

Evidence for Ice VI as an Inclusion in Cuboid Diamonds from High P-T Near Infrared Spectroscopy

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Natural minerals of high-pressure origin with high strength have the potential to retain high internal pressures on material trapped within these crystals. Frequency shifts in IR spectra disclosed that the residual internal pressures for quartz inclusions in cuboid diamonds were 1.5-2.1 GPa (Navon, 1991). The phase diagram of water shows that the high internal pressure retained in diamonds are high enough to crystallize liquid water into ice VI or VII at room temperature. Thus one may expect that water can exist as ice inclusions in diamonds at ambient temperature, but ice inclusions have not been reported although there are numerous reports of liquid water. Previously reported infrared (IR) and Raman spectra have revealed that high internal pressures can be retained in some diamond inclusions. Frequency shifts in IR spectra disclosed that the residual internal pressures for quartz inclusions in cuboid diamonds were 1.5-2.1 GPa (Navon, 1991). In this study, we searched for ice as a solid inclusion in natural diamonds using near infrared (NIR) spectroscopy.

Near infrared absorption spectra of natural morphologically cubic polycrystalline diamonds (cuboid) were obtained at room temperature, and the stretching plus bending combination band of molecular water was observed (Figures 1). The spectrum was composed of the main band at 5180 cm^{-1} due to liquid water and a shoulder at 5000 cm^{-1} . The 5000 cm^{-1} band suggests the presence of a phase with stronger hydrogen bonding in inclusions in the diamond. This shoulder absorption decreased on heating to 120°C. The combination band of H_2O at high pressure and temperature was measured using a resistively heated diamond cell and the pressure dependence of the peak position was obtained. Comparison to the present experimental results indicates that the spectral changes induced by heating of the cuboid corresponded to melting of a high-pressure form of ice, and the shoulder absorption at 5000 cm^{-1} arises from ice VI at 1.9 GPa.

On the other hand, the liquid water, a main component of the fluid inclusions in the cuboid, was not under high pressure judging from the frequency of the combination band. This contrast might relate to the texture of the cuboid diamond. The spectral observation enables us to estimate the residual pressure of mantle fluid encapsulated in these diamonds. The diamond-cell data also provide high-P-T NIR fingerprint spectra that could be useful for identifying H_2O phases and confining pressures in other samples.

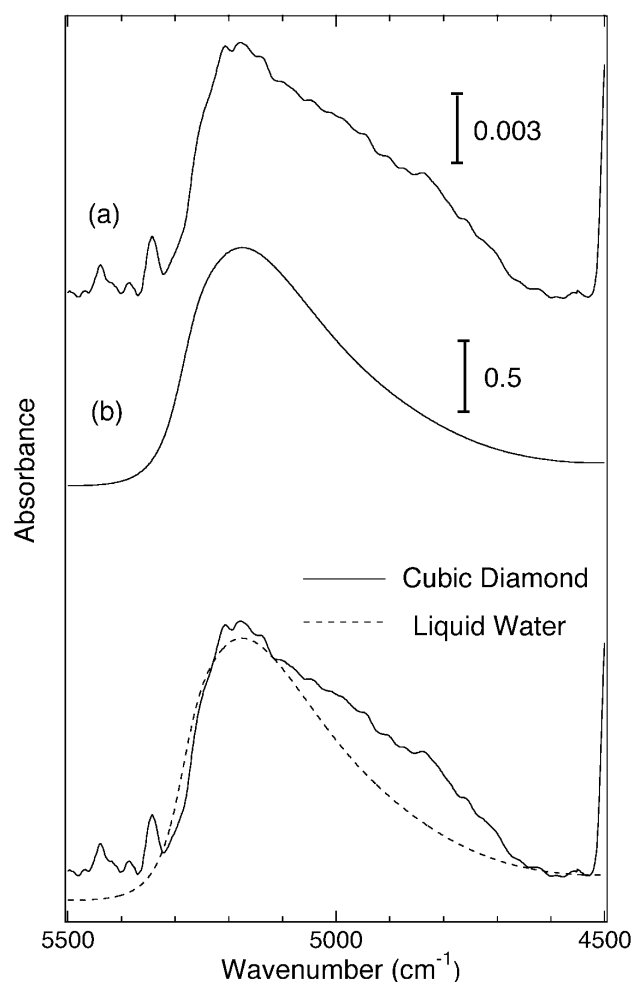


Figure 1: NIR absorption spectra of water involving the stretching plus bending combination band at room temperature. The upper spectrum (a) was from the cuboid diamond, and the lower spectrum (b) was from liquid water. Both spectra show a peak approximately at 5200 cm^{-1} , but the upper spectrum shows a convex upward feature in the low wavenumber side of the band in contrast to the concave upward feature for the lower spectrum. Overlapped these two spectra are illustrated in bottom in order to clarify the difference in band shapes between these two spectra.

Navon O, *Nature*, **353**, 746-748, (1991).