

Abstract Submitted
for the NWS15 Meeting of
The American Physical Society

Stability of Molecular Crystals under High Pressure: Tuning of Hydrogen Bonding by Deuterium Substitution¹ YUCHUAN TAO, ZBIGNIEW DREGER, YOGENDRA GUPTA, Washington State University — Hydrogen bonding (HB) is ubiquitous in many molecular compounds, and is often a key factor in determining the structure and properties of these systems. Because the strength of HB depends on the location of hydrogen atom between two electronegative atoms, external pressure and H/D substitution are very useful tools for controlling and changing the behavior of hydrogen bonding. In this work, we used both factors to gain insight into the role of hydrogen bonding on high-pressure stability of molecular crystals. The pressure effects were examined on two hydrogen-bonded molecular crystals with planar crystal structures, squaric acid ($\text{H}_2\text{C}_4\text{O}_4$, SQA) and diaminodinitroethylene ($[\text{CNO}_2\text{NH}_2]_2$, FOX-7), and their deuterated counterparts. Raman experiments in a diamond anvil cell (DAC) were performed on deuterated SQA and FOX-7 to 25 and 40 GPa, respectively, and compared with our previous results on hydrogenated crystals. We demonstrated that the high-pressure response of these crystals depends on the initial strength of HB, and that the different aspects of high-pressure stability are affected selectively. In particular, we showed that deuteration weakens the hydrogen bonds, affects the pressure onsets for structural phase transitions and lifts vibrational modes coupling.

¹Work supported by DOE/NNSA and ONR

Zbigniew Dreger
Washington State University

Date submitted: 08 Apr 2015

Electronic form version 1.4