SPECTROSCOPY OF AND PHOTOINDUCED ELECTRON TRANSFER IN THE COMPLEXES OF C_2H_4 WITH I AND I_2

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The charge-transfer complex of ethylene and iodine was isolated in a neon matrix and characterized by infrared and electronic spectroscopy, supported by $ab\ initio$ and Density Functional Theory (DFT) calculations which predict the spectra, structure, and binding energy of the complex. The intense charge transfer band of the complex was observed at 247 nm, in good agreement with Time Dependent DFT predictions. Photoinduced electron transfer initiated by laser irradiation at 240 nm gave rise to an intense band at 373 nm which is assigned to bridged ethylene-I atom radical complex. It is postulated that, following excitation of the charge transfer band, rapid back electron transfer leaves the neutral I_2 fragment on an excited repulsive potential surface, which leads to rapid cleavage of the I-I bond. This is consistent with previous gas-phase studies of arene-I_2 complexes. The photolysis of the radical complex, initiated by laser irradiation at 355 nm, led to the reappearance of absorptions due to the ethylene-I_2 complex and the appearance of both the $anti-$ and $gauche-$ conformers of the electrophilic addition product, 1,2-diiodoethane, indicating the importance of a radical addition mechanism.