

Infrared spectra of potential interstellar molecules: protonated PANH and OCS

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The infrared emission from many astronomical objects is dominated by the unidentified infrared (UIR) emission bands, which are characterized by main features at 3.3, 6.2, 7.7, 8.6, and 11.2 μm . Because these features are characteristic of the CH stretching, CC stretching, and CH bending modes of aromatic compounds, polycyclic aromatic hydrocarbons (PAHs) were proposed to be possible emitters. The nitrogen containing PAHs, known as polycyclic aromatic nitrogen heterocycles (PANHs), might be responsible for the 6.2- μm feature of UIR bands because the N atom induces a blue shift to the CC stretching modes of pure PAHs near 6.3 μm [1]. The existence of protonated PANHs is expected because of the large proton affinity at the nitrogen site of PANHs.

We have developed a new method to investigate the infrared spectra of protonated PAHs using electron bombardment during deposition of a PAH/*para*-H₂ mixture at 3.2 K [2]. The electron bombardment of *para*-H₂ produces H₃⁺, which subsequently react with PAH to form protonated PAH (H⁺PAH). We have applied this method to PAHs up to ovalene (C₃₂H₁₄) to obtain infrared spectra of protonated species with narrow lines and excellent signal-to-noise ratio [3]. In this work, we extended our investigation to quinoline and isoquinoline (C₉H₇N) as a first step toward the study of protonated PANHs. The IR spectra of protonated quinoline and isoquinoline (C₉H₇NH⁺) are characterized by features originating from NH stretching, CC stretching, and CH(NH) bending modes. Agreement between observed spectra of C₉H₇NH⁺ and the UIR emission spectrum is unsatisfactory, most probably because the size of molecule is too small; in the case of H⁺PAH, features close to the UIR bands were observed for only large H⁺PAH such as protonated ovalene (C₃₂H₁₅⁺). However, the blue shifts of the CC stretching bands of protonated quinoline and isoquinoline from the corresponding H⁺PAH, protonated naphthalene (C₁₀H₉⁺), are clearly observed. IR spectra of mono-hydrogenated quinoline and isoquinoline (C₉H₇NH[·]) radicals, with hydrogen atom attached on the N atom, were also identified for the first time.

We also applied this method to small molecules such as OCS, which has been postulated to exist in the ISM. The OCS molecule has two possible protonation sites, leading to isomers HOCS⁺ and HSCO⁺. Both HOCS⁺ and HSCO⁺ have been observed with microwave spectroscopy [5], but only the OH stretching mode of HOCS⁺ has been identified with gas-phase IR spectroscopy [6]. We identified three IR absorption lines of HOCS⁺ at 2945.9 (ν_1), 1875.3 (ν_2), and 1041.9 (ν_3) cm⁻¹ and two of HSCO⁺ at 2506.9 (ν_1) and 2074.2 (ν_2) cm⁻¹. Absorption lines of *t*-HOCS at 3563.4, 1394.8, and 1199.0 cm⁻¹ were also identified for the first time. Assignments were achieved according to expected chemistry, comparison between experimental spectra and theoretical predictions, and isotopic substitutions. The large red shift of the ν_1 of HOCS⁺ is attributed to partial proton sharing between OCS and H₂.

References

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