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Vibrational spectra of solid HNFX ($C_6H_8F_8N_8O_4$): Experiments and theory[1] MALCOLM NICOL, CEDRIC GOBIN, EUNJA KIM, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, NV 89154 — Assignment of the vibrational spectra of molecular solids such as HNFX is very complex. We have made a combined experimental and modeling study of the vibrational spectra of solid HNFX. Crystalline HFNX consists of unit cell with 9 HNFX molecules in Ci symmetry. Vibrational modes were calculated by using the PCFF force field method and were directly compared to measured IR and Raman spectra. A complimentary calculation for molecular HNFX allows us to identify the intramolecular motions measured in experiments. Intermolecular motion by F–H bonds between HNFX molecules will be discussed in this talk.

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