NON-LTE INFRARED SPECTRUM OF JET-COOLED NAPHTHALENE

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Polycyclic aromatic hydrocarbons (PAHs) are responsible for the aromatic infrared bands (AIBs) observed in various astronomical objects. Studying their sharp Q-branches associated with the out-of-plane bending vibrational modes under low rotational excitation might be a key for their identification in the interstellar medium (ISM).

IR spectrum of naphthalene was recorded around 12.7 μ m using the jet-AILES setup, coupled to the Fourier transform spectrometer (Bruker IFS 125 HR) equipping the AILES beamline of the synchrotron SOLEIL. In the jet, an efficient rotational relaxation of naphthalene occurs resulting in a rotational temperature of about 25 K, while the vibrational cooling is limited due to an insufficient number of two-body collisions in the supersonic expansion. This leads to an interesting non-LTE situation, favorable for the detection of hot bands: the low rotational temperature drastically simplifies the rotational structure and magnifies the Q-branches, while the higher vibrational excitation allows the presence of many transitions from moderately excited vibrational states. To assign the observed hot bands we have used the AnharmoniCaOs code, which explicitly considers Fermi and Darling Dennison resonances for a better accuracy of the band positions, and the second order dipole derivatives to simulate intensities of overtone, combination, and difference bands. Our program is unique in the sense that it can produce spectrum at a non-zero kelvin temperature unlike standard commercially available quantum chemistry packages. It also enables us to assign arbitrary (non-thermal) populations to individual vibrational states from which transitions originate, allowing us to simulate non-LTE spectra.