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High-Pressure Effects in Benzoic Acid Dimers: Vibrational Spectroscopy YUCHUAN TAO, ZBIGNIEW DREGER, YOGENDRA GUPTA, Washington State University — To understand pressure effects on dimer structure stability, Raman and FTIR spectroscopy were used to examine changes in hydrogen bonded dimers of benzoic acid crystals up to 31 GPa. Raman measurements indicated a phase transition around 7-8 GPa. It is proposed that this transition is caused by a rearrangement of molecules within the dimer leading to a symmetry change from C_{2h} to likely C_2 or C_s. This change was reversible upon pressure release from 15 GPa. Pressures above 15 GPa, induced gradual changes in luminescence and a color change in the crystal from white to brownish. FTIR measurements at 31 GPa revealed the formation of a new broad band centered around 3250 cm^{-1}, which was attributed to the stretching vibrations of the O−H bond. It is proposed that hydrogen bonded dimers of benzoic acid transform partially to a covalently bonded compound composed of benzoic anhydride-like molecules and H_2O. This study demonstrates that application of high pressure can lead to significant changes in the H-bonded dimer structure, including formation of chemical bonding. Work supported by DOE/NNSA and ONR/MURI.

Zbigniew Dreger
Washington State University

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