WEAKLY-BOUND COMPLEXES OF FURAN AND WATER AS INVESTIGATED BY MATRIX ISOLATION FTIR

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Weakly bound complexes containing aromatic species have been the subject of study for many years. Here, a study of the 1:1 complexes of furan (C_4H_4O) with water will be presented. In this work, matrix isolation FTIR and computational methods were used to examine stable geometries of this dimer system. Density functional theory and MP2 methods were used to identify four minimum energy geometries. Three interaction motifs are recognized in these structures: C$-$H$\cdots$O, O$-$H$\cdots$O, and O$-$H$\cdots\pi$. The four structures were found to be within 610 cm^{-1}(7.3 kJ/mol) of each other across all computational methods. Matrix isolation FTIR spectroscopy was used to explore mixtures of furan with H_2O in a nitrogen matrix at 15 K. Spectra acquired show several peaks that were not associated with water or furan monomers and have been assigned to FUW. Additionally, mixtures of furan with D_2O and HDO were deposited and their spectra recorded. Characteristic shifts of each isotopologue were identified and used to characterize the geometry of the FUW complex. Both computational and spectroscopic results point to the formation of a single complex geometry that interacts through a standard O$-$H$\cdots$O hydrogen bond.

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