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## Pressure and temperature dependence of $^{13}\text{C}$ diamond Raman shift determined in-situ to 1.27 GPa and 800 degree C

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The pressure- and temperature-dependent Raman shift of synthetic  $^{13}\text{C}$  diamond was determined in-situ at temperatures to 800 degree C and at pressures to 1.27 GPa. In-situ experiments were conducted using an Ir-gasketed, externally-heated diamond anvil cell (HDAC) fitted to confocal micro-Raman spectrometer. The pressure dependence of the Raman shift was calibrated to the equation-of-state of pure  $\text{H}_2\text{O}$  (IAPWS-95, Wagner and Pruss, J. Phys. Chem. 31, 2002) with a piece of the  $^{13}\text{C}$  diamond aggregate (99% pure) and distilled  $\text{H}_2\text{O}$  loaded in the sample chamber of the HDAC. Temperature was controlled to plus-minus 1 degree C with chromel-alumel thermocouples in contact with the anvils near the sample chamber. To ensure the highest precision of the  $^{13}\text{C}$  diamond Raman shift, the emission of the 585 nm Ne line was recorded simultaneously as reference. The in-situ experiments were repeated along four different isochores to cover a wide coverage of pressures at high temperatures (0.38 to 1.27 GPa at 800 degree C). No carbon-bearing species were detected in the  $\text{H}_2\text{O}$  fluids, which means that the  $^{13}\text{C}$  diamond does not react with  $\text{H}_2\text{O}$  and the diamond anvils as well during these high temperature and pressure measurements.

Multiple regression analysis demonstrated that the pressure and temperature dependence of the  $^{13}\text{C}$  diamond Raman shift can be described by a simple quadratic linear form:  $\nu(P, T) - \nu(0.1, 25) = -1.065 (\text{plus-minus } 0.044) \times 10^{-2} T - 1.769 (\text{plus-minus } 0.046) \times 10^{-5} T^2 + 2.707 (\text{plus-minus } 0.249) \times 10^{-3} P$ , where  $\nu(0.1, 25)$  is the Raman shift at ambient condition ( $1287 \text{ cm}^{-1}$ ),  $T$  is temperature in degree C and  $P$  is pressure in MPa. The average error in the pressure determination with this form is estimated to be plus-minus 0.11 GPa. The pressure derivative and the temperature derivative are both consistent with those of Bassett (Mineral Spectroscopy, 1996) and Schiferl et al. (J. Appl. Phys. 82, 1997), within the uncertainties in the regression analysis. In those previous studies, the pressure dependence was measured at ambient temperature, and the temperature dependence was separately measured at ambient pressure. The present result indicates that the pressure and temperature cross derivatives might be present but are negligibly small over the pressure and temperature conditions investigated.

Keywords: diamond,  $\text{H}_2\text{O}$  fluid, Raman shift, in-situ observation