A THEORETICAL STUDY OF ICE-BOUND PHOTOIONIZATION AND SPECTROSCOPY Of SMALL POLYCYCLIC AROMATIC HYDROCARBONS

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Polycyclic aromatic hydrocarbons (PAHs) are the largest known interstellar molecules identified to date. To complement recent experimental studies, density functional theory calculations were employed to characterize the photoionization behavior of benzene, naphthalene, anthracene, and pyrene in UV-photoprocessed ices. Calculations were performed at the B3LYP/6-31+G** level in conjunction with a continuum solvation model to account for the ice environment. The results indicate that PAH ionization energies are significantly reduced when the molecules are embedded in a water ice matrix. Electronic and vibrational spectra were computed for both neutral and ionized PAHs. For the most part, low-lying electronic transition energies were found to be remarkably unaffected by ice. PAH cations are observed to be long-lived in photoprocessed ices, which may be due to the trapping of electrons at favored sites such as OH radicals formed by photolysis of water.