

MID-INFRARED SPECTROSCOPY OF CYANO-PAH CATIONS FOR ASTROCHEMICAL CONSIDERATION

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The mid-IR spectra observed from different parts of the interstellar medium (ISM) are dominated by a set of IR features referred to as the unidentified infrared bands (UIBs). Although it has been accepted that these emission features originate from polycyclic aromatic hydrocarbon (PAH) molecules and their derivatives, the individual detection of the emitting species is challenging due to their similar IR fingerprint in the 5-15 μm spectral region. Cyano-substituted PAHs were recently detected in the ISM based on their rotational spectra. These species have dominant features (CH and CN stretch) in the less explored 1-5 μm spectral region that can be diagnostic in further detection. However, there is still a lack of laboratory data to compare with the observed mid-IR spectra. Here we present the low temperature gas-phase vibrational spectra of a set of ionised cyano-group containing PAHs in the mid-infrared region. Experimentally, the cyano-PAH ions are cooled below 10 K in a cryogenic ion trapping apparatus, tagged with He atoms and probed with tunable radiation. Quantum-chemical calculations are carried out at a density functional theory level. The spectra are dominated by the CN stretch around 4.5 μm , with weaker CH modes near 3.2 μm .