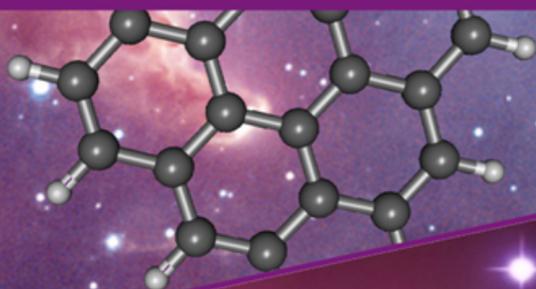


AstropAH

A Newsletter on Astronomical PAHs

Issue 71 • September 2020



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NISMS 2020

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Editorial

Dear Colleagues,

Welcome to our 71st AstroPAH volume! We hope all of you are healthy and have had a nice summer/winter holiday.

We are back from our annual August break and pleased to share a montage of the recent *Not Intentional Seminars on Molecular Spectroscopy* (NISMS) as our cover. NISMS was a remote workshop which ran in June of this year and showed how such virtual meetings can be both efficient and successful. As the prospects of teleworking and isolation are likely to endure in the near-future in many parts of the world, so too will our interactions and scientific collaborations. This month, our In Focus covers these technical aspects and a step-by-step account provided by the organizers of the NISMS virtual conference. We hope this will also be useful to our future colleagues as we make our way through more upcoming remote conferences!

We are also very happy to share several recent publications on diverse topics covering PAH-dust particle surface interactions as well as pyrene and adamantane radical cation infrared and optical spectroscopy.

The proceedings of the first IAU Laboratory Astrophysics Symposium, [IAU S350](#), co-edited by Dr. Farid Salama and Dr. Harold Linnartz, will be made public at the end of the month. Stay tuned!

We hope you enjoy reading our newsletter, and we thank you for your dedication and interest in AstroPAH! In the meantime, please continue sending us your contributions, and if you wish to contact us, feel free to use our [email](#).

Please be safe and stay healthy.

Enjoy reading our newsletter!

The Editorial Team

**Next issue: 22 October 2020.
Submission deadline: 9 October 2020.**

AstroPAH Newsletter

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PAH Picture of the Month

Speakers and session chairs of the Not Intentional Seminars on Molecular Spectroscopy (NISMS), a virtual meeting for spectroscopists organized during the COVID-19 pandemic.

Credits: Pictures and logo by the NISMS organization and the speakers and chairs named in the cover. Picture of the month design by H. R. Hróðmarsson.



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NISMS: A Virtual Meeting for Spectroscopists During COVID-19

by G. Stephen Kocheril, Kin-Long Kelvin Lee, Marie-Aline Martin-Drumel

At the beginning of 2020, no one would have foreseen that nearly all conferences scheduled throughout the year would be canceled or postponed due to a worldwide pandemic — COVID-19. Like many others, we were incredibly sad to see that these conferences and the opportunities that they bring were seemingly lost for the year, if not longer. As early career researchers ourselves, we saw the negative impact of not attending conferences and not sharing our research in scientifically and socially enriching environments.

To remedy this, we organized a virtual conference on molecular spectroscopy held at the end of June 2020. Since early career researchers would likely be among those most affected by this crisis (meeting others outside of their department is already challenging under “normal” circumstances), the *Not Intentional Seminars on Molecular Spectroscopy* (NISMS), was designed to be a meeting where they could showcase their work and facilitate interactions with other like-minded scientists. Consequently, we decided early on that all talks would be given by Master or PhD students and postdocs. We were hoping that this event would help not only to keep track of what kind of work is being done around the world, but also to initiate collaborations.

Pre-COVID-19, organizing a conference required lots of space, time, and money. However, with video conferencing software now widely available, anyone can host a virtual conference at a fraction of the cost. Herein, we will be outlining our experience as organizers of NISMS 2020, which ran from June 22–26 of this year.

[Establishing a scientific program]

Upon starting with this project, our main uncertainty was whether or not scientists beyond our own research groups would be interested in attending; spectroscopy comprises many sub-disciplines and is applied to many different problems. For starters, we contacted many of our collaborators to talk to them about our idea of hosting a virtual conference—from the positive feedback we received it appeared early on that we should be able to organize a

relatively large event. We decided that this year the best dates to organize the meeting were the week of June 22–26, when the [International Symposium on Molecular spectroscopy](#) would have taken place.

Because a virtual meeting can be quite demanding and exhausting to the attendees, we decided to follow a few rules:

1. Scientific sessions should be kept short, on the order of 1 h/session
2. Talks should be concise as well; we opted for the format used during the ISMS conference: 12 min talk + 3 min questions
3. Sessions should occur at times that make attendance reasonable for the speaker (mandatory condition) and the participants (trickier criterion)

Of all criteria, #3 was the only actual challenging one since from the very beginning we knew we would have to accommodate rather large time differences; two of the organizers were on US East Coast while the third was in Europe, and we had attendees from GMT–8 to GMT+10. Instead of forcing many around the world to stay awake at irregular times, we thus decided to restrict ourselves for this first conference to organizing sessions that would mainly accommodate most American and Europeans time zones, with multiple sessions accommodating for researchers working in Australia (GMT+10). Eventually, we settled on 6 sessions:

- 4 USA/Europe-friendly sessions starting at 4 pm UTC (9 am US West Coast, 6 pm Europe)
- 1 USA/Australia-friendly session starting at 10 pm UTC (3 pm US West Coast, *D*+1 8 am Australia)
- 1 Europe/Australia-friendly session starting at 10 am UTC (10 am Europe, 8 pm Australia)

This allowed us to host 24 talks, all solicited (it appeared easier for the inaugural meeting). Again, we had to define some rules and ended up deciding to have one talk per research group (albeit two for very large groups). We either contacted directly early career researchers whom we knew were working in the field of molecular spectroscopy — mainly (but not only) high resolution — or scientific supervisors to propose early career researchers from their groups. With the exception of a couple groups, we received enthusiastic responses and recommendations for speakers. Similarly, we also requested that session chairs be early career scientists.

To ensure that our meeting was attended by many early career researchers, we decided there would not be any registration fee to attend NISMS. We were able to offer this because our home institutions provided us with the tools to host such an event (Brown university zoom account, University of Paris-Saclay mailing list servers).

Once our scientific program was established, to spread the word, we first relied mostly on word-of-mouth — we invited people we know and thought would be interested in attending, and distributed emails to various spectroscopic communities. Eventually, we also used Twitter to attract a broader audience.

[Conferencing tools]

A large portion of conference organization stems around coordinating schedules, communication between organizers and speakers, registration, and updating materials with the newest developments. All of this, of course, builds on top of your regular duties, and so there is much to be said in improving the efficiency of conference organization. Thankfully in this day and age there are many free — and in many cases open-source — solutions to these problems that are highly streamlined and non-redundant. We used Google forms to set up conference registration, which subsequently populated a Google sheet with all of the user details. We used this registration spreadsheet to track who had registered, and for building the website, we exported it as a CSV allowing us to perform a large amount of automation with Python (our preferred language). Through Github pages, we had a free (albeit static) web hosting service, with full creative control over what was displayed and how. The website included an `index.html` for the majority of the content, a CSS stylesheet for formatting, and an auxiliary HTML table for the schedule. There are of course other choices out there: once again, the primary factor for us was keeping it cost-free (and also Kelvin likes to do this kind of thing) as the conference was self-funded.

We compiled abstracts into a book using \LaTeX , for which we created an abstract environment in the default book class (to minimize set-up time).

[Hosting a virtual meeting]

One of the major steps in organizing a virtual conference is choosing a platform to host the daily meetings. There are several different video conferencing apps to choose from, making it important to understand the differences to best suit your needs. We chose Zoom because of its general reliability and ease of use. A licensed version of Zoom can host up to 300 unique viewers at one time and can be password protected to prevent outside disruption. Zoom also has built-in functions like setting breakout rooms or making polls, which fosters smaller, more focused discussions among participants. Zoom also has several quality of life features that make running the meeting easier on the hosts. Zoom meetings can also be scheduled in advance and can have different IDs and passwords if needed. Each session can also be recorded (even though we did not use this feature for NISMS), which puts less pressure on participants to attend every meeting in real time, unlike an in-person meeting.

Virtual meetings tend to be prone to outside disturbances, which can ruin the experience for all involved. Thankfully, Zoom has a set of built-in tools that greatly reduce, if not eliminate any outside disturbances. At the start of every session, all participants were muted by the chair and only the chair was able to unmute them and allow them to share their screen. All other functions outside of the text chat were disabled for the duration of the talk (although Stephen forgot to enable the text chat on the first day). This means that even if someone new joined the meeting, they would automatically be muted and unable to do anything other than type in the text chat.

A nice benefit to hosting a virtual meeting is that after some initial setup, the conference runs itself. As the general flow of the meeting is standard and familiar to experienced conference attendees, there were little to no issues in moving between talks or Q&A sessions after each talk. This fairly straightforward nature also helped participants acclimate to the conference even though we were not altogether in the same place. For the Q&A sessions,

conference attendees could either raise their hand to ask their question directly when allowed by the chair, or write down their questions in the chat (which would then be read by the chair).

[Keeping things relaxed]

While keeping a high bar for the quality of talks is essential to the success of a meeting, a central aspect of a conference participation lies beyond just scientific talks; lunches, dinners, and evenings offer unique opportunities for scientists to connect beyond the strictly scientific sphere. Many scientific collaborations, project ideas, and friendships (as the three authors can attest) actually germinate during these “off-times” at a conference. In order to give a chance to NISMS conference attendees to interact in a relaxed environment, we decided that every scientific session would be followed by a non-scientific one, nominally unlimited in time.

To ensure that there would be a subject of light discussion on the first session (we were afraid people would not know how to initiate conversation) a non-scientific question was added to the registration form, “Are hot-dogs sandwiches?”, and Kelvin launched the first informal session by presenting why hot-dogs are indeed sandwiches and which percentage of the registered participant were correct. This rather stupid question allowed for a very funny discussion which we believe helped the participants feel at ease. During one of the other informal session, Valentina Del’Isolla (student from the university of Bologna) proposed a scientific trivia, which was received with much enthusiasm. Finally, we decided that we would conclude the last session by delivering “awards” as often seen in conferences. However, we did not want to deliver “performance-related” prizes as we believe all of the talks were of great quality, and we did not want to create discrimination between students. Instead, we settled with original awards meant to be non-serious but that would acknowledge significant contributions of people that helped ensure the meeting was a success:

- First Person to Register (Stephan Schlemmer, University of Cologne)
- Best Catch of a Mistake in the Program (Leah Dodson, University of Maryland)
- Most Dedicated Chair & Speaker (Oliver Harper, University of Paris Saclay & Nouredin Osseiran, University of Lille)
- Best Trivia Knowledge (Charles Markus, University of Cologne & Jacob Stewart, Connecticut College)
- Best Trivia Questions (Valentina Dell’Isola, University of Bologna)
- Most Tweets #NISMS2020 #NISMS (University of California, Davis)
- Early Career Scientist Asking Questions (Daofu Yuan, Brown University)
- Best Job at Scaring the Organizers (Michael McCarthy AKA the Arctic Wolf, Center for Astrophysics — Harvard & Smithsonian)

[Some stats and feedbacks on NISMS2020]

- 180 registered participants
 - from about 80 organizations
 - more than 120 early career scientists (bachelor to PhD students, Postdocs)
- about 80 people attending each session, with a peak above 100 attendees
- 24 speakers and 6 chairs, all early career scientists (PhD students, Postdocs)
- 6 sessions (about 1 h of science followed by unlimited discussion time)

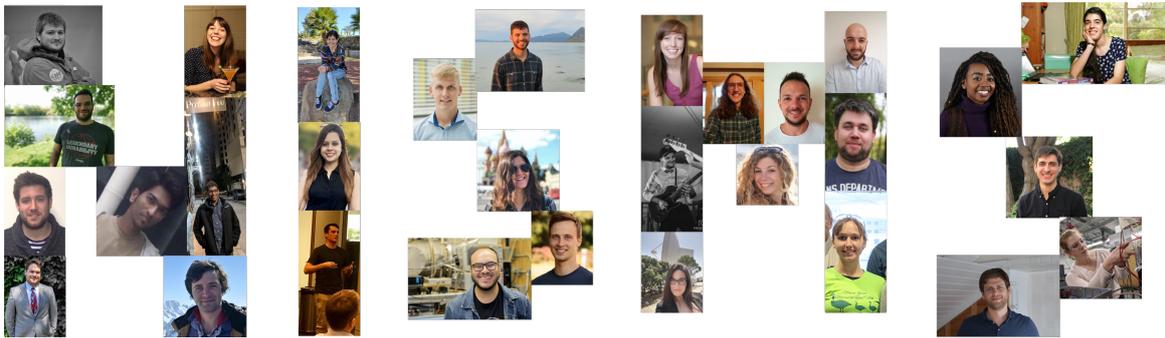


Figura 1: NISMS2020 speakers and chairs

The conference was generally very positively received. All the talks were of excellent quality and yielded enjoyable scientific discussions. At the end of the week, people voted with a vast majority for the NISMS experience to be conducted again in 2021 (and hopefully beyond). We were happy to see that not only young career scientists but also professors and established researchers enjoyed the event.

[There is always room for improvement]

From a technical point a view, the conference organization could be significantly improved, in part to release the organizers from some of the duties. For example, it is much more efficient to be able to implement “[continuous integration](#)” practices widely adopted in modern programming workflows: work is done remotely by multiple contributors and is processed by automated actions triggered by new updates. Organizing a conference using Github will provide you access to [Github actions](#), which allow you to implement these strategies. For instance, the [NISMS conference website](#) is hosted for free on Github pages, albeit statically; you can actually see [all the code here](#). By setting up a Github actions for when the schedule is modified and pushed, we can trigger scripts that update the static website page (as was done locally) and push it up to the web. As it was set up for NISMS 2020, we had to run a Python script to port changes to the schedule (from a CSV file) into the HTML table. The [SciPy conference](#) can be taken as the leading example for this (albeit with many tech savvy people contributing!), which was organized completely over Github, *including building a conference book of abstracts*. This means that any changes to parts of the conference can automatically trigger updates to dependencies, such as authors and scheduling, and if someone updates their conference proceedings paper, automatically rebuild the \LaTeX .

Another aspect that can be improved is certainly communication: this time, we had set up a listserv through the University of Paris–Saclay in the traditional form. This, however, leads to a deluge of emails for all parties involved and made it difficult to track who had submitted what, and so on. Tools like [Slack](#) offer a much more streamlined approach to asynchronous communication compared to email: you would be able to communicate with speakers and organizers directly—even in the event that their Zoom session crashed—in either channels or messaging groups, and because messages won't be lost after the Zoom meeting ends, you can continue to talk on a train of thought hours after a meeting.

The single greatest challenge facing any virtual meeting that is aiming to be international is dealing with time zones. Unlike an in-person conference where all participants are gathered together in one place, anyone can attend a virtual conference from the comfort of their own home. This becomes a significant issue when integrating an international audience as there is no perfect time where it is daytime for everyone in the world. Our approach to dealing with this was to organize specific sessions at times for specific parts of the globe, aiming to gather participants from different time zones for each session. Initially, we were defining session times using various reference location on earth (US West Coast, US East Coast, Central Europe, Sydney) but it resulted in much confusion. It did not help that we changed scheduling multiple times to accommodate the majority of participants... To make the time clear, we eventually chose to report times in Coordinated Universal Time (UTC). However, this too ended up leading to some confusion (mostly on our part) about what time sessions actually started. This led to some people showing up late or at the entirely wrong time.

[Looking to the future]

Immediately following the conclusion of NISMS, we were asked about plans for a second meeting. At the time, the thought of hosting another meeting was too daunting, and we promised to think about it after some time. Several early career scientists who attended the meeting have also reached out to be part of a future meeting, not just to present, but to be involved in the organization of the next meeting: if this sounds like you, please reach out to us as we plan for NISMS 2021; we will be looking for speakers, chairs, scientific organizers, as well as hosts for future sessions, so watch this space!

Acknowledgments

The authors would like to thank all the participants of NISMS for making the meeting a success. Additionally, the authors are thankful for The University of Paris—Saclay for help in setting up the mailing server and to Brown University for providing licensed accounts for conferencing tools used to run the meeting. GSK is thankful for support from a NASA Rhode Island Space Science Consortium Fellowship.



G. Stephen Kocheril received his B.S. in chemistry in 2016 from the University of Illinois at Urbana-Champaign under the supervision of Professor Ben McCall, studying H_3^+ and its deuterated isotopologues. He is currently a graduate student at Brown University under the supervision of Prof. Lai-Sheng Wang, where he studies gas-phase anionic clusters using high resolution photoelectron imaging. Stephen is a recipient of a NASA Rhode Island Space Grant Consortium graduate student fellowship to study the transition of clusters to dust grains in the ISM.

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Dr. Kin Long Kelvin Lee received his B.S. (H1) in 2013 from the University of Sydney and Ph.D. in Physical Chemistry in 2017 from the University of New South Wales; both of these were supervised by Professors Scott Kable (UNSW) and Meredith Jordan and combined velocity-map ion imaging and quasiclassical trajectory simulations to study the photodissociation dynamics of molecules relevant to our atmosphere. He was a postdoctoral fellow at the Center for Astrophysics — Harvard & Smithsonian under the guidance of Drs. Michael McCarthy and Carl Gottlieb, where he worked on a plethora of (astro)chemical projects combining high resolution microwave spectroscopy, quantum chemistry, and machine learning. He is now a senior postdoctoral researcher at the Massachusetts Institute of Technology, working under Professor Brett McGuire on topics in physical chemistry, astrochemistry, and deep learning. Dr. Lee also dedicates time towards a number of open-source projects focused on improving automation and reproducibility in scientific analysis, such as PySpecTools for automated spectroscopic analysis.

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Dr. Marie-Aline Martin-Drumel received her B.S. (2007) and M.S. (2009) in Chemistry from the University of Paris-Sud (France). She earned her PhD in Physics in 2012 under the supervision of Prof. Philippe Brechignac and Dr. Olivier Pirali. She then completed her post-doctoral research in the University of Littoral Cote d'Opale (France), University of Cologne (Germany), where she joined the Group of Prof. Stephan Schlemmer, and at the Harvard–Smithsonian Center for Astrophysics (USA) with Dr. Michael McCarthy. She was appointed in 2017 to a research position at the Centre National de la Recherche Scientifique (CNRS, France). Her research interest focuses on molecular spectroscopy of stable molecules and transient species, and its applications for astrophysics and chemistry.

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Abstracts

Impact of PAH photodissociation on the formation of small hydrocarbons in the Orion Bar and the Horsehead PDRs

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We study whether polycyclic aromatic hydrocarbons (PAHs) can be a weighty source of small hydrocarbons in photo-dissociation regions (PDRs). We modeled the evolution of 20 specific PAH molecules in terms of dehydrogenation and destruction of the carbon skeleton under the physical conditions of two well-studied PDRs, the Orion Bar and the Horsehead nebula which represent prototypical examples of PDRs irradiated by "high" and "low" ultraviolet radiation field. PAHs are described as microcanonical systems. The acetylene molecule is considered as the main carbonaceous fragment of the PAH dissociation as it follows from laboratory experiments and theory. We estimated the rates of acetylene production in gas phase chemical reactions and compared them with the rates of the acetylene production through the PAH dissociation. It is found that the latter rates can be higher than the former rates in the Orion Bar at $A_v < 1$ and also at $A_v > 3.5$. In the Horsehead nebula, the chemical reactions provide more acetylene than the PAH dissociation. The produced acetylene participate in the reactions of the formation of small hydrocarbons (C_2H , C_3H , C_3H^+ , C_3H_2 , C_4H). Acetylene production via the PAH destruction may increase the abundances of small hydrocarbons produced in gas phase chemical reactions in the Orion Bar only at $A_v > 3.5$. In the Horsehead nebula, the contribution of PAHs to the abundances of the small hydrocarbons is negligible. We conclude that the PAHs are not a major source of small hydrocarbons in both PDRs except some locations in the Orion Bar.

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PAH and dust particles surface interaction. Catalytic hydrogenation of PAH molecules under vacuum conditions

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This work reports experiments on the catalytic interaction occurring between Polycyclic Aromatic Hydrocarbon (PAH) molecules and TiO₂ dust grain surfaces under vacuum conditions. The investigation sheds light on the potential catalytic pathways TiO₂ dust surfaces provide in the hydrogenation of PAH molecules, and the chemistry that can be driven by PAH-dust interactions under vacuum conditions. Naphthalene, anthracene, and coronene were chosen as the PAH molecules, while titanium dioxide was selected as the dust analog. PAH samples and dust analog mixtures were studied under vacuum for 24 hours while monitored via Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS). The acquired spectra show that PAH molecules are hydrogenated when in contact with TiO₂ dust particles without the need for external energy or hydrogen sources. Our results suggest that linear PAHs undergo a similar hydrogenation process where the dominant species are fully hydrogenated PAHs. For condensed PAHs, the hydrogenation process yields partially hydrogenated molecules. Fully hydrogenated species can be identified by a band around 2960 cm⁻¹, while partially hydrogenated species produce a band around 2825 cm⁻¹. In the case of the production of hydrogenated species, our results suggest that smaller the PAH the faster the hydrogenation rate.

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Optical Spectrum of the Adamantane Radical Cation

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Known for their stable structural and thermal properties, diamondoids and particularly their radical cations are viable candidates as carriers for diffuse interstellar bands. While previous research has mainly focused on neutral diamondoids and their derivatives, little is known about their radical cations, which may form in interstellar environments by ionizing radiation. We report the first experimental optical spectrum of the simplest diamondoid cation, the adamantane radical cation (C₁₀H₁₆⁺), obtained via electronic photodissociation spectroscopy of cryogenic ions in the 310-1000 nm range. The main fragmentation channels are H loss at low energies and C₃H₇ loss at higher energies. The optical spectrum reveals a broad band spanning the range of 420-850 nm, assigned to the D₂(²E) ← D₀(²A₁)

transition using time-dependent density function theory calculations. Despite a vibrational temperature below 20 K, we observe no vibrational structure because of lifetime broadening and/or Franck-Condon congestion. A second band system originating at 345 nm that shows vibrational progressions is attributed to the overlapping $D_5(^2A_1)/D_6(^2E) \leftarrow D_0(^2A_1)$ transitions split by the Jahn-Teller effect. The lifetime deduced from the widths of these vibronic bands is ~ 30 fs. Comparison of the spectrum with known diffuse interstellar bands suggests that $C_{10}H_{16}^+$ is not likely to be a carrier. However, the strong absorption features in the UV to near IR show promise in the investigation of higher order diamondoids as potential candidates.

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Absorption Spectroscopy of Solid-Phase Fullerene C_{60} between 1.65 and 2.78 μm

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Fullerenes are the largest molecules identified so far in the interstellar medium. The spectroscopic properties of C_{60} and its charge variants, have been extensively studied in the mid-infrared, near ultraviolet and visible regions. On the other hand, the near infrared (NIR) spectral region has remained relatively unexplored, in particular for neutral C_{60} . Here we report the first measurements of the absorption spectra of solid C_{60} from 6052 to 3596 cm^{-1} (from 1.65 to 2.78 μm) recorded over the 11 to 300 K temperature range. NIR spectra of C_{60} microcrystals embedded in solid KBr were measured using a low-temperature helium cryo-cooling setup coupled to a Fourier transform infrared spectrometer. The observed spectra of C_{60} from 1.65 to 2.78 μm show highly structured absorption features. Compared to isolated molecules, the lower symmetry of C_{60} microcrystals optically activates many fundamental vibrational modes which combine (up to 4-quanta) and contribute to the rich observed spectrum. Quantum chemical calculations and group theoretical analysis were performed for a tentative assignment of the observed combination and overtone bands to the calculated transitions of both regions by identifying the IR active T_{1u} symmetries. 3895 combination and overtone transitions were calculated in the region between 1.65 and 2.78 μm amongst which 1862 transitions belong to the IR active T_{1u} symmetry, expected to be observed in the absorption spectrum of gas-phase C_{60} . This work offers some guidance for future low temperature gas-phase NIR absorption spectroscopic studies of C_{60} . Measurements of vibrational overtone bands of C_{60} are extremely timely for the identification of the carriers of NIR DIBs (Diffuse Interstellar Bands) in the context of the upcoming launch of the James Webb Space Telescope.

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Structural investigation of doubly-dehydrogenated pyrene cations

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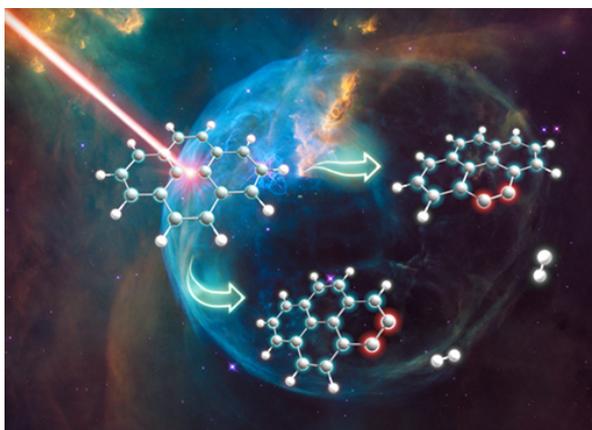
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The vibrationally resolved spectra of the pyrene cation and doubly-dehydrogenated pyrene cation ($C_{16}H_{10}^+$; Py^+ and $C_{16}H_8^+$; $ddPy^+$) are presented. Infrared predissociation spectroscopy is employed to measure the vibrational spectrum of both species using a cryogenically cooled 22-pole ion trap. The spectrum of Py^+ allows a detailed comparison with harmonic and anharmonic density functional theory (DFT) calculated normal mode frequencies. The spectrum of $ddPy^+$ is dominated by absorption features from two isomers ($4,5-ddPy^+$ and $1,2-ddPy^+$) with, at most, minor contributions from other isomers. These findings can be extended to explore the release of hydrogen from interstellar PAH species. Our results suggest that this process favours the loss of adjacent hydrogen atoms.



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Energetics of Formation of Cyclacenes from 2,3-Didehydroacenes and Implications for Astrochemistry: A TAO-DFT Study

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The carriers of the diffuse interstellar bands (DIBs) are still largely unknown although polycyclic aromatic hydrocarbons, carbon chains, and fullerenes are likely candidates. A recent analysis of the properties of *n*-acenes of general formula $C_{4n+2}H_{2n+4}$ suggested that these could be potential carriers of some DIBs. Dehydrogenation reactions of *n*-acenes after absorption of an interstellar UV photon may result in didehydroacenes. Here the reaction energies and barriers for formation of *n*-cyclacenes from 2,3-didehydroacenes (*n*-DDA) by intramolecular Diels-Alder reaction to dihydro-etheno-cyclacenes (*n*-DEC) followed by ejection of ethyne by retro-Diels-Alder reactions are analyzed using thermally assisted occupation density functional theory (TAO-DFT) for $n = 10 - 20$. It is found that the barriers for each of the steps depend on the ring strain of the underlying *n*-cyclacene, and that the ring strain of *n*-DEC is about 75 % of that of the corresponding *n*-cyclacene. In each case, ethyne extrusion is the step with the highest energy barrier, but these barriers are smaller than CH bond dissociation energies, suggesting that formation of cyclacenes is an energetically conceivable fate of *n*-acenes after multiple absorption of UV photons.

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