Abstract

The interstellar medium is filled with very cold and dense molecular clouds. These icy clouds contribute to the structure and evolution of the interstellar medium. Among various molecular clouds, the ones containing hydrogen bonds have special importance. Propargyl alcohol and methyl amine are two such molecules. Propargyl alcohol further gains importance because of the known propargyl radical pathway for benzene formation. Matrix isolation infrared spectroscopy corroborated with quantum chemical calculations serves as a powerful tool to study weak interactions in a system. This technique is characterized to give very sharp spectral features, making it possible to identify and study various conformations and complexes formed by weak interactions. In this thesis, propargyl alcohol with methyl amine system has been explored experimentally and supported with computational calculations. Calculations were performed at B3LYP, MP2 and M06-2x levels of theory using the 6-311++G(d,p) basis set to obtain optimized structures, stabilization energies and vibrational frequencies of the intuitive structures. The calculated results were used to support the experimental results. The O-H…N and the C≡C-H…N structures which are global and local minima respectively were identified in the matrix. Methyl amine and water system was also studied in a similar manner. 1:1 and 1:2 adducts of methyl amine with water were identified in the matrix.