INFRARED SPECTRA OF γ-BUTYROLACTONE DIMERS AND TRIMERS ISOLATED IN INERT GAS MATRICES

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The infrared spectra of matrix-isolated γ-butyrolactone and γ-butyrolactone-d_6 were obtained. The carbonyl stretching mode appears as a doublet at 1803 and 1775 cm^{-1} (1797 and 1788 cm^{-1} for the deuterated isotopomer) in an argon matrix. Other peaks, including the ester and C-H (C-D) stretching modes also exhibit comparable splitting. These features may be enhanced with annealing and can be attributed to dimers and trimers formed during deposition of the matrix.
Vibrational frequencies predicted by DFT are in agreement with the observed values. The dimer geometries are influenced by multiple hydrogen bonds to the carbonyl oxygens, and stacking of the monomer rings. Binding energies of 20-22 kJ mol^{-1} are predicted. Similar stacked structures are predicted for trimers (37-39 kJ mol^{-1}), but cyclic trimers (50 kJ mol^{-1}) are more stable.