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High Pressure Raman Spectroscopy of Hydrogen Bonded, Layered Crystal of Squaric Acid ZBIGNIEW DREGER, JUEFEI ZHOU, YUCHUAN TAO, YOGENDRA GUPTA, Washington State University — High pressure Raman spectroscopy experiments were carried out on squaric acid ($H_2C_4O_4$) to understand the role of hydrogen bonding on the structural and chemical stability of layered molecular crystals. Measurements in a diamond anvil cell up to 70 GPa revealed several instances of structural changes: (1) disappearance of some lattice modes at 0.6-0.9 GPa, indicating a change in the crystal structure symmetry from monoclinic to tetragonal, (2) disappearance of some intramolecular modes at 3 GPa, indicating possible symmetrization of hydrogen bonding in crystal layers, and (3) appearance of new intramolecular modes at 13-14 GPa. The latter changes were accompanied by a gradual increase in the Raman intensity and changes in the widths of lattice and intramolecular modes. No chemical changes were observed over the pressure range examined. These results suggest that hydrogen bonding network in layers is preserved to the highest applied pressures. However, the layers could be distorted with respect to each other above 13 GPa. Work supported by DOE/NNSA and ONR/MURI.

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