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

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Weakly-bound complexes containing aromatic species have been the subject of study for many years. Here, a study of the weakly-bound complexes of thiophene (C_4H_4S) with water will be presented. In this study, matrix isolation FTIR and computational methods were used to examine stable 1:1 complexes of thiophene : water (Tp:H_2O). Multiple density functional theories along with MP2 calculations were used to find four stable geometries. Two geometries can be described by C$-$H$\cdots$O interaction, one by O$-$H$\cdots\pi$ interaction, and one by O$-$H$\cdots$S interaction. These geometries were found to be within 10 kJ/mol of each other by all computational methods. Matrix isolation FTIR experiments identified several peaks that were not associated with isolated water or thiophene, implying the bands are due to weakly-bound complexes of the two. In addition to normal water, D_2O and HDO complexes with thiophene were also observed. Possible interpretations of the experimental and computational results will be presented. Comparisons to the structure of furan (C_4H_4O) : water[a] will also be discussed.

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[a]Lockwood, S. P.; Fuller, T. G.; and Newby, J. J. *J. Phys. Chem. A* **2018**, 122, 36, 7160-7170