

AB INITIO AND EXPERIMENTAL STUDIES OF ISOMERISM IN He-CH₃X COMPLEXES

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The existence of multiple minima on the intermolecular potential energy surface of rare gas-molecule complexes appears quite general. Localization of the rare gas atom in the various potential energy minima results in several "isomeric" forms of a single complex. Studying these isomers provides detailed information about a much larger portion of the potential energy surface than can be gained through the study of the ground state. We find He-molecule complexes particularly advantageous for the study of this problem. The weak He-molecule interaction energy and the low mass of the helium atom combine to make the zero point energy an appreciable fraction of the total well depth, and this leads to several low-lying states that are separated by energies in the microwave to millimeter-wave region. Although the states are high up on the potential surface, they do tend to show localization in the various potential energy minima. We present a combined *ab initio* and experimental study of He-CH₃F and He-CH₃Cl. High-level *ab initio* calculations show three potential energy minima for each of the species: one on either end of the C-X axis and one in which the helium is in a T-shaped configuration relative to the C-X axis. In He-CH₃F the global minimum is at the C end of the C-F axis, whereas in He-CH₃Cl the global minimum is in the T-shaped configuration. Bound state calculations on the *ab initio* surfaces show the ground state for both species to be T-shaped, with higher energy states localized at either end of the C-X axis. Results from on-going microwave and millimeter-wave experimental studies on both species will be presented and compared with the *ab initio* calculations.