



AstropAH

A Newsletter on Astronomical PAHs

Issue 90 • July 2022



JWST Starts Its Science!



Editorial

Dear Colleagues,

This is AstroPAH volume 90!

Our cover features the first images from the James Webb Space Telescope (JWST). These images mark the beginning of its scientific observations. We expect even more amazing observations and great results in the coming months!

The 'In Focus' section features the contribution from Prof. Heloisa M. Boechat-Roberty, who heads the Astrochemistry Research Group at the Observatorio do Valongo, Universidade Federal do Rio de Janeiro (UFRJ), in Brazil. The article is co-authored by Dr. Heidy M. Qutián-Lara, who was a researcher in Rio and is now a visiting researcher at the University of Kent, UK.

Do not miss any of the papers in our Abstracts section. This month, many cover experimental work such as PAH growth in a benzene discharge, spectroscopy of PAH cations and mass spectrometry of ionized PAHs.

If you are on Instagram, be sure to check out our next [PAH of the Month!](#) This month we feature the nitrogen heterocycle and anthracene-related PAH, acridine.

We hope you enjoy reading our newsletter, and we thank you for your dedication and interest in AstroPAH! Please continue sending us your contributions, and if you wish to contact us for a future In Focus, Picture of the Month, or other ideas, feel free to use our [email](#).

We hope you enjoy reading our newsletter.

The Editorial Team

**Next issue: 22 September 2022.
Submission deadline: 9 September 2022.**

AstroPAH Newsletter

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PAH Picture of the Month

First images from the James Webb Space Telescope (JWST). The background picture features the star forming region NGC 3324 in the Carina Nebula. The upper, middle and bottom pictures show the Stephan's Quintet, the galaxy cluster SMACS 0723 and the Southern Ring planetary nebula (NGC 3132), respectively.

Credits: Images of the Carina nebula, Stephan's Quintet, Southern Ring nebula, and SMACS 0723: [NASA](#), [ESA](#), [CSA](#) and [STsci](#). JWST artist conception: [Northrop Grumman](#).

PAHs in Highly Dissociative Regions

by Heloisa M. Boechat-Roberty and

Heidy M. Qutián-Lara

Polycyclic aromatic hydrocarbons (PAHs) are molecular archetypes that can be classified according to the number of fused benzene (C_6H_6) rings that make up the base structure. Both neutral and ionised forms of these macro-molecules have been identified in different astrophysical environments inside and outside the Milky Way (Tielens, 2008; Sales et al., 2010; Yang et al., 2017; Peeters et al., 2021). Benzene (C_6H_6) and benzene-derived molecules such as benzonitrile (C_7H_5N) and cyanonaphthalene ($C_{10}H_7CN$) have also been identified in space thanks to their infrared (IR) spectroscopic characteristics and their rotational transitions in the radio frequency region (McGuire et al., 2021; McGuire, 2022).

PAHs and benzene-derived systems exist in space in the gas-phase or frozen on the surface of dust grains. They are constantly exposed to the effects of a strong flux of ultraviolet (UV) photons, X-rays and charged particles, which induce processes of excitation, ionisation, dissociation, and molecular desorption. The mechanisms by which these structures manage to maintain their molecular integrity in such highly dissociative regions are still not fully understood. To shed light on the structural stability of PAHs in astrophysical environments, our research group performs laboratory experiments where the harsh conditions of these regions are simulated.

Experimental Setups

The ionisation and dissociation measurements of PAHs, benzene, and related molecules were performed using UV and X-ray photons from different experimental beamlines of the Brazilian Synchrotron Light Laboratory (LNLS) at the Brazilian Centre for Research in Energy and Materials, located in Campinas, Brazil. For photons at UV (5-100 eV) and at soft X-ray (250-1000 eV) ranges, we used the Toroidal Grating Monochromator (TGM) and Spherical Grating Monochromator (SGM) beamlines, respectively. For 2500 eV photons, we used the Soft X-ray Spectroscopy (SXS) beamline, which operates in the 1000–5000 eV energy range. The selection of the specific photon energies covered in this work was also due to the fact that they are amongst the highest photon fluxes in each beamline, which ultimately results in better ion counting and low signal-to-noise ratio. Mass spectra of ionic fragments were obtained using time-of-flight mass spectrometry (TOF-MS). Currently, LNLS is being replaced by a new state-of-the-art, fourth-generation synchrotron laboratory called Sirius (Figure ??, Shin 2021), with which it will be possible to perform new and improved experiments.



Figure 1 – Aerial photo of the new synchrotron laboratory 'Sirius', <https://www.lnls.cnpm.br/sirius-en/>.

We have examined experimentally the photo-ionisation and photo-stability of benzene (C_6H_6), toluene ($C_6H_5CH_3$), biphenyl ($C_{12}H_8$), naphthalene ($C_{10}H_8$), anthracene ($C_{14}H_{10}$), 2-methylanthracene ($C_{14}H_9CH_3$), and pyrene ($C_{16}H_{10}$) upon interaction with photons at energy ranges of UV (10–200 eV), soft X-rays (280–310 eV), and 2500 eV. We determined the absolute photo-ionisation and photo-dissociation cross-sections as a function of the incident photon energy; the production rates of singly, doubly, and triply charged ions; and the molecular half-lives in some astronomical environments such as photo-dissociation regions and circumnuclear regions of active galactic nuclei (AGN).

PAHs in Circumnuclear Regions

IR signatures of PAHs are observed in a variety of astrophysical objects, including the circumnuclear medium of AGNs. In these regions, the flux of high-energy photons (0.2-10 keV) interacts continuously and aggressively with PAHs, and strong destruction of the molecular structures is to be expected. Therefore it is necessary to study the mechanisms of PAH protection. Recently, we examined the photo-ionisation and photo-stability of a set of small PAHs upon interaction with 275, 310 and 2500 eV photons (Monfredini et al., 2019). We determined the absolute photo-ionisation and photo-dissociation cross-sections as a function of the incident photon energy; the production rates of singly, doubly, and triply charged ions; and the molecular half-lives in the regions surrounding selected AGN sources. Inspection of the results indicates that even considering X-ray photon flux attenuation by dust grains, the estimated half-lives are not long enough to account for PAH detection. We suggest that a more sophisticated interaction between PAHs and dust grains should be present to avoid severe molecular destruction. Since the carbon content of the PAHs comprised in this study varied merely from 10 to 16, it was not possible to observe any significant difference in the estimated molecular half-lives with respect to PAH size. On the other hand, we observed an increase in the formation of multiply-charged cationic parental ions with increasing PAH size at 2500 eV (Figure 2). This result suggests that enrichment of multiply charged ions triggered by high energy X-ray photons may occur in AGNs.

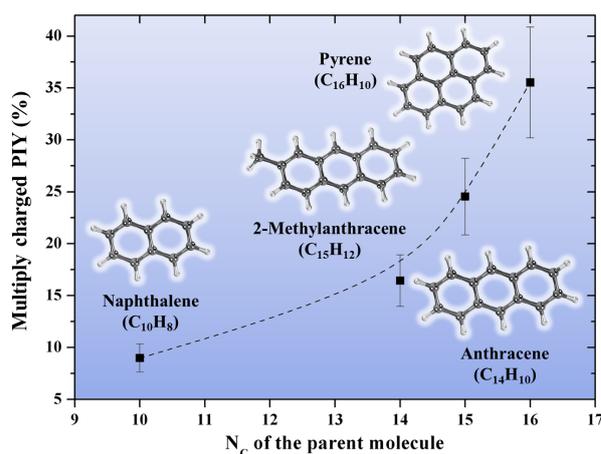


Figure 2 – Multiply charged partial ion yield (PIY) as a function of the PAH carbon content at photon energy of 2500 eV. (Monfredini et al., 2019).

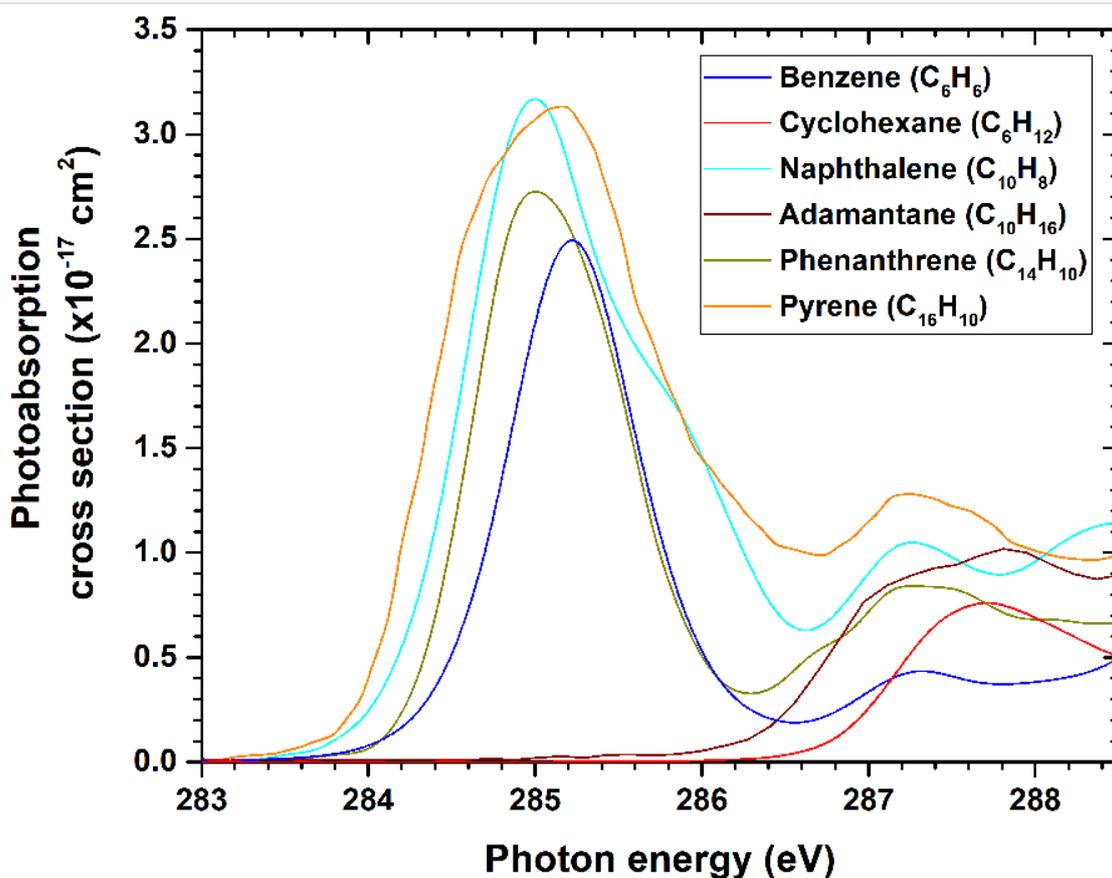


Figure 3 – Absolute photoabsorption cross sections of selected molecules. Adapted from *Quiján-Lara et al. (2018)* using data from the Hitchcock database (*Hitchcock, 1994*).

Effect of PAH Hydrogenation

The PAH aromatic band at 3.3 μm is generally accompanied by the 3.4 μm band assigned to the vibration of the aliphatic C–H bonds. These features are usually associated with PAH-based compounds featuring an excess of peripheral H-atoms, labelled Hn-PAHs. This motivated us to investigate the effect of hydrogenation of PAHs on their X-ray photo-absorption, photo-ionisation and photo-dissociation cross-sections. Particularly, we experimentally analysed cyclohexane, C₆H₁₂, (*Quiján-Lara et al. 2018*) by simulating the impact of stellar radiation in the photo-dissociation region of a planetary nebula. Using synchrotron radiation and TOF-MS experiments, the ionisation and dissociation processes of C₆H₁₂ in the UV (10-200 eV) and soft X-ray (280-310 eV) energy ranges were investigated. Partial ion yield (PIY) analyses evidenced the higher tendency towards dissociation of cyclohexane compared to benzene, as expected due to the weakening of the carbon backbone following saturation of the C=C bonds and removal of aromaticity. However, the successive hydrogenation of the PAH structure leads to a systematic decrease in the photo-absorption cross-section around the C1s resonance edge (Figure 3), which consequently decrease their dissociation efficiency. These results suggest that hydrogenation could work as a protection mechanism for interstellar PAHs, a hypothesis also corroborated by other authors (*Reitsma et al., 2014*).

Biphenyl in Protoplanetary Nebulae

Biphenyl ($C_{12}H_{10}$) is special type of molecule where two benzene rings are connected by a C–C single bond (Figure 4). This species is considered an important precursor in the formation of larger PAHs through a series of hydrogen abstraction/acetylene addition (HACA) mechanistic steps. Given the possible relevance of biphenyl in astrophysical environments, we investigated its ionisation and dissociation processes upon interaction with soft X-ray photons in the edge of the inner-shell C1s resonance energy (Quitíán-Lara et al., 2020). The results were discussed in the context of PAH-rich planetary nebulae, namely BD+30°3639, NGC 7027, NGC 5315, and NGC 40. For the photon energies of 275 and 310 eV, the half-lives of biphenyl span from 10^5 to 10^7 yr. These values are, at best, two orders of magnitude lower than those related to interstellar injection time-scales of carbonaceous materials by AGB stars (Jones et al., 1994). These results suggest that processes such as density inhomogeneities should be present in order to facilitate biphenyl survival in the circumstellar regions of protoplanetary nebulae.



Figure 4 – Biphenyl ($C_{12}H_{10}$).

Final Remarks

Laboratory studies play a crucial role in the understanding of the chemical composition and nature of different astrophysical objects. With our experiments, we aim at contributing to the investigation of the stability of PAHs under UV and X-ray photon fluxes. Despite considerable advances in recent decades, there are still many questions to be fully addressed and solved concerning interstellar PAH chemistry. Recently, Gatchell et al. (2021) showed that PAHs, when dismembered by strong energetic collisions, can rebuild their structure in an amorphous form and survive in thermal equilibrium in the interstellar medium indefinitely. This finding, together with the results obtained by us and by other groups, highlights the importance of experimental investigation for a better understanding of PAHs, a very important class of carbon-based molecules, in interstellar, circumstellar and circumnuclear environments.

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We would like to thank the other members of our Astrochemistry group at Universidade Federal do Rio de Janeiro (UFRJ), Brazil, that brings together experimental and theoretical researchers and students working in the fields of Astronomy, Physics and Chemistry: Franciele Kruczkiewicz (PhD student at Aix-Marseille University, France); Julia C. Santos (PhD student at Leiden University, Netherlands); Dr. Edgar Mendoza (Universidad de Huelva, Spain); Dr. Felipe Fantuzzi (University of Kent, UK); Dr. Rafael Pinotti (UFRJ and Petrobras); Dr. Thiago Monfredini; Prof. Diana Andrade (Observatorio do Valongo - OV/UFRJ); Prof. Fabio Ribeiro (IFRJ); Prof. Marco Antônio Chaer do Nascimento (Instituto de Quimica - IQ/UFRJ); Prof. Maria Luiza Rocco (IQ/UFRJ); Prof. Ricardo R. Oliveira (IQ/UFRJ); Prof. Wania Wolff (Instituto de Fisica/UFRJ).



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Abstracts

Polycyclic aromatic hydrocarbon growth in a benzene discharge explored by IR-UV action spectroscopy

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Infrared signatures of polycyclic aromatic hydrocarbons (PAHs) are detected towards many phases of stellar evolution. PAHs are major players in the carbon chemistry of the interstellar medium, forming the connection between small hydrocarbons and large fullerenes. However, as details on the formation of PAHs in these environments are still unclear, modeling their abundance and chemistry has remained far from trivial. By combining molecular beam mass-selective IR spectroscopy and calculated IR spectra, we analyze the discharge of benzene and identify resulting products including larger PAHs, radicals and intermediates that serve as promising candidates for radio astronomical searches. The identification of various reaction products indicates that different gas-phase reaction mechanisms leading to PAH growth must occur under the same conditions to account for all observed PAH-related species, thereby revealing the complex and interconnected network of PAH formation pathways. The results of this study highlight key (exothermic) reactions that need to be included in astrochemical models describing the carbon chemistry in our universe.

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Quantification of molecular aromaticity as a predictive factor of astrophysical significance

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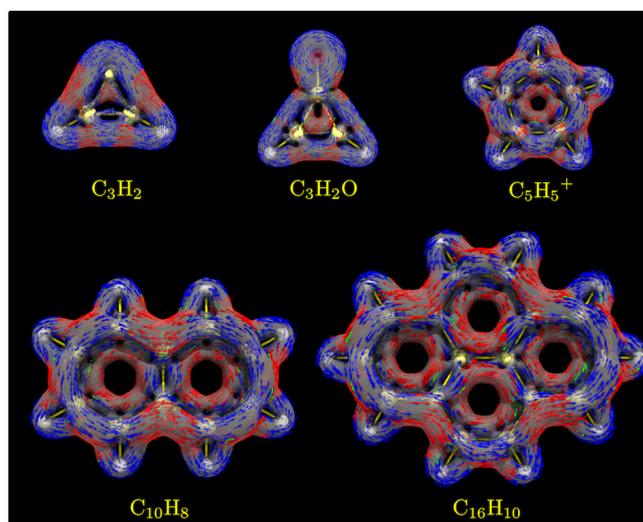
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This study reports the index of aromaticity calculated by numerical integration of the magnetically-induced current density for cyclic hydrocarbon molecules both known to exist in astrophysical media as well as those proposed to exist. This study promotes the ring current strength (RCS) value for quantifying aromaticity as a means of predicting astrophysical detectability. Density functional theory (DFT) calculations at the B3LYP/aug-cc-pVTZ level provide optimized structures and the wavefunctions needed to provide the RCS values for the molecules analyzed. The known interstellar molecules examined *c*-C₃H₂, *c*-(O)C₃H₂, *c*-C₃HC₂H, *o*-benzynes, benzonitrile, 1-cyano and 2-cyanonaphthalene all have RCS values of 9.9 nA T⁻¹ (nanoAmpère per Tesla) or above. The known antiaromatic species have RCS values of less than 0.0 nA T⁻¹ as expected. Several proposed interstellar molecules likely will not persist if they form due to low RCS values including *c*-(C)C₃H₂. Other species such as *p*-benzynes and *c*-HCNN⁺ have high RCS values of 19.9 nA T⁻¹ and 14.4 nA T⁻¹, respectively. Cyclic hydrocarbons previously observed in astrophysical media have high RCS values. Those with low or negative RCS values have yet to be observed implying that such a metric can indicate astrophysical significance.



Aromaticity of some selected PAHs: streamline representations of the current density flow. The magnitudes of the currents are indicated by a decreasing scale: white-yellow-red-black. Copyright: Alvarez-Thon et al., A&A, 2022, reproduced with permission ©ESO

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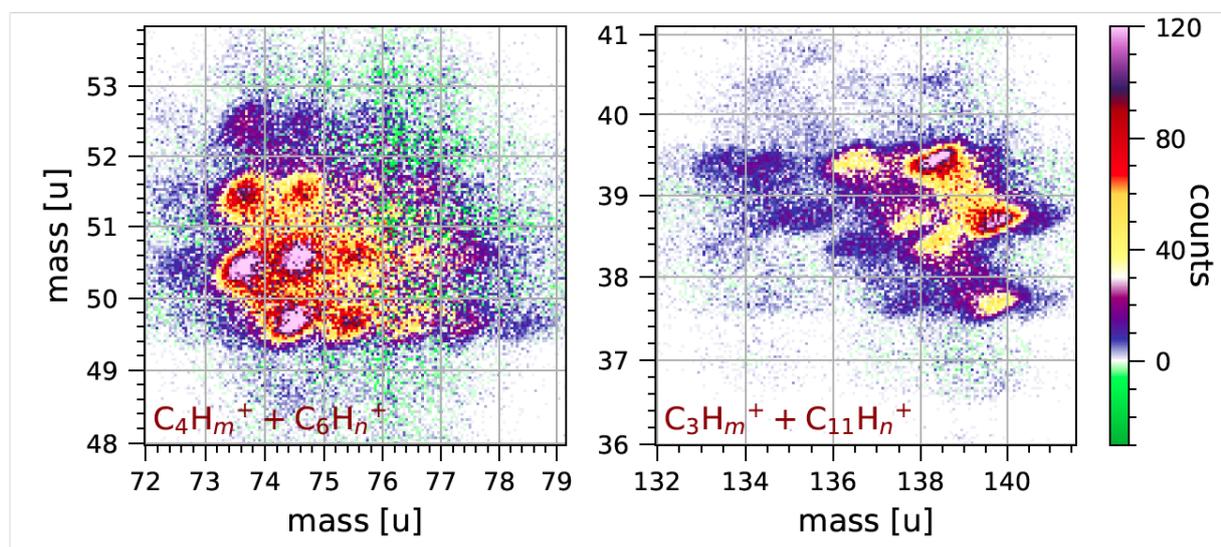
<https://doi.org/10.1051/0004-6361/202243253>

Coincidence mass spectrometry study of double ionization of anthracene by 70 eV electron impact

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Double ionization of anthracene molecules by 70 eV electron impact results in a number of prominent fragmentations producing two singly ionized fragments. In our experiment, ionized fragments were detected using a reflectron time-of-flight mass spectrometer. A field programmable gate array was used for the timing and the recording of mass spectra on an event-by-event basis. A detailed model of the coincidence data acquisition was developed, enabling us to reliably obtain the map of true coincidences. Our measurements show that fragmentations for which the total number of carbon atoms in the two singly ionized fragments is even are generally significantly stronger than fragmentations for which the total is odd. No fragmentations are observed for a total number of 13 carbon atoms. There are only very weak fragmentations where one of the fragments only contains one carbon atom. Most of the fragments have 2 or 3 hydrogen atoms. There are several fragmentations in which the larger fragment has 9, 10, 11 or 12 carbon atoms and 5, 6, 7 or 8 hydrogen atoms. Fragments with only carbon atoms and no hydrogen atoms are not present, and only few fragmentations are observed with a fragment containing only one hydrogen atom.



The figure shows two of the coincident groups observed in the map of true coincidences. Each section contains 160×160 bins and corresponds to $2 \times 2 \mu s$ in ion flight time. Because of the Coulomb explosion, many of the fragments are not detected, resulting in the bimodal distributions observed. Reproduced with permission of the authors and publisher under CC4 regulations.

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Penetration of non-energetic hydrogen atoms into amorphous solid water and their reaction with embedded benzene and naphthalene

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Chemical processes on the surface of icy grains play an important role in the chemical evolution in molecular clouds. In particular, reactions involving non-energetic hydrogen atoms accreted from the gaseous phase have been extensively studied. These reactions are believed to effectively proceed only on the surface of the icy grains; thus, molecules embedded in the ice mantle are not considered to react with hydrogen atoms. Recently, Tsuge et al. suggested that non-energetic hydrogen atoms can react with CO molecules even in ice mantles via diffusive hydrogenation. This investigation was extended to benzene and naphthalene molecules embedded in amorphous solid water (ASW) in the present study, which revealed that a portion of these molecules could be fully hydrogenated in astrophysical environments. The penetration depths of non-energetic hydrogen atoms into porous and nonporous ASW were determined using benzene molecules to be > 50 and ~ 10 monolayers, respectively (1 monolayer ≈ 0.3 nm).

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Infrared Spectra of 1-quinolinium ($C_9H_7NH^+$) Cation and Quinoliny Radical (C_9H_7NH and 3-, 4-, 7-, 8- HC_9H_7N) Isolated in Solid para-Hydrogen

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Large protonated polycyclic aromatic hydrocarbons (H^+PAH) and the corresponding nitrogen heterocycles (H^+PANH) have been proposed as possible carriers of unidentified infrared (UIR) emission bands from galactic objects. The nitrogen atom in H^+PANH is expected to induce a blue shift of the band associated with the CC-stretching mode of H^+PAH near $6.3 \mu m$ so that their emission bands might agree better with the UIR band near $6.2 \mu m$. We report the IR spectrum of protonated quinoline (1-quinolinium cation, $C_9H_7NH^+$) and its neutral species (1-quinoliny radical, C_9H_7NH) measured upon electron bombardment during deposition of a mixture of quinoline (C_9H_7N) and para-hydrogen ($p-H_2$) at 3.2 K, indicating that the protonation and hydrogenation occur mainly at the N-atom site. Additional experiments on irradiation of $C_9H_7N/Cl_2/p-H_2$ matrices at 365 nm to generate Cl atoms, followed by irradiation with IR light to generate H atoms via $Cl + H_2 (v = 1)$, were performed to induce the reaction $H + C_9H_7N$. This method proved to be efficient for hydrogenation reactions in solid $p-H_2$; we identified, in addition to C_9H_7NH observed in electron-bombardment experiments, four radicals with hydrogenation at the C-atom site – 3-, 4-, 7-, and 8- HC_9H_7N . Spectral assignments were achieved according to the behavior on secondary photolysis and a comparison of experimental results with vibrational wavenumbers and IR intensities predicted with the B3LYP/6-311++G(d,p) method. The observed lines at 1641.4 , 1598.4 , and 1562.0 cm^{-1} associated with the CC-stretching mode of $C_9H_7NH^+$ are blue-shifted from those at 1618.7 , 1580.8 , 1556.7 , and 1510.0 cm^{-1} of the corresponding protonated naphthalene ($C_{10}H_9^+$).

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