American Mineralogist, Volume 82, pages 682–688, 1997

The equation of state and high-pressure behavior of magnesite

Nancy L. Ross

Research School of Geological and Geophysical Sciences, University College London, Gower Street, London WC1E 6BT, U.K.

Abstract

Unit-cell parameters of magnesite have been measured to high precision between 0 and 7 GPa using single-crystal X-ray diffraction. The isothermal bulk modulus of magnesite determined from fitting a Birch-Murnaghan third-order equation of state to the volume compression data is K_T = 117(3) GPa with K_T' = 2.3(7), and K_T = 111(1) GPa if K_T' is constrained to a value of 4. Crystal structure parameters have been determined from X-ray intensity data at room pressure, 2.26, 3.09, 4.16, 4.77, and 6.05 GPa. The principal structural change with increasing pressure is compression of the MgO_6 octahedra while the CO_3 group remains invariant (within the experimental uncertainty) throughout the pressure range studied. The effect of the polyhedral compression is reflected in the anisotropic compression of the unit-cell parameters with the *c* axis approximately twice as compressible as the *a* axis. The polyhedral bulk modulus of the MgO_6 octahedron is 113 GPa, which is greater than that observed in other rhombohedral carbonates, but significantly smaller than values observed in many oxides and silicates. The distortion of the octahedra, though already small, decreases slightly with pressure. No phase change or change in compression behavior was observed throughout the pressure range studied.