Bonding and electronic changes in rhodochrosite at high pressure

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ABSTRACT

Atmospheric carbon is critical for maintaining the climate and life equilibrium on Earth. The concentration of this carbon is controlled by the deep carbon cycle, which is responsible for the billion year-scale evolution of the terrestrial carbon reservoirs of the planet. Understanding the crystal chemistry and physical properties of carbonates at mantle conditions is vital as they represent the main oxidized carbon-bearing phases in the Earth's mantle. Here we present data on the crystal chemistry and physical properties of rhodochrosite at high pressure.

Rhodochrosite (MnCO₃) exhibits a series of high-pressure transitions between 15 and 30 GPa and at 50 GPa at ambient temperature as observed by in situ Raman spectroscopy, X-ray diffraction (XRD), and X-ray emission spectroscopy (XES). A transition is observed to begin at 15 GPa and complete at 30 GPa, which may be due to several possibilities: modifications in the magnetic order, changes in the compression mechanism, and/or a structural transition resulting from disorder. We also observed a first-order phase transition of MnCO₃ at 50 GPa, which is not accompanied by any changes in the electronic spin state. These results highlight the unique behavior of MnCO₃, which we found to be quite different from other common carbonates such as siderite, magnesite, and calcite.

Keywords: Rhodochrosite, deep carbon, Raman spectroscopy, XES, XRD, high pressure, carbonate