Spectroscopic and Computational Insight into Weak Noncovalent Interactions in Crystalline Pyrimidine

Ashley M. Wright, Lynn V. Joe, Austin A. Howard, Gregory S. Tschumper, and Nathan I. Hammer

Department of Chemistry and Biochemistry, University of Mississippi, University, Mississippi 38677

Supplementary Data

Figure S-1 shows polarized Raman spectra of pyrimidine in the C-H stretching region compared to simulated spectra from B3LYP/6-311++G(2df, 2pd) B3LYP/aug-cc-pVTZ, and MP2/6-311++G(2df, 2pd) harmonic vibrational frequencies. The simulated spectra are constructed by summing Lorentzian functions centered at each computed normal mode with a consistent width. The frequencies have been scaled with appropriate scaling factors for each method/basis set combination.

Figure S-2 shows solid and liquid phase Raman spectra of pyrimidine that include Lorentzian functions whose sums have been fit to the full experimental spectra. The center frequencies of the Lorentzians were used to define the spectral locations of each overlapped peak.
Figure 1: Polarized Raman spectra of pyrimidine in the C-H stretching region compared to simulated (sum of Lorentzian functions) spectra from B3LYP/6-311++G(2df, 2pd) (scaled by 0.963), B3LYP/aug-cc-pVTZ (scaled by 0.964), and MP2/6-311++G(2df, 2pd) (scaled by 0.945) harmonic vibrational frequencies.
Figure 2: Solid and liquid phase Raman spectra of pyrimidine including Lorentzian fit functions