

Research Highlights

Molecular Science

The researchers on molecular science are engaged in various projects on the spectra and reaction dynamics of molecules and transient species. Recent research has explored new phenomena and provided basic understanding relevant to the photochemistry of the interstellar medium, to photodissociation and to inner-shell photoexcitation. We investigate spectra and chemical dynamics using various experimental probes including photofragment-translational spectra coupled with a crossed molecular-beam apparatus, matrix-isolation spectra, near-edge X-ray absorption spectra, resonant photoemission spectra, and uv/visible dispersed fluorescence. Progress in this research will contribute significantly to a fundamental understanding of the chemical reactivity of molecules and the elementary processes involved in photoexcitation and photodissociation.

Y. J. Wu and B. M. Cheng undertook a project to investigate the photodissociation of C₂H₂ at low temperature; the results are useful in the development of photochemical models to simulate the composition of the atmosphere of Titan and the source of aerosols. The absorption spectrum of ethyne, C₂H₂, in solid Ar was measured in the wavelength region 107–220 nm with light from a synchrotron. Based on that absorption, irradiation of samples of ethyne dispersed in neon with vacuum-ultraviolet (VUV) radiation yielded various products that were identified through their infrared absorption spectra including C_n (n = 3–12), C₂H, C₂H₃, C₄H, C₄H₂, C₈H⁺, and C₈H₂. As C₂H₂ has been proposed to assist the decomposition of CH₄ in Titan's atmosphere, the photochemistry of C₂H₂ plays an important role there.

S. H. Lee investigated the photodissociation dynamics of tetrahydrofuran (c-C₄H₈O) at 193.3 nm in a molecular-beam apparatus using photofragment-translational spectra. Five dissociation channels leading to products with *m/z* ratios appropriate for CH₂CH₂CH₂ + H₂CO, CH₂CHCH₂ + CH₂OH, H + CH₂CH₂ + CH₂CHO, CH₂CH₂ + CH₃ + HCO and CH₂CH₂ + CH₂CO + H₂ were identified, and their branching ratios were determined. The distributions of product kinetic energy, average kinetic-energy release, and fractions in translation were measured for each dissociation channel. The photodissociation of tetrahydrofuran into five channels is proposed to proceed mainly on the potential-energy surface of the ground state following ring opening and efficient internal conversion.

