

Infrared Spectra of Matrix-Isolated Heterocyclic Aromatic Compounds and their Ions

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Polycyclic Aromatic Hydrocarbons (PAHs) are present in the interstellar environment. Nitrogen is the fourth most abundant chemically reactive element in the interstellar medium. Thus it is reasonable that nitrogen compounds may be present in interstellar environment. The mid-infrared spectra of a variety of argon matrix isolated Nitrogen Heterocyclic Aromatic Compounds (NHACs) - polycyclic aromatic compounds with one or more nitrogen atoms incorporated into the aromatic framework of the molecule - are presented in this paper. The experimental data are compared to theoretically calculated values obtained using density functional theory (DFT) at the B3LYP/4-31G level, unless otherwise indicated. In general, the neutral NHAC compounds exhibited behavior similar to that observed in ionized PAHs, the most intense spectral features were those in the CC stretching and CH in-plane bending regions (1500 to 1300 cm^{-1}). The NHAC compounds. The implications of these results for astrophysical infrared spectroscopy are discussed.