

INFRARED SPECTROSCOPIC INVESTIGATION ON CH BOND ACIDITY IN CATIONIC ALKANES

YOSHIYUKI MATSUDA, MIN XIE, ASUKA FUJII, *Department of Chemistry, Tohoku University, Sendai, Japan.*

We have demonstrated large enhancements of CH bond acidities in alcohol, ether, and amine cations through infrared predissociation spectroscopy based on the vacuum ultraviolet photoionization detection. In this study, we investigate for the cationic alkanes (pentane, hexane, and heptane) with different alkyl chain lengths. The σ electrons are ejected in the ionization of alkanes, while nonbonding electrons are ejected in ionization of alcohols, ethers, and amines. Nevertheless, the acidity enhancements of CH in these cationic alkanes have also been demonstrated by infrared spectroscopy. The correlations of their CH bond acidities with the alkyl chain lengths as well as the mechanisms of their acidity enhancements will be discussed by comparison of infrared spectra and theoretical calculations.