AstroPAH

A Newsletter on Astronomical PAHs

Issue 100! • July 2023

Celebrating the 100th Edition of AstroPAH!

Editorial

Dear Colleagues,

AstroPAH has reached its 100th edition!

We are very grateful to all who have contributed to this milestone – past and current editors, and of course the PAH community! Your hundreds of contributions and In Focus topics have been at the core of AstroPAH's operations. If we are still here today, it is because of your amazing science and your support to our initiative. So, we want to take this moment to thank you all for your contributions to AstroPAH!

In this special issue, we have two In Focus! Our first In Focus, entitled *"AstroPAH at 100"* and written by Alexander Tielens, our Editor-in-Chief, stresses the importance of our community and how much we can contribute to science. Our second In Focus, is centered around SOFIA and its legacy to the fields of astrophysical and planetary sciences. "Looking Back at SOFIA" was written by Maggie McAdam and Naseem Rangwala, from NASA Ames Research Center.

In our abstract section, you can read about newly published papers on emission spectra of fullerenes, cyanonaphthalene, and charged PAHs.

We also wish to draw your attention to the meeting "Laboratory Astrophysics Workshop ICE 2024", which will be held in Hawaii in February of next year. Registration deadline is November 1, 2023.

If you are on Instagram, be sure to check out our next PAH of the Month!

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 or other ideas, feel free to use our email.

AstroPAH will take its traditional break in August, but will be back in September!

The Editorial Team

Next issue: 21 September 2023.
Submission deadline: 8 September 2023.

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PAH Picture of the Month

With our AstroPAH cover, this month we are celebrating our 100th edition of AstroPAH.

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This newsletter is edited in LaTeX. Newsletter Design by: Isabel Aleman. Image Credits: Background image in this page: NASA, ESA, and the Hubble Heritage Team (STScI/AURA). Headers background: X-ray and optical image composition. X-ray by Chandra: NASA/CXC/Univ.Potsdam/L.Oskinova et al; Optical by Hubble: NASA/STScI; Infrared by Spitzer: NASA/JPL-Caltech.

In Focus

AstroPAH at 100

Alexander Tielens

This is the 100th issue of AstroPAH, the newsletter for studies of Polycyclic Aromatic Hydrocarbon (PAH) molecules in space. AstroPAH has brought you close to ten years of abstracts of relevant articles, announcements of interesting conferences and summer schools, and a host of job opportunities, while the in-focus articles have introduced you to experimental techniques, observational opportunities, and quantum chemical insights that, together, present a general overview of the field and that can serve as the starting point for more in depth exploration of new developments. Looking back over these ten years, by all means, AstroPAH has mapped out this important corner of the molecular Universe.

Well over 100 years ago, the first diatomic molecules were discovered, and this brought Sir Arthur Eddington, the preeminent astrophysicist of his time, to lament that “atoms are physics, but molecules are chemistry”. Ever since, astrophysicists rued the moment that simple physical formulas had to give way to complex chemical solutions in a molecular universe. Over the last two decades, the opening up of the infrared and submillimeter spectral windows – driven by rapid increase in detector technologies and ever-increasing telescope sizes – has provided us with a view of the richness of the molecular Universe. I am convinced that if Sir Arthur Eddington had been alive at this day, he would have well recognized the advantages of studying molecules in the Universe. We are truly living in a Molecular Universe where molecules are abundant and widespread and play an important role in the evolution of galaxies. Moreover, regions of planet formation contain a rich organic inventory that may well have provided a prebiotic jump-start to life on Earth and perhaps other planets in the solar system and beyond. Finally, molecules provide an excellent tool to measure the physical conditions and probe the dynamics of many astronomically interesting objects and phenomena. Hence, molecular astrophysics has come into its own right as a key subdiscipline within astronomy.

Interstellar PAHs take a special place in the pantheon of the molecular Universe. Molecules containing 50 to 100 atoms were inconceivable in Eddington’s time and their presence reveals a richness and complexity undreamt of even 40 years ago when I first entered this field. Nowadays, interstellar PAHs are recognized as an important component of the interstellar medium. Interstellar PAHs dominate the emission characteristics of regions in size from the kiloparsec scale of entire star forming galaxies, to the parsec scale of individual regions of massive star formation, and down to the 100 AU scale of planet-forming disks. At all these scales, PAHs provide a probe of their morphology and the interaction of nearby stars with the surrounding circumstellar and interstellar gas. PAHs also control key processes in the ISM. Specifically, they dominate the energy balance of gas in diffuse interstellar clouds, hence, are at the basis of the phase structure of the ISM. By the same token, PAHs direct the radiative feedback of massive stars in the photodissociation regions, that separate ionized from molecular gas in their immediate environments. Likewise, PAHs regulate the ionization balance in molecular clouds and, therefore, the magnetic support of molecular clouds against gravitational collapse. Moreover, the ultraviolet (UV) driven fragmentation of PAHs may be an important source of small hydrocarbon species in diffuse clouds and in photodissociation regions. By the same token, PAH fragmentation may be at the basis of the presence of large carbon clusters and fullerenes in space. PAHs may also play a catalytic role in the formation of the most abundant molecule in space, H_2. Very excitedly, observations have revealed that, inside the shielded environment of dense cores, ion-molecule and radical- neutral chemistry can build up small PAHs. Finally, as the PAH spectral characteristics reflects the local physical conditions, astronomers have recognized PAHs as convenient tools to study the Universe in UV-rich environments. Specifically, astronomical interest centers on the use of PAHs to measure the (obscured) star formation rate and as a way to separate star formation activity from black hole activity throughout the history of the Universe.

Determining the properties of PAHs in space and understanding their role in the Universe requires a close collaboration between observers, modelers, theoreticians, and experimentalists. The study of interstellar PAHs is a highly interdisciplinary field, where astronomy and astrophysics intersect with molecular physics, molecular spectroscopy, physical chemistry, reaction dynamics, quantum physics, geophysics, geochemistry, planetary science, surface science, and solid-state physics. There is no scientist who can overview all these fields and can keep track of all new developments. This is where AstroPAH plays a central role. AstroPAH aims to provide a forum where the latest developments in the field are presented to a wide-ranging audience in a language that can be understood by all. From my perspective, Isabel Aleman, the managing editor, and her group of dedicated editors, David Dubois, Alessandra Candian, Helgi Rafn Hrodmarsson, Rijutha Jaganathan, Kin Long Kelvin Lee, Donatella Loru, Elisabetta Micelotta, Julianna Palotás, Anemieke Petrignani, Ella Sciamma-O'Brien, Ameek Sidhu, Amanda Steber, and Sandra Wiersma, have succeeded exceedingly well in this endeavor and we all owe a deep debt of gratitude to them for their tireless efforts to link us all into a “universal PAH family”.

Celebrating 100 editions of AstroPAH

The AstroPAH editors thank you for your contributions!

Looking back at SOFIA

Maggie McAdam and Naseem Rangwala

Introduction

The Stratospheric Observatory for Infrared Astronomy (SOFIA, Figure 1) was NASA's far-infrared observatory from the mission's first light in 2010 until its conclusion in 2022. SOFIA was a joint mission between NASA and the German Space Agency at DLR. The observatory conducted a broad range of astrophysical and planetary science investigations using unique, state-of-the-art, mid- and far-infrared capabilities to address NASA's key astrophysics objectives.


Credit: NASA/ SOFIA/Monika Rose

Figure 1 *– The Stratospheric Observatory for Infrared Astronomy (SOFIA).*

Much of the radiant energy from planets, star-forming clouds, and galaxies emerges in the mid-infrared (mid-IR; 5-40 μm) and far-infrared (far-IR; 40-650 μm), but water vapor in the Earth's atmosphere blocks mid-IR and far-IR at even the best terrestrial sites. By flying above 99.9% of the atmosphere's IR-absorbing water, SOFIA observed the infrared spectrum from about 1 to 1000 μm and tapped into the wealth of astrophysical information accessible only at these wavelengths. SOFIA's instrument suite exploited the full mid-IR/far-IR wavelength range with continuum imaging, high-resolution spectroscopy, and polarization mapping.

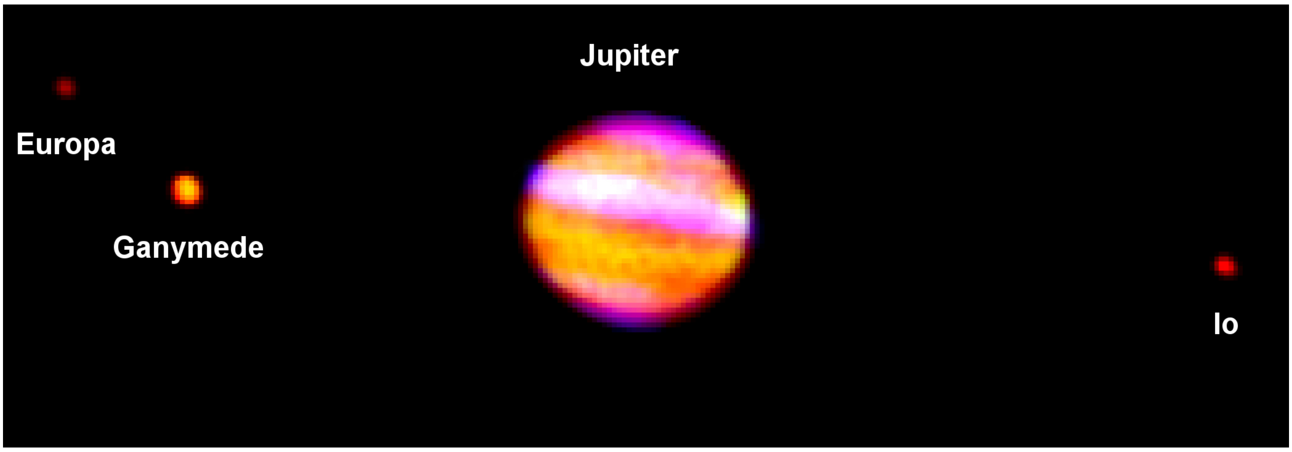

Figure 2 *– SOFIA's first-light image of Jupiter. Original image caption: SOFIA image of Jupiter and three of the Galilean moons composed of multiple frames taken at wavelengths of 5.4, 24 and 37 μm with the FORCAST infrared camera (P.I. Terry Herter, Cornell University). These data and other measurements from SOFIA's "first light" flight show that the observatory aircraft and telescope were remarkably stable on their first night out. (Image is oriented with Jupiter's north pole at the top.) Image credit: (NASA/SOFIA/USRA/FORCAST Team/James De Buizer).*

SOFIA's capability for polarization mapping in the far-infrared revolutionized the way scientists think about the role of magnetic fields. Such novel measurements tested theories in a variety of cosmic ecosystems, from the formation of stars and planets to the evolution of galaxies and clusters. SOFIA's unparalleled spectroscopic observations made unambiguous detections of distinct molecular fingerprints and investigated complex physics across a wide array of astrophysical environments.

From SOFIA's first-light images of Jupiter (Figure 2) to adapting instruments with new modes, SOFIA impacted many areas of astrophysics.

Cosmic magnetic fields in galaxies

Magnetic fields are notoriously difficult to detect. SOFIA's specialized instrumentation detected the polarization of dust particles. These tiny particles spinning in space align themselves with the magnetic fields around them. When they do this, the nature of the light interacting with them is also changed. The HAWC+ instrument on SOFIA was specially designed to observe magnetic fields to learn how they affect star formation, accretion onto black holes, and galactic mergers.

Through the SALSA legacy program, the team of scientists have shown that magnetic fields detected by HAWC+ are much more chaotic than previously understood (Figure 3). These fields can suppress or enhance star formation and accretion onto black holes in ways that were previously unknown.

SOFIA also studied the effects of magnetic fields in other astrophysical regions, especially galactic filaments, star forming regions, and our galactic center.

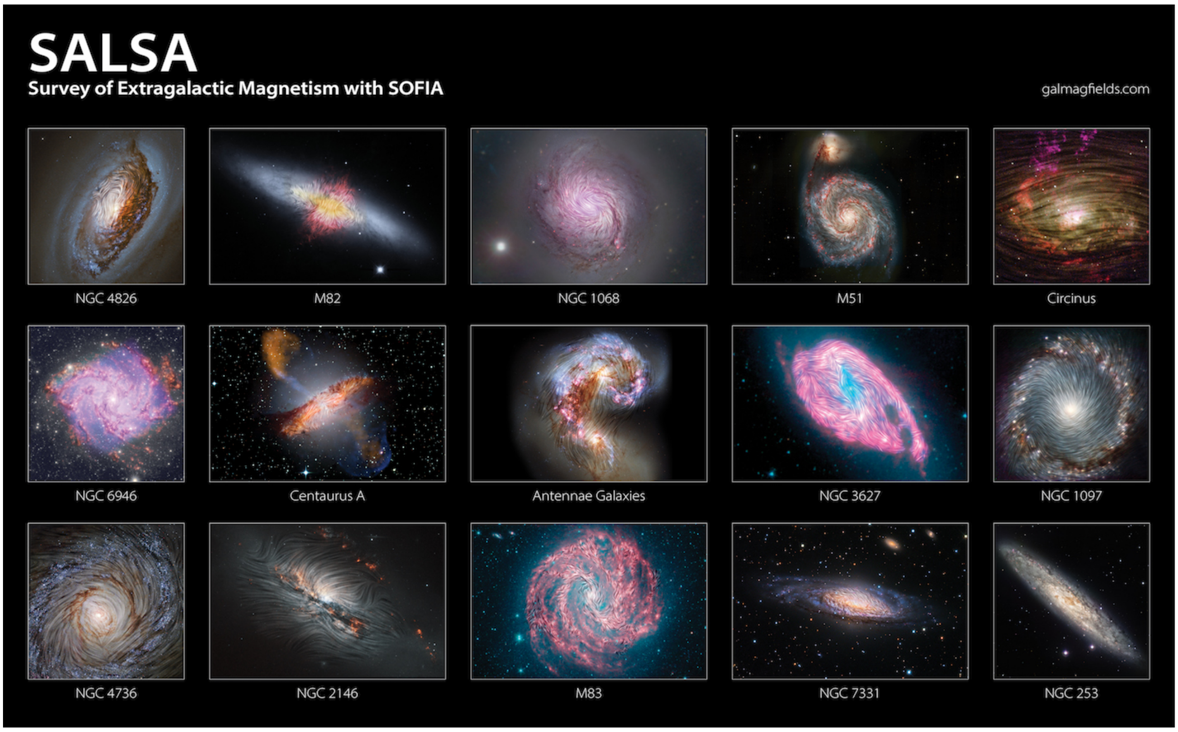

Figure 3 *– Cosmic magnetic fields as detected by HAWC+. Original image caption: The magnetic fields of M51, M82, M83, NGC 253, NGC 1068, NGC 1097, NGC 2146, NGC 3627, NGC 4736, NGC 4826, NGC 6946, NGC 7331, Antennae galaxies, Centaurus A, and Circinus obtained by SALSA (Survey of extragALactic magnetiSm with SOFIA). Image credit: M51: (NASA, the SOFIA science team, A. Borlaff; NASA, ESA, S. Beckwith (STScI) and the Hubble Heritage Team (STScI/AURA)); M82: NASA/SOFIA/E. Lopez-Rodriguez; NASA/Spitzer/J. Moustakas et al.; M83: NASA/JPL-Caltech/E. Lopez-Rodriguez; NGC 253: ESO/A.S. Borlaff; NGC 1068: NASA/SOFIA; NASA/JPL-Caltech/Roma Tre Univ.; NGC 1097: NASA, the SOFIA science team, E. Lopez-Rodriguez et al.; ESO/Prieto et al.; NGC 2146: ESA/Hubble & NASA/E. Lopez-Rodriguez; NGC 3627: NASA/JPL-Caltech/R. Kennicutt (University of Arizona) and the SINGS Team/E. Lopez-Rodriguez; NGC 4736: ESA/Hubble & NASA/A.S. Borlaff; NGC 4826: ESA/Hubble & NASA, J. Lee and the PHANGS-HST Team, Acknowledgement: Judy Schmidt/A.S. Borlaff; NGC 6946: ESA/Hubble/NASA/JPL-Caltech/L.Proudfit/A.S. Borlaff; NGC 7331: Adam Block/Mount Lemmon SkyCenter/University of Arizona/E. Lopez-Rodriguez; Antennae galaxies: ESA/Hubble & NASA/E. Lopez-Rodriguez; Centaurus A: Optical: European Southern Observatory (ESO) Wide Field Imager; Submillimeter: Max Planck Institute for Radio Astronomy/ESO/Atacama Pathfinder Experiment (APEX)/A.Weiss et al.; X-ray and Infrared: NASA/Chandra/R. Kraft; JPL-Caltech/J. Keene; SOFIA; Circinus:Andrew S. Wilson (University of Maryland); Patrick L. Shopbell (Caltech); Chris Simpson (Subaru Telescope); Thaisa Storchi-Bergmann and F. K. B. Barbosa (UFRGS, Brazil); and Martin J. Ward (University of Leicester, U.K.) and NASA/ESA/A.S. Borlaff. Poster design: NASA/SOFIA/L. Proudfit.*

For more information on SALSA visit the Legacy Project page and see selected references:

References

1. *"Extragalactic Magnetism with SOFIA (SALSA Legacy Program): The Magnetic Fields in the Multiphase Interstellar Medium of the Antennae Galaxies", Lopez-Rodriguez, Enrique, et al., 2023/01, ApJL, 942, L13. DOI: 10.3847/2041-8213/acaaa2; ADS Bibliographic Code: 2023ApJ...942L..13L*
2. *"Extragalactic Magnetism with SOFIA (SALSA Legacy Program). IV. Program Overview and First Results on the Polarization Fraction", Lopez-Rodriguez, Enrique, et al., 2022/09, ApJ, 936, 92. DOI:10.3847/1538-4357/ac7f9d; ADS Bibliographic Code: 2022ApJ...936...92L*
3. *"Extragalactic Magnetism with SOFIA (SALSA Legacy Program). III. First Data Release and On-the-fly Polarization Mapping Characterization", Lopez-Rodriguez, Enrique, et al., 2022/09, ApJ, 936, 65. DOI: 10.3847/1538-4357/ac83ac; ADS Bibliographic Code: 2022ApJ...936...65L*

Lunar observations that made a splash

SOFIA's most high-profile result was the first detection of molecular water on the sunlit surface of the Moon in 2020 (Figure 4). The presence of water on the lunar surface has been hypothesized for over a decade, particularly after the LCROSS mission sent an impactor into a permanently shadowed basin at the lunar South Pole. This experiment proved that there was water ice hidden in these cold traps. However, water had never been unambiguously detected elsewhere on the lunar surface.

The study of water on the Moon's surface is ongoing. Recently, the same team produced new maps showing the distribution of water on the lunar surface, around the landing site of the VIPER mission.

For more information, see the Moon Water Legacy Project page and selected references:

References

1. *"Regional Map of Molecular Water at High Southern Latitudes on the Moon Using 6 μm Data From the Stratospheric Observatory for Infrared Astronomy", Honniball, C. I., et al., 2022/04, GeoRL, 4997786H. DOI: 10.1029/2022GL097786; ADS Bibliographic Code: 2022GeoRL..4997786H*
2. *"Molecular water detected on the sunlit Moon by SOFIA", Honniball, C. I., et al., 2021, Nature Astronomy, 5, 121. DOI: 10.1038/s41550-020-01222-x; ADS Bibliographic Code: 2021NatAs...5..121H*
3. *"The Distribution of Molecular Water in the Lunar South Polar Region Based upon 6 μm Spectroscopic Imaging", Reach, William T., et al., 2023/03, Planetary Science Journal, , 4. DOI: 10.3847/PSJ/acbdf2; ADS Bibliographic Code: 2023PSJ.....4...45R*

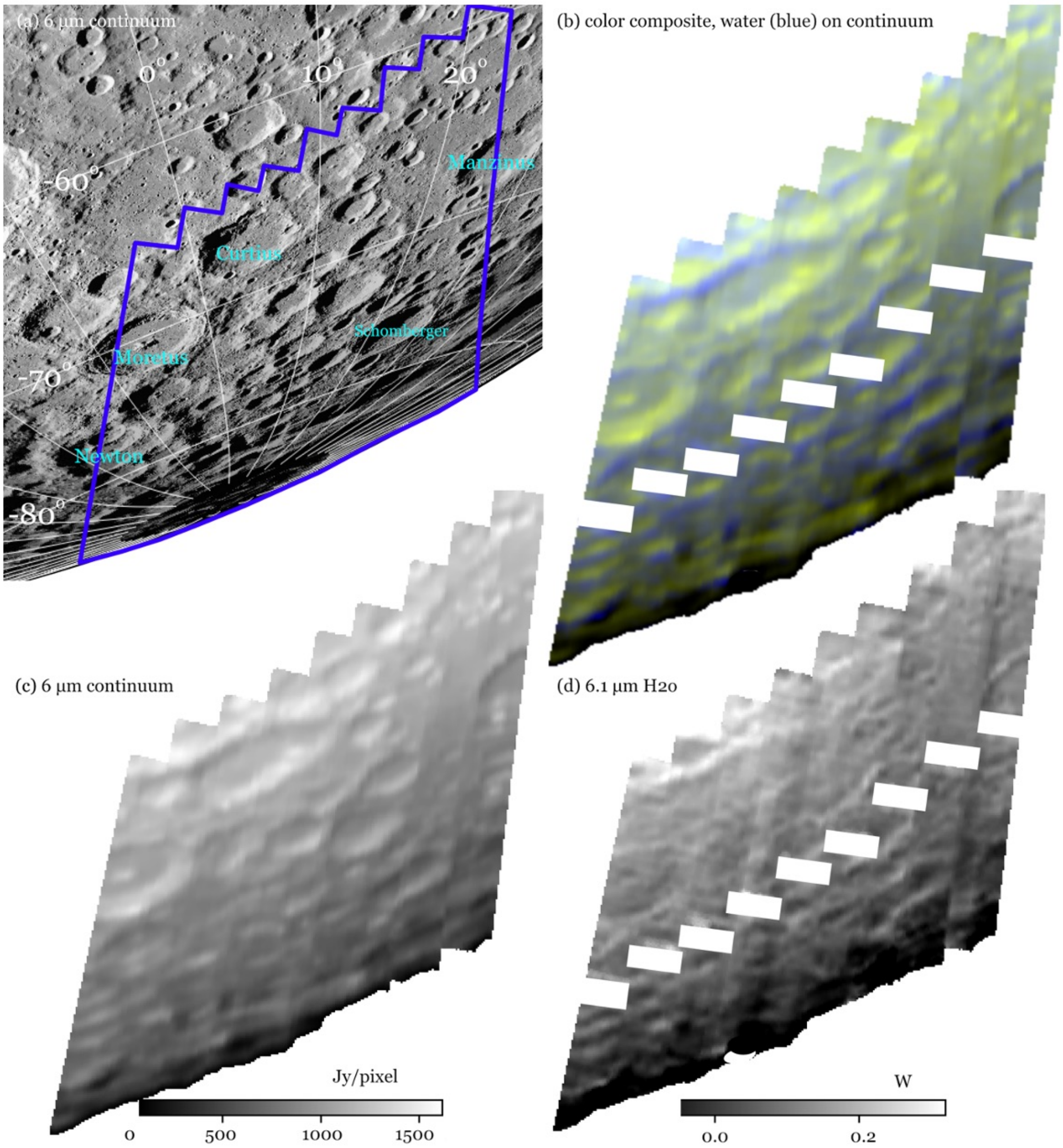

Figure 4 *– Mapping molecular water on the lunar surface. Original image caption: (a) Lunar Reconnaissance Orbiter Wide Angle Camera image of the southern limb of the Moon, oriented with the celestial pole at the top as appropriate for 2022 February 17, with lunar coordinate grid overlaid and an outline of the region observed with SOFIA (blue lines). (b) Color rendition of SOFIA water and continuum emission. The color image combines the 6-micron continuum surface brightness (green) and the 6-micron water feature strength (blue). The diagonal empty regions on the water image mask a partially transparent defect on the surface of the detector that leads to significantly higher noise. (c) The 6-micron continuum surface brightness in Jy/pixel. (d) The 6-micron integrated water band strength, W. Image credit: (Reach et al., 2023).*

Cosmic molecular fingerprints

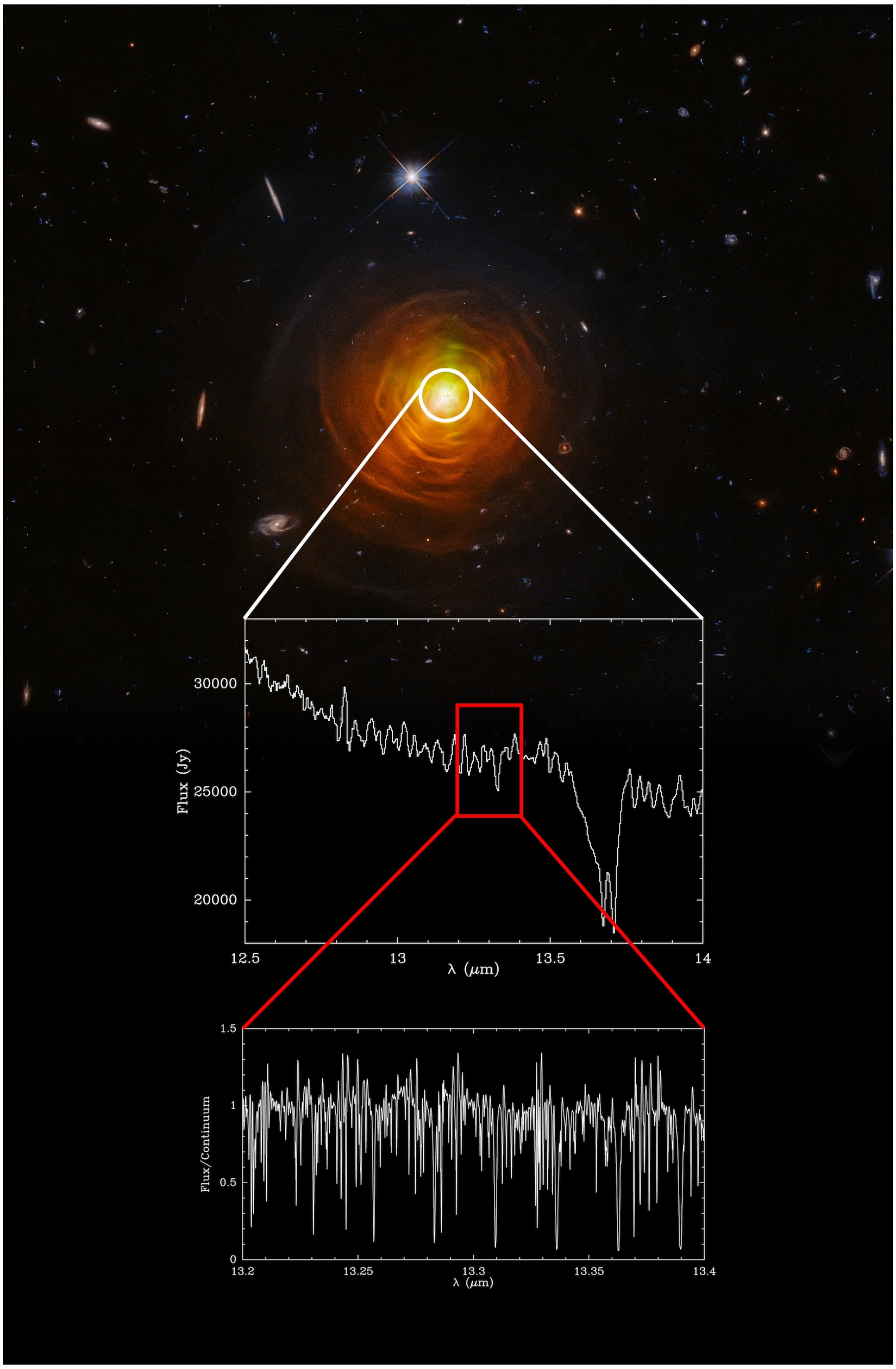

Figure 5 *– Cosmic fingerprints. Original caption: Hubble Space Telescope image of IRC+10216 together with a small portion of the SOFIA/EXES high-resolution spectrum around 13.3 μm. The low-resolution spectrum taken with the Infrared Space Observatory is similar to the results expected from JWST. Image credit: (ESA/Hubble, NASA, and Toshiya Ueta (University of Denver), Hyosun Kim (KASI); Cernicharo et al., 1999; Montiel et al. (in prep); Fonfría et al (in prep))*

SOFIA's powerful mid- and far-infrared capabilities allowed scientists to inventory molecules in a variety of astrophysical environments. Many molecules are visible to telescopes in the submillimeter wavelength range. However, symmetric molecules like H_2, do not have rotational transitions and so can only be observed in the mid-infrared.

The EXES instrument on SOFIA was capable of detecting symmetric molecules that emit in the mid-infrared, providing a key observation of abundances of many molecules otherwise invisible to submillimeter and interferometer telescopes. Using EXES, low abundance molecules could be detected thanks to the instrument's high resolution.

In one recent study, 95 molecules were detected in an evolved carbon-rich star, IRC+10216 (Figure 5). This ongoing work and other studies with the EXES instrument will help constrain circumstellar chemistry models, date the ages of stars, and provide insights into the evolution of the interstellar medium.

For more information, see the EXES Legacy programs pages, Hot Core Spectral Surveys and EXES High-Resolution Spectral Library, and selected references:

References

1. *"Infrared H_2O Absorption in Massive Protostars at High Spectral Resolution: Full Spectral Survey Results of AFGL 2591 and AFGL 2136", Barr, Andrew G., et al., 2022/08, ApJ, 935, 165. DOI: 10.3847/1538-4357/ac74b8; ADS Bibliographic Code: 2022ApJ...935..165B*
2. *"High-resolution Infrared Spectroscopy of Hot Molecular Gas in AFGL 2591 and AFGL 2136: Accretion in the Inner Regions of Disks around Massive Young Stellar Objects", Barr, Andrew G., et al., 2020/09, ApJ, 900, 104. DOI: 10.3847/1538-4357/abab05; ADS Bibliographic Code: 2020ApJ...900..104B*
3. *"The H_2O Spectrum of the Massive Protostar AFGL 2136 IRS 1 from 2 to 13 μm at High Resolution: Probing the Circumstellar Disk", Indriolo, Nick, et al., 2020/05, ApJ, 894, 107. DOI: 10.3847/1538-4357/ab88a1; ADS Bibliographic Code: 2020ApJ...894..107I*
4. *"The First Mid-infrared Detection of HNC in the Interstellar Medium: Probing the Extreme Environment toward the Orion Hot Core", Nickerson, Sarah, et al., 2021/01, ApJ, 907, 51. DOI: 10.3847/1538-4357/abca36; ADS Bibliographic Code: 2021ApJ...907...51N*
5. *"The Mid-infrared Molecular Inventory toward Orion IRc2", Nickerson, Sarah, et al., 2023/03, ApJ, 945, 26. DOI: 10.3847/1538-4357/aca6e8; ADS Bibliographic Code: 2023ApJ...945...26N*

Cosmic bubbles

How do massive stars affect their surroundings? This is the key question for the team investigating stellar feedback through the FEEDBACK Legacy Program. Through their work, scientists are finding that massive stars can trigger the formation of other smaller stars as their stellar winds blow into the surrounding interstellar medium (Figure 6). As these bubbles grow, they transfer energy into turbulent and kinetic motions in the surrounding dust clouds, causing the formation of new stars. Their work also shows that this transfer of energy is most efficient when the massive star is very young. After the bubble pops, the hot ionized gas leaks into the surroundings and the transfer of kinetic energy becomes less efficient.

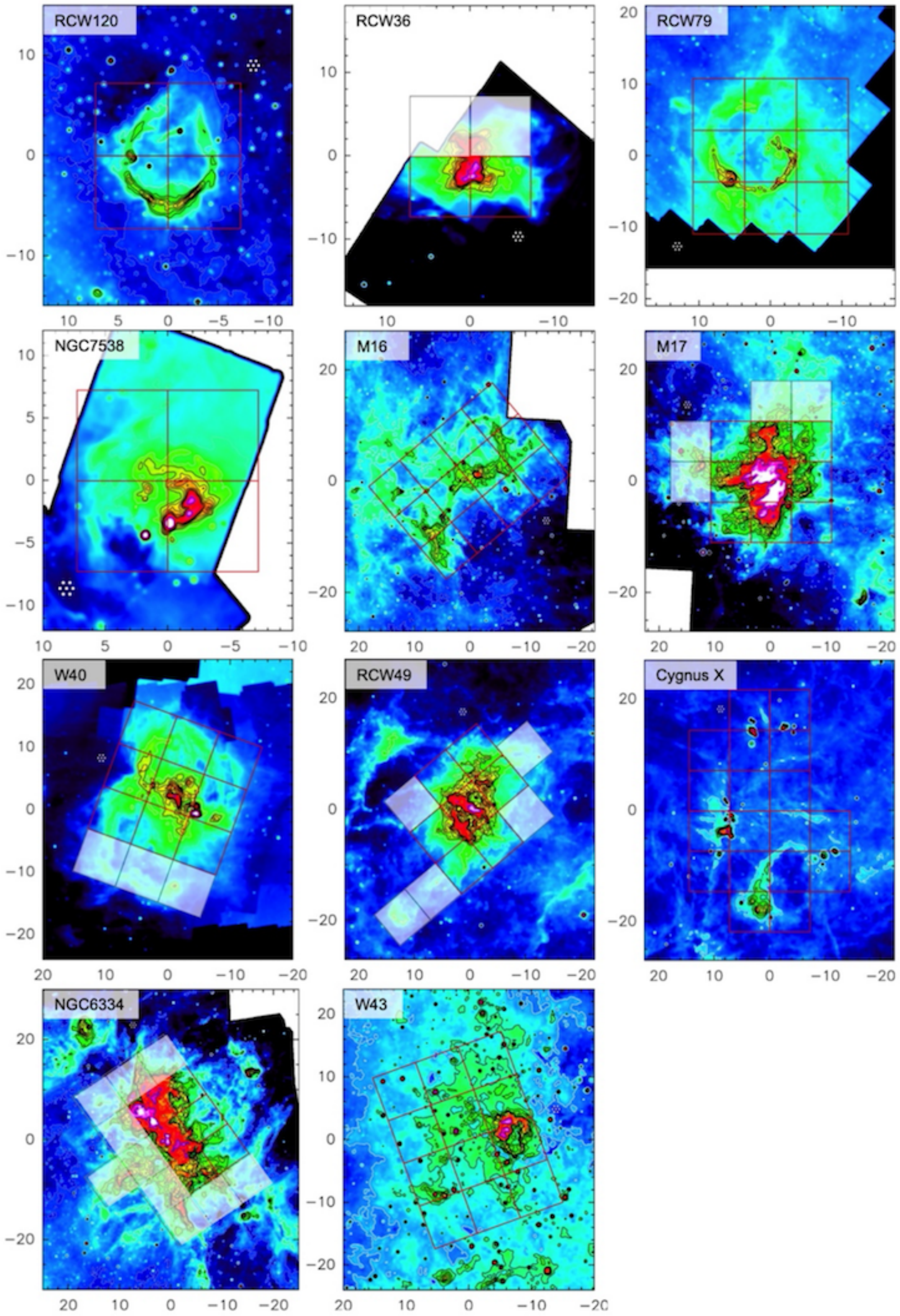

Figure 6 *– Cosmic bubbles around massive stars. Original caption: Feedback source sample. The red boxes outline the tiles proposed to be observed for each source. The slightly opaque ones were not observed. Colored background: The IRAC 8*μ*m map of the sources tracing the PDRs in these regions convolved to the 14*$''$ *upGREAT beam. Contours are predicted [C II] 1.9 THz integrated line intensity based upon the [C II]-8* μ*m relation derived for L1630, Orion, and 30 Dor. Contour levels are: white dashed (50 K km/s), white (100 K km/s), black (150(50)400 K km/s), red (500 K km/s), blue (1000 K km/s). Box units are in arcmin. The upGREAT 7 beam pattern is plotted alongside the outlined area in each box, illustrating that much finer detail than visible in these images can be traced. Image credit: (Robert Simon, University of Cologne)*

For more information see the FEEDBACK Legacy Program page and selected references:

References

1. *"SOFIA FEEDBACK survey: PDR diagnostics of stellar feedback in different regions of RCW 49", Tiwari, M., et al., 2022/10, AJ, 164, 150. DOI: 10.3847/1538-3881/ac8a44; ADS Bibliographic Code: 2022AJ....164..150T*
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4. *"FEEDBACK from the NGC 7538 H II region", Beuther, H., et al., 2022/03, A&A, 659A, A77. DOI: 10.1051/0004-6361/202142689; ADS Bibliographic Code: 2022A&A...659A..77B*

SOFIA's human element

SOFIA, a specially modified Boeing 747SP aircraft with a 2.7-meter telescope, was the largest airborne observatory ever built. SOFIA was operated by an 80/20 partnership between NASA and DLR (German Aerospace Center). The Science and Mission Operations center, located at NASA's Ames Research Center (ARC), provided comprehensive support for SOFIA users. The SOFIA team mastered the unique and complex operations of the observatory and worked continuously to improve operational efficiency and scientific effectiveness.

No space-based missions nor ground-based observatories are exact analogs to SOFIA. SOFIA was a crewed mission that employed an onboard team to fly the aircraft and operate the observatory. SOFIA flight operations were based at NASA's Armstrong Flight Research Center (AFRC). SOFIA deployed to Southern Hemisphere sites to observe targets that are not accessible from the north.

SOFIA's impact was influential and far-reaching. SOFIA stood out compared to its sibling astrophysical missions because of its human element. Being a crewed airborne mission involved the expertise and skills of a wide variety of individuals from multiple professions, including scientists, engineers, pilots, navigators, flight planners, meteorological support, life support, software engineers, mission directors, instrument operators, avionics, and aircraft mechanics.

SOFIA's public outreach activities and targeted initiatives captured the imagination of people around the world and provided opportunities for the next generation to pursue their interest in STEM fields. Through the partnership between DLR and NASA, SOFIA significantly impacted the American and German scientific communities as well as the citizens of both countries.

Teachers and students

SOFIA had a long and very successful history of providing critical support for the Airborne Astronomy Ambassadors Program (AAA) and its equivalent German program through which teachers received professional development, training, and support for implementing new STEM curricula for middle school, high school, and community college classrooms.

Prior to the conclusion of SOFIA, over 200 U.S. teachers had flown on SOFIA and shared their new skills and knowledge with their students. These teachers have reached over 20,000 students since 2011, in 37 states plus the District of Columbia. About 50 German school teachers participated, and through their initiatives reached about 50,000 young people. The AAA program partners with school districts chosen based partly on their participation in the National School Lunch Program. Due to the historical context of the United States, these districts also disproportionately serve students of color.

Figure 7 *– A group of Airborne Astronomy Ambassadors plus their flight facilitator aboard SOFIA.*

On board SOFIA, teachers interacted with scientists, mission crew, and pilots to learn about SOFIA science and operations. Once they returned to their schools, these teachers were equipped to provide their communities with specialized educational opportunities that were designed to measurably enhance STEM learning and engagement of their students. One of the major findings from a recent study was that the students whose teachers were in the AAA program and flew on SOFIA internalized that there are multiple ways of becoming a STEM professional, that STEM is collaborative (rather than solitary), and that STEM requires many different skills. These students also had a marked increased interest in becoming STEM professionals after their teachers participated in the AAA program.

This text is based on excerpts taken from the report SOFIA: Status and Future Prospects authored by Naseem Rangawala et al. and various science highlights. We would like to acknowledge Abby Tabor, Science Communication Specialist at NASA Ames Research Center, for proof-reading this article.

Dr. Maggie McAdam is an early career planetary scientist working at NASA Ames Research Center since 2020. Maggie served as the Associate Project Scientist for SOFIA from 2020 – 2023.

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Dr. Naseem Rangwala is the Chief of the Astrophysics Branch at NASA's Ames Research Center since March 2023. She has also been serving as the NASA Project Scientist for the SOFIA airborne observatory since 2019, which ended science operations in September 2022. During her tenure on SOFIA, Naseem worked closely with NASA HQ, Ames and Armstrong center management, the German space agency, DLR, and the astrophysics community and advisory groups. Naseem's current research focuses on observational astrochemistry. She is leading the effort to build a large database of observed molecular transitions from infrared space missions to enable a wide range of astrophysics and laboratory astrophysics applications. She led a large SOFIA observing campaign on the first high-resolution molecular line survey in the mid-infrared that has detected new molecular lines in the interstellar medium and is providing a key chemical inventory in the infrared – essential for studying chemical networks, understanding organic astrochemistry associated with star formation, and providing clues on supply pathways of key organic molecules from the ISM to exoplanets. Previously, she has led several observing programs using the Atacama Large Millimeter Array and the Herschel Space Observatory to characterize the molecular gas in the nuclear regions of luminous infrared galaxies.

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Emission spectra of fullerenes: computational evidence for blackbody-like radiation due to structural diversity and electronic similarity

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The spectral emission of hot C_{60} has been experimentally shown to be broad and continuous, in apparent contradiction with the discrete and narrow absorption spectrum associated with the high symmetry of buckminsterfullerene. In the present work we computationally model the emission spectrum of isolated carbon clusters, assuming a broad distribution of isomers that are likely populated under the experimental conditions. The contributions of individual structures to the global spectrum correspond to the relaxation via recurrent fluorescence and vibrational emission, electronic and vibrational structures being described by a simple but efficient density-functional-based tight-binding scheme. The model predicts a blackbody-like emission spectrum that is naturally broad and correctly accounts for the experimental measurements, except for a maximum that is quantitatively shifted with respect to Wien's displacement law. To quantify such differences, we introduce an emissivity parameter ε as the ratio between the spectral emittance and the corresponding exact blackbody spectrum; ε is numerically found to scale as $(\lambda T)^{-2}$ at leading order with increasing temperature T and for wavelengths $\lambda > 350$ nm, and we provide a theoretical justification for this behavior. Our results are discussed in the light of the astrophysical detection of interstellar fullerenes, as well as in combustion environments where carbon clusters are relevant in the context of nascent soot particle formation.

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The largest fullerene

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Fullerenes are lowest energy structures for gas phase all-carbon particles for a range of sizes, but graphite remains the lowest energy allotrope of bulk carbon. This implies that the lowest energy structure changes nature from fullerenes to graphite or graphene at some size and therefore, in turn, implies a limit on the size of free fullerenes as ground state structures. We calculate this largest stable single shell fullerene to be of size $N=1\times10^4$, using the AIREBO effective potential. Above this size fullerene onions are more stable, with an energy per atom that approaches graphite structures. Onions and graphite have very similar ground state energies, raising the intriguing possibility that fullerene onions could be the lowest free energy states of large carbon particles in some temperature range.

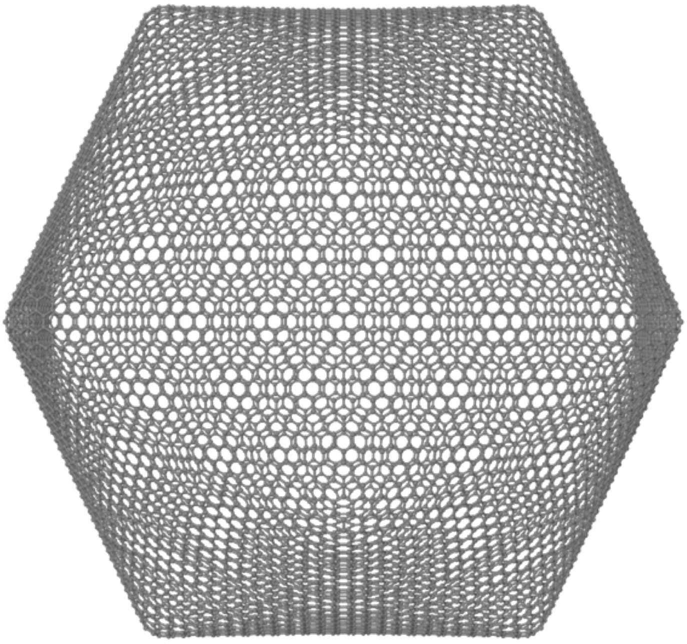

Figure 8 *– Optimized structure of the* C_{10140} *icosahedral fullerene.*

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Autoionization from the plasmon resonance in isolated 1-cyanonaphthalene

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Polycyclic aromatic hydrocarbons have widely been conjectured to be ubiquitous in space, as supported by the recent discovery of two isomers of cyanonaphthalene, indene, and 2-cyanoindene in the Taurus molecular cloud-1 using radioastronomy. Here, the photoionization dynamics of 1-cyanonaphthalene (1-CNN) are investigated using synchrotron radiation over the $h\nu = 9.0$–19.5 eV range, revealing that prompt autoionization from the plasmon resonance dominates the photophysics for $h\nu = 11.5$–16.0 eV. Minimal photo-induced dissociation, whether originating from an excited state impulsive bond rupture or through internal conversion followed by a statistical bond cleavage process, occurs over the microsecond timescale (as limited by the experimental setup). The direct photoionization cross section and photoelectron angular distributions are simulated using an ezDyson model combining Dyson orbitals with Coulomb wave photoejection. When considering these data in conjunction with recent radiative cooling measurements on 1-CNN$^+$, which showed that cations formed with up to 5 eV of internal energy efficiently stabilize through recurrent fluorescence, we conclude that the organic backbone of 1-CNN is resilient to photodestruction by VUV and soft XUV radiation. These dynamics may prove to be a common feature for the survival of small polycyclic aromatic hydrocarbons in space, provided that the cations have a suitable electronic structure to support recurrent fluorescence.

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Experimental radiative cooling rates of a polycyclic aromatic hydrocarbon cation

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Several small Polycyclic Aromatic Hydrocarbons (PAHs) have been identified recently in the Taurus Molecular Cloud (TMC-1) using radio telescope observations. Reproducing the observed abundances of these molecules has been a challenge for astrochemical models. Rapid radiative cooling of PAHs by Recurrent Fluorescence (RF), the emission of optical photons from thermally populated electronically excited states, has been shown to efficiently stabilize small PAHs following ionization, augmenting their resilience in astronomical environments and helping to rationalized their observed high abundances. Here, we use a novel method to experimentally determine the radiative cooling rate of the cation of 1-cyanonaphthalene ($C_{10}H_7CN$, 1-CNN), the neutral species of which has been identified in TMC-1. Laser-induced dissociation rates and kinetic energy release distributions of 1-CNN cations isolated in an cryogenic electrostatic ion-beam storage ring are analysed to track the time evolution of the vibrational energy distribution of the initially hot ion ensemble as it cools. The measured cooling rate is in good agreement with the previously calculated RF rate coefficient. Improved measurements and models of the RF mechanism are needed to interpret astronomical observations and refine predictions of the stabilities of interstellar PAHs.

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C–H Stretch Vibrational Modes: Tracers of Interstellar PAH Geometries?

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Polycyclic Aromatic Hydrocarbon (PAH) molecules have been long adjudged as carriers of the frequently detected interstellar emission features in the 3-20 µm region. In the present work, PAHs with straight edges having solo-duo ($\mathrm{PAH_D}$) and solo-duo-trio ($\mathrm{PAH_T}$) C-H modes along with PAHs with irregular edges ($\mathrm{PAH_I}$) have been studied theoretically to understand the effect of molecular geometry on the interstellar C-H stretch vibrations at 3.3 µm. The C-H out-of-plane bending vibrations at 11.2 and 12.7 µm are also included for completeness. Using *NASA Ames PAH IR Spectroscopic Database*, the mid-infrared spectra have been studied for 125 PAH molecules of varying molecular geometries, sizes, charge states and symmetries. Results show that the individual solo, duo and trio C-H stretches follow an order in the peak wavelength ($\lambda_{3.3(\mathrm{solo})} > \lambda_{3.3(\mathrm{duo})} > \lambda_{3.3(\mathrm{trio})}$) and intensity ($I_{3.3(\mathrm{solo})} < I_{3.3(\mathrm{duo})} < I_{3.3(\mathrm{trio})}$). If only $\mathrm{PAH_D}$s are considered, the contribution of each charge state is required to account for the observed peak wavelength of the 3.3 µm band, or, if only neutrals are contributors, $\mathrm{PAH_D}$ and $\mathrm{PAH_T}$ neutrals can explain the 3.3 µm band variations. The observed emission at 11.2 and 12.7 µm is found to match effectively with $\mathrm{PAH_D}$ with increasing size, and the 11.2 µm band is present at longer wavelengths for $\mathrm{PAH_T}$ contributing to the red-wing. When the solo to duo hydrogens ratio is nearly equal or greater than 1.0, $\mathrm{PAH_D}$ neutrals yield better 3.3 µm peak positions. The ratio has a lower limit of 0.8 for the 11.2 µm band and converges at 1.5, indicating a size range of $\mathrm{PAH_D}$ neutrals with 80 to larger numbers of carbon atoms. The present work examines the presence of solo, duo and trio modes in the C-H stretching band, which must be taken into consideration when interpreting accurate data from *James Webb Space Telescope (JWST)* to further explain the observed variations in the interstellar 3.3 µm.

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Theoretical microwave spectra of interstellar nitrogen-containing PAHs

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The recent discovery of naphthalene ($C_{10}H_8$) in cyano-substituted polycyclic aromatic hydrocarbon (CN-PAH) form in the Taurus Molecular Cloud (TMC-1) sparks curiosity for the search of other nitrogen-containing naphthalenes in similar interstellar environments. In this light, naphthalene having N atoms in the structure are promising candidates to be searched in cold, dark molecular clouds such as TMC-1. Since obtaining data on such samples in the laboratory is complicated, the present work reports theoretical microwave spectra of naphthalene in all N-substituted forms. The density functional theory (DFT) calculations are employed to calculate the spectroscopic constants and simulate the rotational spectra with hyperfine splitting. For cold temperature regions such as TMC-1 (about 5 K), the considered N-naphthalene species show the strongest transition around centimetre wavelengths, a typical range for PAH-related species in dark molecular clouds. Accurate rotational data provided here may act as a guide for laboratory experiments and astronomical searches.

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Buckyball-metal complexes as potential carriers of astronomical unidentified infrared emission bands

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Efforts over 40 yr still leave the source of astronomical infrared emission bands largely unidentified. Here, we report the first laboratory infrared (6-25 µm) spectra of gas-phase fullerene-metal complexes, [C_{60}-Metal]$^+$ (Metal = Fe, V) and show with density functional theory calculations that complexes of C_{60} with cosmically abundant metals, including Li, Na, K, Mg, Ca, Al, V, and Fe, all have similar spectral patterns. Comparison with observational infrared spectra from several fullerene-rich planetary nebulae demonstrates a strong positive linear cross-correlation. The infrared features of [C_{60}-Metal]$^+$ coincide with four bands attributed earlier to neutral C_{60} bands and in addition also with several bands unexplained to date. Abundance and collision theory estimates indicate that [C_{60}-Metal]$^+$ could plausibly form and survive in astrophysical environments. Hence, [C_{60}-Metal]$^+$ are proposed as promising carriers, in supplement to C_{60}, of observational bands, potentially representing the largest molecular species in space other than C_{60}, C_{60}^+ , and C_{70}.

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Polycyclic aromatic hydrocarbon size tracers

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We examine the dependence of polycyclic aromatic hydrocarbon (PAH) band intensity ratios as a function of the average number of carbon atoms and assess their effectiveness as tracers for PAH size, utilising the data, models, and tools provided by the NASA Ames PAH Infrared Spectroscopic Database. To achieve this, we used spectra from mixtures of PAHs of different ionisation fractions, following a size distribution. Our work, congruent with earlier findings, shows that band ratios that include the 3.3 µm PAH band provide the best PAH size tracers for small-to-intermediate sized PAHs. In addition, we find that band ratios that include the sum of the 15-20 µm PAH features ($I_{\Sigma_{15-20}}$) and the 6.2 or 7.7 µm bands also serve as good tracers for PAH size in the case of small-to-intermediate sized PAHs, for objects under a similar PAH size distribution as with the presented models. For different PAH size distributions, the application of a scaling factor to the $I_{6.2}/I_{\Sigma_{15-20}}$ ratio can provide estimates for the size of the small-to-intermediate PAH population within sources. Employment of the $I_{6.2}/I_{\Sigma_{15-20}}$ and $I_{7.7}/I_{\Sigma_{15-20}}$ ratios can be of particular interest for *JWST* observations limited only to ∼5-28 µm MIRI(-MRS) coverage.

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https://arxiv.org/abs/2307.03743

Machine-learning identified molecular fragments responsible for infrared emission features of polycyclic aromatic hydrocarbons

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A machine learning model was employed to identify the sources of infrared emission features of polycyclic aromatic hydrocarbons (PAHs). The model was trained on the spectra of 14,124 neutral PAHs to assess the significance of 10,632 molecular substructures for 171 bands in the spectral region between 2.761 and 1172 µm. The molecular fragments deemed most important are summarized in two Tables, to serve as a new reference for investigating potential neutral PAH carriers of aromatic infrared bands.

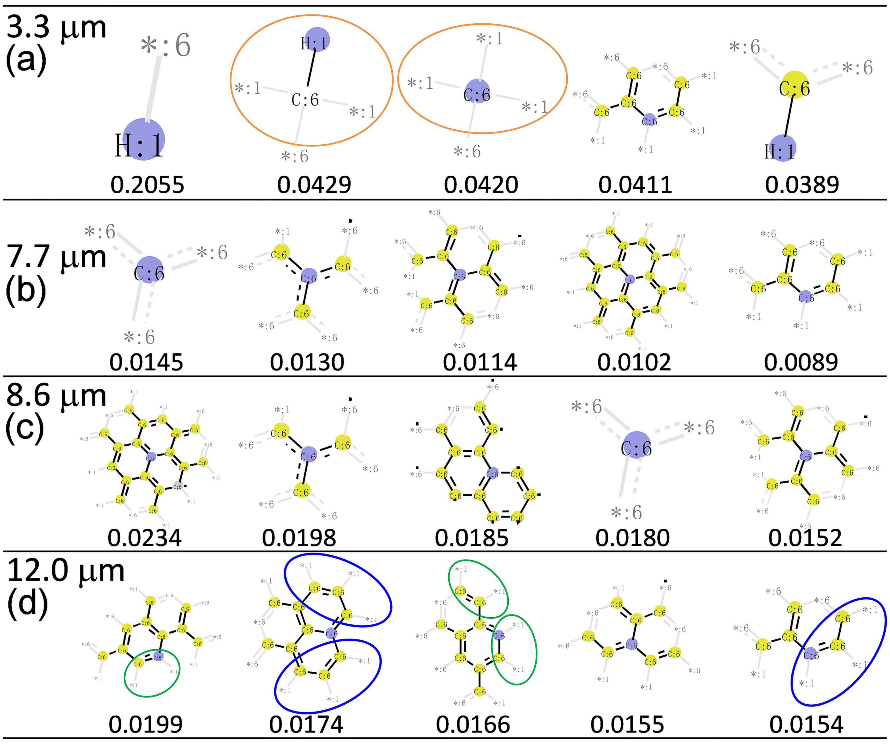

Figure 9 *– Five most important fragments for bands with established sources.*

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Fullerene-indene adducts (ICMA & ICBA) in an astrochemical perspective part 1: chemical thermodynamics, stability and electronic absorption spectroscopy

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Both C_{60} fullerene and indene were detected in certain astrophysical objects. It is then possible that these two molecules may react together in space forming adducts like indene-C_{60} mono-adduct (ICMA) as well as the indene-C_{60} bis-adducts (ICBA). In view of the potential detection of such adducts in space, the chemical thermodynamics of the reaction between C60 and indene was analyzed using the thermochemical group increment approach. ICMA and ICBA were synthesized and their composition and stability was studied with thermogravimetric analysis and derivative thermogravimetry (TGA-DTG). ICBA and moreover ICMA resulted stable and strong adducts. In particular, the latter is stable up to 350 °C and this fact increases the chances to find it in space. Furthermore, the retro Diels-Alder reaction was accurately studied on ICMA with differential scanning calorimetry (DSC) and an unusually high activation energy for the decomposition was determined and explained with the chemical thermodynamic data. The electronic absorption spectra of ICMA and ICBA were studied in n-hexane and the molar extinction coefficients of the main absorption bands have been determined. A possible way to detect such adducts is through electronic absorption spectroscopy, while the infrared spectroscopy of ICMA and ICBA is analyzed and discussed in the following second part of this work.

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https://doi.org/10.1080/1536383X.2023.2220841

Fullerene-indene adducts (ICMA ICBA) in an astrochemical perspective. Part 2: FT-IR spectroscopy from -180 °C to +250 °C

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It is likely that indene-C_{60} mono-adduct (ICMA) as well as the indene-C_{60} bis-adducts (ICBA) could exist in space. With this astrochemical perspective in mind, the FT-IR spectra of these two compounds were recorded in a wide range of temperatures from -180 °C to +250 °C. Furthermore, the molar extinction coefficients and integrated molar absorptivity of the main infrared absorption bands of ICMA and ICBA have been measured. The infrared data presented in this work may allow the astrochemists and astrophysicists an easy qualitative and quantitative potential identification of ICMA and ICBA in space.

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Laboratory Astrophysics Workshop

ICE 2024

Kauai, Hawaii, USA
19–22 February, 2024

http://uhmreactiondynamics.org/ICE2024.html

Registration is now open for ICE 2024. Significant new experimental techniques have been developed to investigate the interaction of ionizing radiation (UV, VUV, gamma rays, charged particles) and of neutrals (atoms, radicals, molecules, grains) with surfaces of solids (ices, minerals, carbonaceous compounds) in the Solar System and in the Interstellar Medium (ISM). These processes provide new fundamental insights – sometimes on the molecular level – into the processes that are critical to the chemistry in the ISM, star and planet forming regions, and on/in icy objects in the Solar System from the formation of the simplest molecule (molecular hydrogen) to astrobiologically important species such as amino acids and sugars. There is an increasing convergence of interests of these fields, so a 'united' workshop is highly desired.

Based on the successful workshops in 2013 and 2015, the third workshop features invited (senior and junior researchers) as well as contributed talks covering the interaction of ionizing radiation (UV, VUV, gamma rays, charged particles) and neutrals (atoms, radicals, molecules, grains) with low temperature solids (ices, minerals, organics). The talks can be extended to observations, modeling, and electronic structure calculations, if these topics can be linked – as evident from the abstract – to laboratory experiments.

Accommodation: Several hotels are within walking distance of the conference center including the ISO Mokihana, Aston Islander on the Beach, Waipouli Beach Resort, Kauai Shores Hotel, and the Sheraton Coconut Beach Resort.

Conference: The workshop will take place in the Sheraton Coconut Beach Resort in Kapaa, Kauai, Hawaii, starting with a reception and registration on February 18, 2024, at 6 pm (Sunday) followed by presentations on February 19-22. Presenters may choose between oral or poster presentation formats.

Registration: The registration fee of $ 400 includes the reception, a morning and evening snack break, and a book-of-abstracts. The late registration fee after November 1, 2023, is $ 600. No refunds will be given after November 1, 2023.

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AstroPAH Newsletter

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