

LETTER

A high pressure X-ray diffraction study of aragonite and the post-aragonite phase transition in CaCO₃

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ABSTRACT

CaCO₃-aragonite has been examined to pressures of 50 GPa using angle-dispersive synchrotron X-ray diffraction at 300 K. A progressive pressure-induced change takes place in the diffraction patterns, with the (021) and (111) diffraction lines of aragonite converging toward one another with compression. The ultimate convergence of these lines and shifts in intensity in the diffraction pattern imply that CaCO₃-aragonite undergoes a transition to a trigonal structure near 50 GPa. This transition is similar to that occurring in BaCO₃ at 7 GPa and SrCO₃ at 35 GPa. Indeed the *b/a* ratio of aragonite at 50 GPa is $\sqrt{3}$: the critical value for producing a transition to a trigonal structure, and similar to that of BaCO₃ at low pressure. The occurrence of this phase transition is in general accord with systematics in aragonite-structured divalent cation carbonates. If free CaCO₃ exists in the deep mantle, either as a consequence of subduction or carbonatite melt fractionation, we anticipate that it is likely to occur as a trigonal phase.