American Mineralogist, Volume 90, pages 1669–1673, 2005

LETTER

An infrared study of carbon-oxygen bonding in magnesite to 60 GPa

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ABSTRACT

Infrared spectra of magnesite, $MgCO_3$, have been measured in the diamond anvil cell from 0 to 60 GPa at 300 K. Mode shifts were determined for the in-plane bend, the asymmetric-stretch, and the out-of-plane bend of the carbonate group, as well as a magnesium ion translational mode. The in-plane bend shows a small positive shift and ultimately merges with the out-of-plane bend, exhibiting an accidental degeneracy by 60 GPa. The asymmetric stretch exhibits highly nonlinear behavior, shifting monotonically to pressures of ~30 GPa, at which point its shift markedly decreases to ~50 GPa. At 50 GPa, it again shifts strongly with pressure. We calculate force constants for the carbonate group under pressure from our data, and correlate these with the C-O bond length. Our data are consistent with a slight lengthening (~0.01 Å) of the C-O bond between 30 and 50 GPa to a maximum bond distance of ~1.27 Å. Although our finding of bond lengthening is in general agreement with previously published Rietveld refinements of X-ray diffraction data for magnesite under pressure, our data indicate that the lengthening is likely substantially smaller than previously proposed. The expansion of the C-O bond in magnesite can be produced by rotations of the MgO_6 octahedra, and such non-ionic crystal-chemical effects may be a key contributor to the remarkable stability of $R\overline{3}c$-structured carbonates to very high pressures.