume variation with *P* and *T* can be modeled as a function of θ(*P*,*T*) and *r*(*P*,*T*). These relationships are investigated for diopside, hedenbergite, acmite, jadeite, and kosmochlor. The model reproduces observed unit-cell volumes of these phases recorded at *P* to within 0.09% and at *T* to within 0.10%, at simultaneous *P* and *T* for jadeite to within 0.57%, and at simultaneous *P* and *T* for diopside to within 1.20%. K_o and K' from third-order Birch-Murnaghan fits to the observed volume vs. pressure relationships and those calculated from the Thompson-Downs model are statistically the same. The fit of the Thompson-Downs EOS to the observed data is compared to the fit of the third order Birch-Murnaghan. The model is used to create an algorithm that estimates volumes for *C*2/*c* pyroxenes as a function of *P*, *T*, and *x*.