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Thermodynamics of cation ordering in karrooite ($MgTi_2O_5$)

MARK S. GHIORSO,[1,*] HEXIONG YANG,[2] AND ROBERT M. HAZEN[2]

[1]Department of Geological Sciences, Box 351310, University of Washington, Seattle, Washington 98195-1310, U.S.A.
[2]Geophysical Laboratory and Center for High Pressure Research, Carnegie Institution of Washington, 5251 Broad Branch Road, N.W., Washington, D.C., 20015-1305, U.S.A.

ABSTRACT

A thermodynamic model of non-convergent cation-ordering in karrooite ($MgTi_2O_5$) has been calibrated from the single-crystal X-ray structure refinements of Yang and Hazen (1998) and from estimates of the dependence of the bulk modulus on ordering state (Hazen and Yang 1997). Derived values of the Gibbs free energy, enthalpy, entropy, and heat capacity of disordering of karrooite are reported as a function of temperature at 1 bar and at elevated pressures.