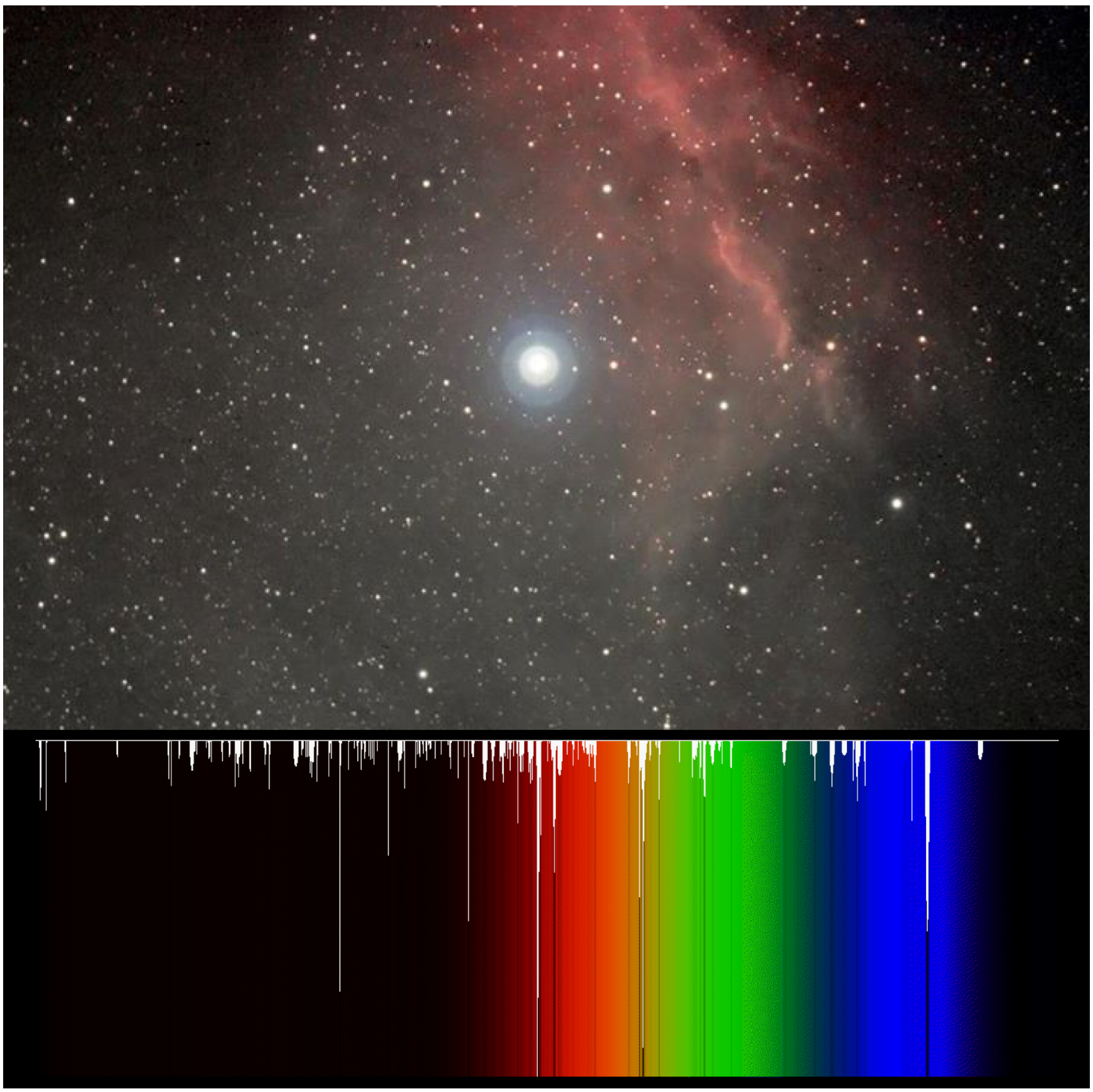
Issue 6 | April 2014

AstroPAH

A Newsletter on Astronomical PAHs



Editorial

Dear Colleagues,

Welcome to the 6th release of AstroPAH with the *Picture of the Month* featuring the Diffuse Interstellar Bands (DIBs; see the caption in p. 3), which is the topic of our *In Focus* this month. *In Focus* presents the highlights of the recently held conference on the Diffuse Interstellar Bands (IAU Symposium 297), a conference dedicated entirely to these enigmatic features. We thank Jan Cami and Nick Cox for providing us with this very interesting read.

This month's abstracts section features papers on PAHs in a range of astronomical objects and on new results from laboratory and calculation. We would also like to draw your attention to the *Job Opportunities* section, which may be of interest to you.

We would like to thank you all for your contributions and please keep them coming. You can send your contributions to AstroPAH any time – abstracts, *In Focus* suggestions, awards, future events, or other information you would like to share with the community.

The deadline for contributions to appear in the next issue is 9 May 2014. The next issue of AstroPAH will be out on 20 May 2014.

For more information on AstroPAH, visit our website:

http://astropah-news.strw.leidenuniv.nl.

Best regards

The Editorial Team

AstroPAH Newsletter

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PAH Picture of the Month

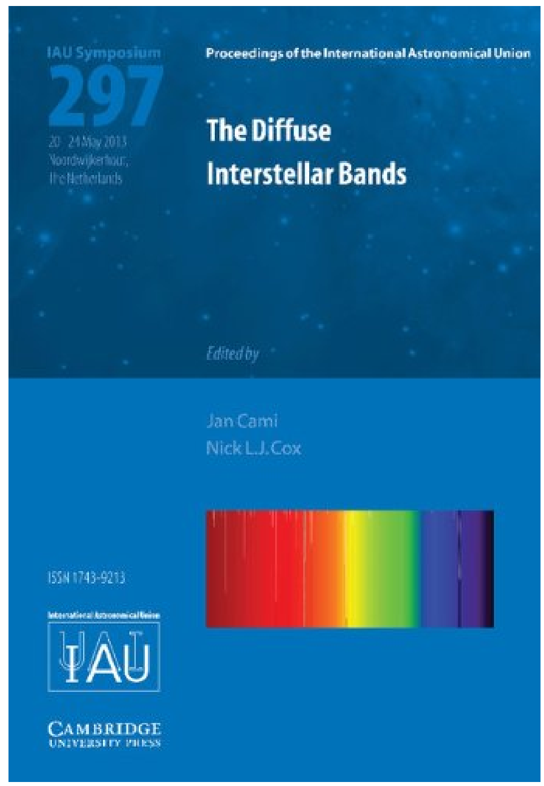
Top: σ Scorpii, also known as Al Niyat, is a bright star surrounded by diffuse nebulosity in the Scorpion constellation. It represents, together with ζ Perseii, one of the two prototypical line of sights from where Diffuse Interstellar Bands (DIBs) are detected. Credits: Claudio Vallerani 2012

Bottom: Visualisation of the Jenniskens-Desert Catalog of Diffuse Interstellar Bands (http://leonid.arc.nasa.gov/DIBcatalog.html). See *In Focus* section for more on DIBs. Credits: P. Jenniskens & F.-X. Desert

In Focus:

Nick Cox and Jan Cami Present Impressions and Proceedings of the IAU Symposium 297 "The Diffuse Interstellar Bands"

"Almost one year ago, from 20-24 May 2013, more than a hundred observational astronomers, laboratory astrophysicists, chemists and various theorists met in Noordwijkerhout, the Netherlands, to participate in **IAU Symposium 297 "The Diffuse Interstellar Bands"**. This international conference was the long awaited follow-up to the very successful **first DIB meeting in 1994 in Boulder**. Once again, the mysterious diffuse interstellar bands (DIBs) took center stage at this symposium. The meeting ran very smoothly thanks to the tireless efforts of the LOC chair, Harold Linnartz (Leiden).



The DIB problem is old (dating back to 1922) and is easily described: the DIBs are a set of hundreds of absorption bands that commonly appear in the spectra of reddened objects at optical to near-infrared wavelengths. Their interstellar origin is well established, but the identity of the DIB carriers – the material causing these absorption bands – remains a mystery to date. Observational studies suggest that the carriers are most likely stable carbonaceous molecules that reside ubiquitously in the interstellar medium. Such characteristics are reminiscent of PAHs, whose mid-IR emission bands provide an abundant glow in the Universe near and far, and thus **PAHs have been considered as very promising DIB carrier candidates for many years now**. This possible connection between PAHs and DIBs was one of the common threads in the talks, posters and discussions held during IAUS 297, and many contributions were therefore relevant to PAH researchers. **Many readers of the AstroPAH newsletter may thus be interested in the conference proceedings that were published the first week of April by Cambridge University Press.**

The IAUS 297 proceedings provide a lasting record collecting the current state of affairs in the field of DIB-related research. More than 70 contributions (organized in six topical themes described below) cover a broad range in topics in observational astronomy and astrophysics; laboratory astrophysics and spectroscopy; astrochemistry; and theoretical, experimental and computational chemistry. This interdisciplinary overview contains all the required background material (in a series of review papers) to make the volume an ideal starting point for researchers and graduate students to learn about the various aspects of DIBs and related topics. In addition, there are many more focused contributed papers highlighting modern approaches to DIB research.

At the end of each topical theme session, participants were invited to join in a discussion to explore the limits of current DIB research and brainstorm about new avenues forward. Invariably, these discussion sessions led to lively yet very constructive and fruitful debates involving senior and junior researchers alike. We found these discussion sessions very stimulating, and recognized a growing interest, enthusiasm and participation from relative ”outsiders” in the field, including from early and mid-career scientists. A synthesis of these discussions was the basis to create a road map toward the identification of the DIB carriers that is included at the end of the volume.

DIB research has a long and rich history and tradition, with contributions by many different eminent researchers. **We dedicate these proceedings to the memory of George H. Herbig, who passed away on October 12, 2013.** He was a monument in astronomy, and one of the pioneers of modern DIB research.

We also found it fitting to have the organizers of the 1994 Boulder meeting open and close our 2013 meeting. And thus, Ted Snow provided a historic overview of DIB research and ideas (p. 3), while Xander Tielens closed the meeting with an engaging outlook (p. 399).

Below are some highlights for the six topical themes:

Properties of the Diffuse Interstellar Bands

This part provides most of the background on the observational properties of DIBs including overall survey results and environmental behaviour (p. 13, 51); families and correlations (p. 23); DIB band profiles (p. 34); extra-galactic DIBs (p. 41). Some recurring themes in the other contributions are explorations beyond the Galaxy (p. 74, 79, 106); analysis of large survey data sets (p. 58, 68, 84, 110, 113, 117); detections of new DIBs in the near-infrared (p. 64, 100, 103); relations between DIBs and other quantities (p. 121, 125, 128, 132, 135, 138) and detailed analyses of peculiar lines-of-sight (p. 89, 94, 141). In the latter category, the star of the meeting was undoubtedly Herschel 36, whose line of sight exhibits DIBs with very anomalous profiles. Analysis of these profiles shows a differentiation between polar and non-polar DIB carriers for different bands. This new invigorating discovery illustrates that striking new results are still found after a century of observations!

The relation of DIBs to other interstellar components and astronomical phenomena

DIBs are not an isolated astrophysical problem, and in fact many other phenomena share some of the DIB characteristics or show a clear relation to the DIB properties: the most commonly discussed in this context are extinction due to interstellar dust; gas-phase components in the interstellar medium; molecular interstellar species as seen at longer wavelengths; Blue Luminescence and Extended Red Emission (the latter sharing a similar distribution as the DIBs); the Red Rectangle Bands and the Infrared Emission Bands, commonly attributed to PAHs (p. 147, 153, 163, 173, 180, 187,197). Furthermore, the recent detection of the fullerene species C60 and C70 has sparked a renewed interest in exploring their potential as DIB carriers (p. 203, 208, 223, 339, 370). Relations with other proposed or unidentified species have been considered as well (p. 213, 219), while other researchers have looked for DIBs in peculiar objects or lines of sight (p. 216, 226).

Laboratory Astrophysics studies of DIB carrier (related) candidates

The proceedings give a comprehensive overview on the state-of-affairs of laboratory spectroscopy of potential DIB carriers. Species considered in the lab include carbon chains and rings (p. 237, 258); PAHs, PAH cations and polyynyl-substituted PAHs (p. 247, 265, 276, 286, 294). Several new experimental techniques were introduced by representatives of the astrophysical laboratories of Boulder (p. 258), Leiden (p. 281, 297), Toulouse (p. 286), Tokyo (p. 291), and Catania (p. 294).

Astrochemistry: theoretical modeling approaches

A good theoretical understanding of the interplay between the physical conditions and the chemistry occurring in diffuse clouds is crucial to assess the viability of certain [classes of] DIB carriers for various environments and to understand the response of the DIB carriers to their environments. Modeling of diffuse clouds has advanced rapidly but many difficult challenges remain (p. 303, 311, 321). Theoretical work in this context also includes studies on the formation and stability of possible DIB carrier candidates (p. 339, 353). Finally, theoretical and computational chemistry methods can be used to obtain accurate spectroscopic properties of specific DIB carriers (e.g. anions) as well (p. 330, 344, 349).

The DIB carrier candidates

This part addresses several specific classes of molecules or structures and evaluates their potential as DIB carriers. This includes a critical review of two of the most often named DIB carrier candidate: PAHs (p. 364) and fullerene analogues (p. 370), and a contribution that explores spectroscopy of DIB carriers in ices (p. 359). Furthermore, this part also describes less accepted and somewhat more exotic alternative suggestions (p. 375, 378, 381, 384).

Future directions in DIB research

We conclude the conference proceedings with an outlook on what future observatories and instruments may add to the DIB field (p. 389), and with a strong appeal to the community to work together more intensely and share data through joint networking and research efforts (p.

399). Finally, a road map for the identification of the DIB carriers presents a synthesis of the discussions that were held throughout the symposium (p. 412); our wish is that this editorial contribution will help organize research efforts.

We hope that you will enjoy reading these conference proceedings!

The Editors,

Jan Cami & Nick Cox

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Nick Cox *is a postdoctoral research scientist at KU Leuven (Belgium)*

Proceedings of the IAU Symposium 297 The Diffuse Interstellar Bands

Cambridge University Press
ADS - The SAO/NASA Astrophysics Data System

Recent Papers

Observational Studies on the Near-Infrared Unidentified Emission Bands in Galactic HII regions

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Using a large collection of near-infrared spectra (2.5-5.4 μm) of Galactic HII regions and HII region-like objects, we perform a systematic investigation of the astronomical polycyclic aromatic hydrocarbon (PAH) features. 36 objects were observed by the use of the infrared camera onboard the AKARI satellite as a part of a director's time program. In addition to the well-known 3.3-3.6 μm features, most spectra show a relatively-weak emission feature at 5.22 μm with sufficient signal-to-noise ratios, which we identify as the PAH 5.25 um band previously reported. By careful analysis, we find good correlations between the 5.25 μm band and both the aromatic hydrocarbon feature at 3.3 μm and the aliphatic ones at around 3.4-3.6 um. The present results give us convincing evidence that the astronomical 5.25 μm band is associated with C-H vibrations as suggested by previous studies and show its potential to probe the PAH size distribution. The analysis also shows that the aliphatic to aromatic ratio of $I_{3.4-3.6\,\mu\mathrm{m}}/I_{3.3\,\mu\mathrm{m}}$ decreases against the ratio of the 3.7 μm continuum intensity to the 3.3 μm band, $I_{3.7\,\mathrm{cont}}/I_{3.3\,\mu\mathrm{m}}$, which is an indicator of the ionization fraction of PAHs. The mid-infrared color of $I_{9\,\mu\mathrm{m}}/I_{18\,\mu\mathrm{m}}$ also declines steeply against the ratio of the hydrogen recombination line Brα at 4.05 μm to the 3.3 μm band, $I_{\mathrm{Br}\alpha}/I_{3.3\,\mu\mathrm{m}}$. These facts indicate possible dust processing inside or at the boundary of ionized gas.

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ApJ, 784, 53 (2014)

http://iopscience.iop.org/0004-637X/784/1/53/
http://arxiv.org/abs/1401.7879

Data Catalogue

AKARI Near-infrared Spectral Atlas of Galactic HII Regions Public Release (in English)
AKARI Near-infrared Spectral Atlas of Galactic HII Regions Public Release (in Japanese)

PAH formation in O-rich Planetary Nebulae

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Polycyclic aromatic hydrocarbons (PAHs) have been observed in O-rich planetary nebulae towards the Galactic Bulge. This combination of oxygen-rich and carbon-rich material, known as dual-dust or mixed chemistry, is not expected to be seen around such objects. We recently proposed that PAHs could be formed from the photodissociation of CO in dense tori. In this work, using *VISIR/VLT*, we spatially resolved the emission of the PAH bands and ionised emission from the [SIV] line, confirming the presence of dense central tori in all the observed O-rich objects. Furthermore, we show that for most of the objects, PAHs are located at the outer edge of these dense/compact tori, while the ionised material is mostly present in the inner parts of these tori, consistent with our hypothesis for the formation of PAHs in these systems. The presence of a dense torus has been strongly associated with the action of a central binary star and, as such, the rich chemistry seen in these regions may also be related to the formation of exoplanets in post-common-envelope binary systems.

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Accepted by MNRAS

http://arxiv.org/abs/1403.1856

C/O abundance ratios, iron depletions, and infrared features in Galactic planetary nebulae

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We study the dust present in 56 Galactic planetary nebulae (PNe) through their iron depletion factors, their C/O abundance ratios (in 51 objects), and the dust features that appear in their infrared spectra (for 33 objects). Our sample objects have deep optical spectra of good quality, and most of them also have ultraviolet observations. We use these observations to derive the iron abundances and the C/O abundance ratios in a homogeneous way for all the objects. We compile detections of infrared dust features from the literature and we analyze the available

Spitzer/IRS spectra. Most of the PNe have C/O ratios below one and show crystalline silicates in their infrared spectra. The PNe with silicates have C/O < 1, with the exception of Cn 1-5. Most of the PNe with dust features related to C-rich environments (SiC or the 30 μm feature usually associated to MgS) have C/O $\gtrsim$ 0.8. Polycyclic aromatic hydrocarbons are detected over the full range of C/O values, including 6 objects that also show silicates. Iron abundances are low in all the objects, implying that more than 90% of their iron atoms are deposited into dust grains. The range of iron depletions in the sample covers about two orders of magnitude, and we nd that the highest depletion factors are found in C-rich objects with SiC or the 30 μm feature in their infrared spectra, whereas some of the O-rich objects with silicates show the lowest depletion factors.

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ApJ, 784, 173 (2014)

http://arxiv.org/abs/1402.6376
http://iopscience.iop.org/0004-637X/784/2/173/

Laboratory Determination of the Infrared Band Strengths of Pyrene Frozen in Water Ice: Implications for the Composition of Interstellar Ices

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Broad infrared emission features (e.g., at 3.3, 6.2, 7.7, 8.6, and 11.3 μm) from the gas phase interstellar medium have long been attributed to polycyclic aromatic hydrocarbons (PAHs). A significant portion (10%−20%) of the Milky Way's carbon reservoir is locked in PAH molecules, which makes their characterization integral to our understanding of astrochemistry. In molecular clouds and the dense envelopes and disks of young stellar objects (YSOs), PAHs are expected to be frozen in the icy mantles of dust grains where they should reveal themselves through infrared absorption. To facilitate the search for frozen interstellar PAHs, laboratory experiments were conducted to determine the positions and strengths of the bands of pyrene mixed with H_2O and D_2O ices. The D_2O mixtures are used to measure pyrene bands that are masked by

the strong bands of H_2O, leading to the first laboratory determination of the band strength for the CH stretching mode of pyrene in water ice near 3.25 μm. Our infrared band strengths were normalized to experimentally determined ultraviolet band strengths, and we find that they are generally ∼50% larger than those reported by Bouwman et al. based on theoretical strengths. These improved band strengths were used to reexamine YSO spectra published by Boogert et al. to estimate the contribution of frozen PAHs to absorption in the 5−8 μm spectral region, taking into account the strength of the 3.25 μm CH stretching mode. It is found that frozen neutral PAHs contain 5%−9% of the cosmic carbon budget, and account for 2%−9% of the unidentified absorption in the 5−8 μm region.

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ApJ, 784, 172 (2014)

http://iopscience.iop.org/0004-637X/784/2/172/article

The Far-Infrared Spectrum of Azulene and Isoquinoline and Supporting Anharmonic Density Functional Theory Calculations to High Resolution Spectroscopy of Polycyclic Aromatic Hydrocarbons and Derivatives

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In the laboratory, the acquisition and analysis of the rotationally resolved spectra of large molecular systems remain challenging. We report in this paper the rotational analysis of the ν_{30} -GS band of azulene and the ν_{41} -GS band of isoquinoline recorded with synchrotron-based Fourier transform absorption spectroscopy in the far-IR. As a support to rotational analyses, we employed a method based on standard density functional theory calculations performed at the anharmonic level which accurately reproduced the rotational constants of 28 vibrational states of 16 Polycyclic Aromatic Hydrocarbons (PAHs) and aza-derivatives. This method appears as an invaluable support for the spectral assignment of the very congested rotational structures of the infrared bands of PAH species and should be very helpful in the active search of these molecules in space through their pure rotational or rovibrational spectra.

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J. Chem. Phys., 140, 044322 (2014)

http://dx.doi.org/10.1063/1.4862828

Spitzer Observations of Dust Emission from H II Regions in the Large Magellanic Cloud

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Massive stars can alter physical conditions and properties of their ambient interstellar dust grains via radiative heating and shocks. The H II regions in the Large Magellanic Cloud (LMC) offer ideal sites to study the stellar energy feedback effects on dust because stars can be resolved, and the galaxy's nearly face-on orientation allows us to unambiguously associate H II regions with their ionizing massive stars. The Spitzer Space Telescope survey of the LMC provides multi-wavelength (3.6-160 μm) photometric data of all H II regions. To investigate the evolution of dust properties around massive stars, we have analyzed spatially resolved IR dust emission from two classical H II regions (N63 and N180) and two simple superbubbles (N70 and N144) in the LMC. We produce photometric spectral energy distributions (SEDs) of numerous small subregions for each region based on its stellar distributions and nebular morphologies. We use DustEM dust emission model fits to characterize the dust properties. Color-color diagrams and model fits are compared with the radiation field (estimated from photometric and spectroscopic surveys). Strong radial variations of SEDs can be seen throughout the regions, reflecting the available radiative heating. Emission from very small grains drastically increases at locations where the radiation field is the highest, while polycyclic aromatic hydrocarbons (PAHs) appear to be destroyed. PAH emission is the strongest in the presence of molecular clouds, provided that the radiation field is low.

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http://iopscience.iop.org/0004-637X/784/2/147/

Nucleation and stabilization of carbon-rich structures in interstellar media

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We study conditions under which carbon clusters of different sizes form and stabilize. We describe an approach to equilibrium by simulating tenuous carbon gas dynamics to long times. First, we use reactive molecular dynamics simulations to describe the nucleation of long chains, large clusters, and complex cage structures in carbon and hydrogen rich interstellar gas phases.

We study how temperature, particle density, presence of hydrogen, and carbon inflow affect the nucleation of molecular moieties with different characteristics, in accordance with astrophysical conditions. We extend the simulations to densities which are orders of magnitude lower than current laboratory densities, to temperatures relevant to circumstellar environments of planetary nebulae, and to longtime (microsecond) formation timescales. We correlate cluster size distributions from dynamical simulations with thermodynamic equilibrium intuitions, where at low temperatures and gas densities, entropy plays a significant role.

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http://arxiv.org/abs/1402.0534

Anthracene Clusters and the Interstellar Infrared Emission Features

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The unidentified infrared bands are ubiquitous in the interstellar medium and typically attributed to emission from neutral and ionized polycyclic aromatic hydrocarbons (or PAHs). The contribution of neutral PAH clusters to these bands has been impossible to determine due to a paucity of infrared spectral data. Here we investigated neutral clusters of the three-ring PAH anthracene using FTIR absorption spectroscopy of anthracene matrix-isolated at varying concentrations in solid argon. In order to determine likely cluster structures of the embedded molecules, we also calculated theoretical absorption spectra for the anthracene monomer through hexamer using density functional theory with a dispersion correction (DFT-D). The DFT-D calculations have been calibrated for the anthracene dimer using the second-order Møller-Plesset approach. Because there is some support for the hypothesis that three or four-ring PAHs are present in the Red Rectangle nebula, we discuss the application of our results to this nebula in particular as well as to the interstellar infrared emission in general.

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ApJ, 783, 97 (2014)

http://iopscience.iop.org/0004-637X/783/2/97/article

The infrared spectra of $C_{96}H_{25}$ compared with that of $C_{96}H_{24}$

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The addition of one H atom to $C_{96}H_{24}$ has been studied for the neutral, cation, and anion. Hydrogen atom binding at the solo site is the most favorable for all three charge states. The solo and duo sites are significantly more strongly bound than the endo positions. One extra hydrogen atom has very little effect on the infrared spectra. It is unlikely that species with one extra hydrogen could be identified from the astronomical emission spectra.

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Theor. Chem. Acc., 133, 1454 (2014)

http://link.springer.com/article/10.1007%2Fs00214-014-1454-0

Job Oportunities

Post Doctoral Research Position in Experimental Physical Chemistry and Chemical Physics

One postdoctoral position in experimental physical chemistry and chemical physics (reaction dynamics, astrobiology, astrochemistry) is open at the Department of Chemistry, University of Hawai'i at Manoa, for the period of initially one year to investigate the evolution of organics under a simulated Martian environment. The salary is competitive and commensurate with experience ranging from $39,000 to $45,000. Successful applicants should have a strong back-ground in experimental reaction dynamics, surface scattering, UHV technology, and VUV laser systems, optical spectroscopy (FTIR, Raman, UVVIS), and gas phase detection techniques (time-of-flight and quadrupole mass analyzer). Programming experience in C, labview, and/or autocad and knowledge in the generation of tunable UVVUV radiation is desirable. The prime directive of this research project is to investigate the chemical fate of molecules in the extreme environments representative of the surface of Mars. Solid communication skills in English (written and oral) and a strong publication record in internationally circulated, peer-reviewed journals are mandatory. Only self-motivated and energetic candidates are encouraged to apply; please send a letter of interest, three letters of recommendation, CV, which includes a publication list to Brant Jones (brantmj@hawaii.edu), Department of Chemistry & W.M. Keck Research laboratory in Astrochemistry, University of Hawaii at Manoa, Honolulu, HI 96822-2275, USA. Only complete, electronic applications in pdf format will be considered. The review of applications will start June 1, 2014, with an expected start state of September 2014.

Advertised by: Brant Jones
Deadline for Application: May 1, 2014
Webpages: http://www.chem.hawaii.edu/Bil301/welcome.html
http://www.chem.hawaii.edu/Bil301/KLA.html
Email for contact: brantmj@hawaii.edu

AstroPAH Newsletter

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astropah@strw.leidenuniv.nl

Next issue: 20 May 2014
Submission deadline: 9 May 2014