

## **Raman modes of carbonate minerals as pressure and temperature gauges up to 6 GPa and 500 °C**

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### **ABSTRACT**

Diamond-anvil cell (DAC) experiments focusing on the solubility of carbonates and aqueous carbon speciation at subduction zones require pressure monitoring with sensitive, chemically inert sensors. Commonly used pressure indicators are either too insensitive or prone to contaminate pressure-transmitting media due to their increased solubility at high pressure and/or temperature ( $P$ - $T$ ). Here, the  $P$ - and  $T$ -induced frequency shifts of the Raman vibrational modes of natural crystalline carbonate minerals aragonite, calcite, dolomite, magnesite, rhodochrosite, and siderite have been calibrated for application as Raman spectroscopic  $P$  and  $T$  sensors in DACs up to 500 °C and 6 GPa. The shifts of all modes are quasi-constant over the observed  $P$  and  $T$  ranges and are generally less prominent for internal modes than for external modes. Our method provides a sensitive and robust alternative to traditional pressure calibrants, and has three principal advantages: (1) higher sensitivity (for particular Raman vibrational modes), (2) monitoring  $P$ - $T$ -induced shifts of several modes allows even more accurate  $P$ - $T$  determination, and (3) no contamination of pressure-transmitting media by foreign materials can occur. Additionally, the isobaric and isothermal equivalent of the Grüneisen parameter and the anharmonic parameter for each of the traced modes have been determined.

**Keywords:** Aragonite, calcite, diamond-anvil cell, dolomite, high pressure, high temperature, magnesite, pressure sensor, Raman spectroscopy, rhodochrosite, siderite, temperature sensor