

MATRIX-ISOLATION SPECTROSCOPY OF POLYCYCLIC AROMATIC HYDROCARBON (PAH) IONS:  
HYDROGENATED-PAH CATIONS AND THE PENTACENE IONS

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We are currently extending the size, structure, and charge state of polycyclic aromatic hydrocarbons (PAHs) studied spectroscopically in the laboratory to develop a more complete understanding of the physical conditions and the chemical evolution within the interstellar medium. We report here the UV/Visible spectroscopy of a series of PAHs containing excess H atoms ( $H_n$ -PAHs) and their photoproducts isolated in a neon matrix and compare them to the spectra of their chromophores. We also report supporting time-dependent density-functional theory (TD-DFT) calculations that allow new and revised assignments for pentacene ions. These calculations indicate that in the specific case of the pentacene cation, the HOMO to LUMO transition leads to the lowest excited electronic state. This is the first time such an effect is reported for the acenes.