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A high-pressure phase transition of calcite-III

KRYSTLE CATALLI* AND QUENTIN WILLIAMS

Department of Earth Sciences, University of California, Santa Cruz, 1156 High Street, Santa Cruz, California 95064, U.S.A.

ABSTRACT

We document the presence of a high pressure phase transition in metastable calcite-III using infrared spectroscopy. The post-calcite-III transition initiates at a pressure of 15.5 (±2) GPa, and is completed between 25 and 30 GPa. The transition is particularly apparent in the ν_4-in-plane bending vibration of the carbonate group, in which two new peaks progressively supplant the doublet associated with calcite-III. Additionally, both the ν_3-asymmetric and ν_1-symmetric stretches of the carbonate group in the high-pressure phase occur at substantially lower frequencies than the extrapolated positions of the corresponding calcite-III peaks. The geometry of the carbonate unit within the high-pressure phase is likely closer to trigonal symmetry than in the calcite-III structure, and the C-O bond is probably longer than in the lower pressure calcite-III phase.