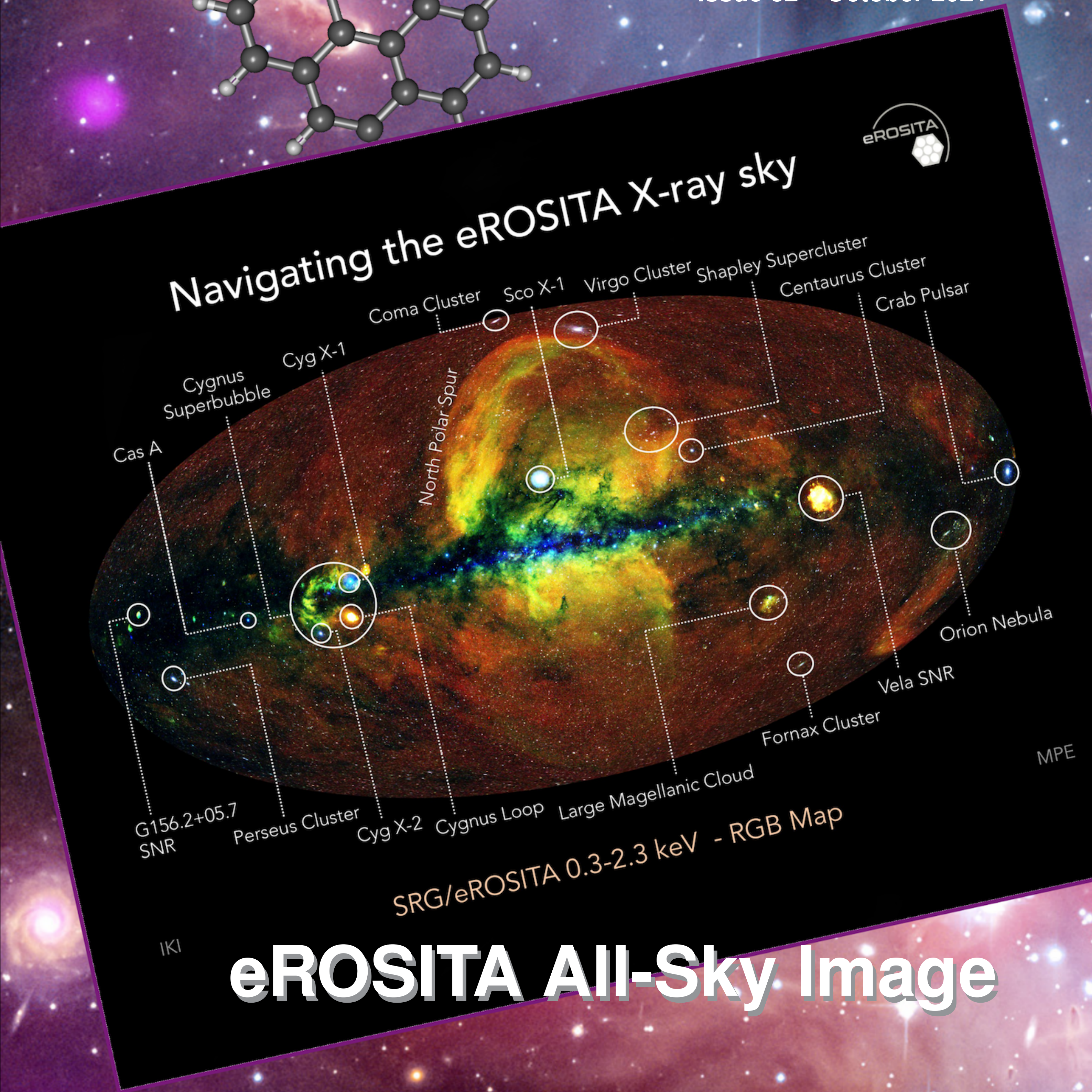
AstroPAH

A Newsletter on Astronomical PAHs

Issue 82 • October 2021



eROSITA All-Sky Image

Editorial

Dear Colleagues,

Welcome to our new AstroPAH volume! We hope all of you are healthy and doing well!

This month, we dedicate our cover and the In Focus to X-Rays! On the cover the amazing all-sky X-ray image taken by eRosita, an instrument built by the Max Planck Institute for Extraterrestrial Physics (MPE), Germany, which is part of the Russian–German Spektr-RG space observatory. The In Focus, written by Sascha Zeegers and Elisa Costantini, shows how observations of X-ray binaries can lead to information on interstellar dust properties.

Benzene, small hydrocarbons, Cyclopropenylidene, fluorene, fullerenes, and even a new detection of benzyne are in the Abstracts menu this month. For the dessert, the announcement of the upcoming online workshop 'Evolved Stars and their Circumstellar Environments' and two open postdoc positions at IAC, Spain.

We hope you enjoy reading our newsletter and our brand new webpage. If you are on Instagram, be sure to check out our next PAH of the Month!

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.

The Editorial Team

Next issue: 18 November 2021.
Submission deadline: 5 November 2021.

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PAH Picture of the Month

Annotated version of the eROSITA First All-Sky image. In this picture the prominent X-ray features are marked. These range from distant galaxy clusters (Coma, Virgo, Fornax, Perseus) to extended sources such as Supernova Remnants (SNRs) and Nebulae to bright point sources, e.g. Sco X-1, the first extrasolar X-ray source to be detected. Find more about the X-ray view on interstellar dust in the In Focus section.

Credits: Jeremy Sanders, Hermann Brunner, Andrea Merloni and the eSASS team (MPE); Eugene Churazov, Marat Gilfanov (on behalf of IKI). The image is available here.

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The X-ray view on interstellar dust

by Sascha Zeegers (ASIAA) and Elisa Costantini (SRON)

Interstellar dust plays important roles in various processes in galaxies and although we roughly understand its properties, there are many details we are still missing. For example, it is still unclear how the properties of dust influence the life cycle of stars and vice versa and how dust is processed and destroyed in the interstellar medium (ISM). Our current understanding of dust in the ISM is based mostly on infrared absorption spectra from a relatively limited number of sight lines.

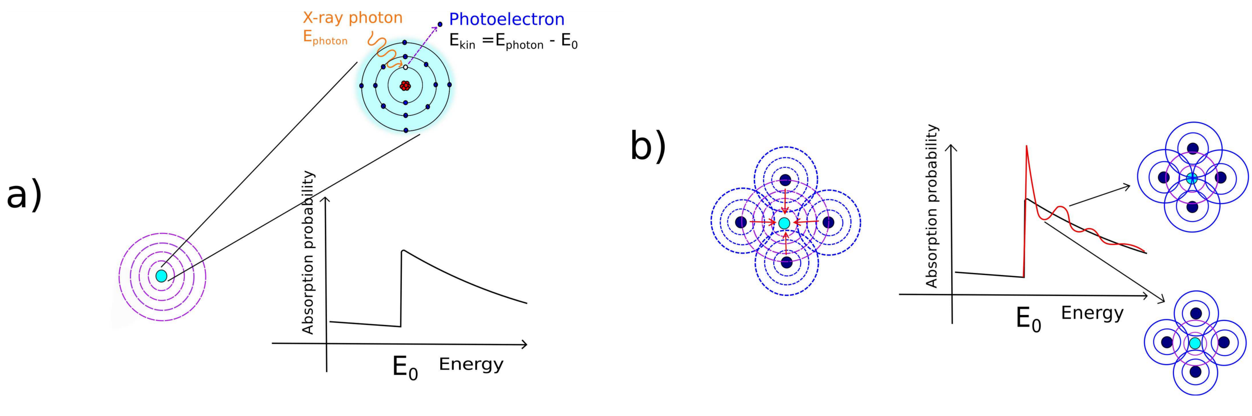

Figure 1 *– a) Above: photoelectric effect. Left: the photoelectron is shown as a wave emanating from the site of the atom (purple circles). Right: resulting absorption probability versus energy, which increases at the binding energy and then decays with increasing energy. b) The initial wave now is scattered by the neighboring atoms and new waves emanate from these sites (blue circles). Right: modified absorption (i.e. XAFS, red line). The scattered blue waves are superimposed on the initial purple wave causing alternating constructive or destructive interference at the absorbing atom. Figure by S. Zeegers.*

The X-rays provide an interesting view on dust properties, enabling us to study crystallinity, composition and dust particle size. This wavelength range not only provides additional information to what is already known from infrared wavelengths, but it gives us a whole new perspective on the dust properties. A unique aspect is the possibility to measure the column densities of dust and gas simultaneously. Of course to do so, we need suitable X-ray background sources shining through the ISM. Nature provides us with X-ray binaries scattered over the Galactic plane.

The spectral features that reveal all this information are the so-called ”X-ray edges”. These discontinuities, that occur at wavelengths where the energy of an absorbed photon corresponds to an electronic transition or ionization potential, show characteristic substructures, called XAFS (X-ray absorption fine structure). As can be seen in Figure 1, the XAFS features uniquely depend on the neighbouring atoms: the type of elements and the distances between them. These fingerprints of the dust particles along the line of sight tell us about the crystallinity, chemical composition and dust size.

The *Chandra* and *XMM Newton* X-ray observatories are especially suitable to study silicates because the edges O K, Fe L, Mg K and Si K fall within their detection range (where K and L stand for the corresponding electron shells). However, although we have the telescopes available to observe these edges, it has been realized that a lack of interstellar dust models prevented us from a detailed interpretation of these absorption edges. In the SRON dust team, lead by Elisa Costantini, we performed a series of measurements at synchrotron facilities all over Europe to remedy this situation. This took us on trips to Paris (Soleil Synchrotron Facility), Grenoble (European Synchrotron Radiation Facility) and Cadiz (STEM facility at the University of Cadiz). Every synchrotron beamline is specialized in a specific energy band and therefore optimized for different absorption edges. The samples were kindly provided by the Jena AIU dust laboratory and contained both amorphous and crystalline interstellar dust analogues. Some of these samples were synthesized and others came from natural sources (e.g. Zeegers et al. 2019). The resulting sample set contained olivines and pyroxenes, but also quartz types and aluminates. The obtained laboratory spectra were then transformed to extinction spectra and implemented in a spectral fitting tool (SPEX, Kaastra et al. 1996) for further analysis.

Exploring the Galaxy

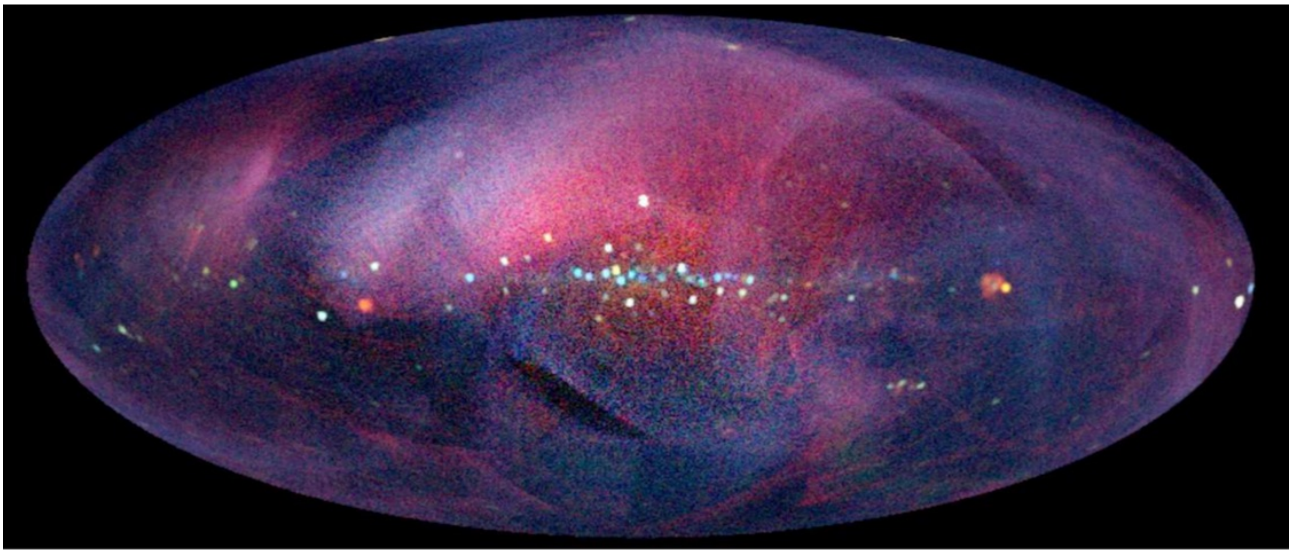

Figure 2 *– The Galaxy in the X-rays showing X-ray sources: 0.5-16 keV MAXI all-sky survey. Image credits: JAXA/RIKEN/MAXI team.*

The absorption features of spectra of bright X-ray background objects, we can explore dust in the Galaxy as can be seen in Figure 2. When moving to higher energies we explore denser environments as can be seen in Figure 3, where we display the transmitted continuum affected by a broad band photoelectric absorption as a function of energy and column density. The column density can be considered a measure of the amount of dust along the line of sight. The lower the energy of the edge, the more diffuse the environment in which we observe the dust.

A pilot study was carried out after the first laboratory measurement run on the silicon K-edge using observational data of the bright X-ray binary GX 5-1 (Figure 4) by the *Chandra* observatory. After that, a larger sample of nine different sight-lines was used to explore the central Galactic environment (Zeegers et al. 2019). Rogantini et al. (2020) then extended this study to include the magnesium K-edge and further expanded the number of sources to even include a source in the Large Magellanic Cloud.

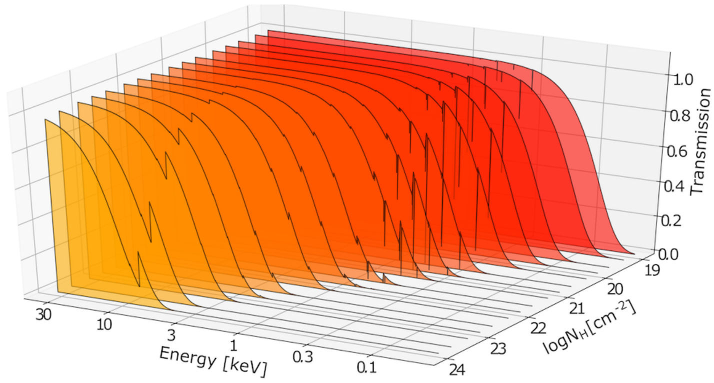

Figure 3 *– Transmission models with different values of hydrogen column densities, indicating how the observation of edges changes for dense to diffuse sightlines. Figure by D. Rogantini.*

The results from these studies, which focused on relatively dense environment near the Galactic bulge, all pointed toward a dominant contribution of olivine. However, surprisingly, different sightlines did show differences in the contribution of crystalline olivine, sometimes even reaching values as high as 10-15%. This result seems to contradict results from the analysis of infrared spectra, but could be a consequence of the nature of the X-rays, where we measure short range interactions between the atoms, instead of the more long range resonances of the bending and stretching modes detected in the infrared.

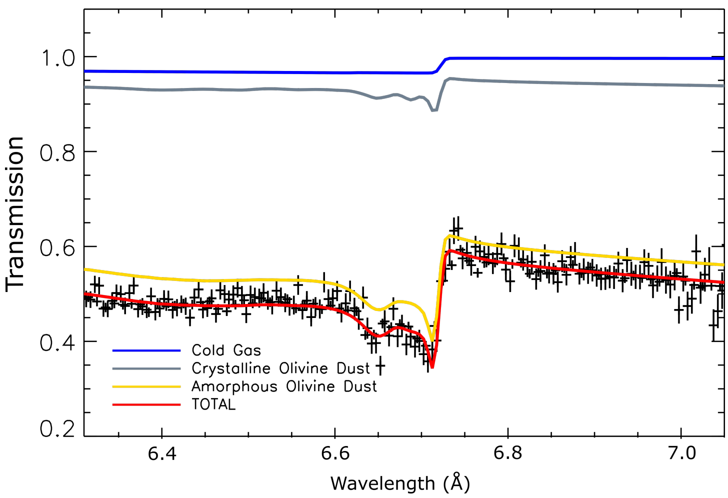

Figure 4 *– The Si K-edge of X-ray binary GX 5-1. The best fitting dust mixture is shown by the yellow line (amorphous olivine) and the grey line (crystalline olivine dust). The cold gas contribution is shown by the blue line and the total, cold gas and dust, by the red line (Zeegers et al. 2019).*

Explorations of the more diffuse ISM were first undertaken by e.g. Lee et al. (2009), Pinto et al. (2010) and Costantini et al. (2012). The X-ray binary 4U 1820-30 observed with *XMM Newton* showed that in this environment the dust along the line of sight was well fitted by a mixture of metallic iron and pyroxenes (Costantini et al. 2012). This may indicate the presence of GEMS in the ISM, i.e. metallic iron or iron sulfide globules embedded in a glassy silicate matrix (e.g. Bradley 1994). Such a configuration has also been observed in interplanetary dust particles with an interstellar origin and primitive meteorites.

More recently the oxygen K-edge was analyzed by Psaradaki et al. (2020) with new models based on recent measurements with the STEM at Cadiz, Spain. This study contains a detailed analysis of oxygen along the line of sight toward Cygnus X-2. Both the iron and oxygen edge show significant dust depletion. A new analysis of the Fe L-edge which includes the new laboratory data is ongoing.

The X-ray observatory future looks bright with new telescopes coming to the scene. There will be XRISM in early 2023 and Athena in the early 2030s, providing us with more detailed spectra of the edges over an even broader wavelength range. In the meantime the laboratory measurements are still ongoing to make sure we are well prepared for these upcoming mission.

Dr. Sascha Zeegers (below) is a postdoctoral researcher at the Institute of Astronomy and Astrophysics of Academia Sinica in Taiwan (ASIAA). She investigates the properties of interstellar dust with every tool available. During her PhD at SRON and Leiden Observatory in the Netherlands, she worked on X-ray spectroscopy of interstellar dust and continues this line of research in Taiwan. Beside X-ray spectroscopy she also specializes in infrared spectroscopy and will use the upcoming James Webb Space Telescope to explore dust in the nearby diffuse ISM.

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Dr. Elisa Costantini (above) is a senior research scientist at SRON, Netherlands Institute for Space Research. She is interested in experimental and observational studies of interstellar dust as seen in the X-rays.

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The C_{60}:C_{60}^+ ratio in diffuse and translucent interstellar clouds

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Context. Insight into the conditions that drive the physics and chemistry in interstellar clouds is gained from determining the abundance and charge state of their components.

Aims. We propose an evaluation of the C_{60}:C_{60}^+ ratio in diffuse and translucent interstellar clouds that exploits electronic absorption bands so as not to rely on ambiguous IR emission measurements.

Methods. The ratio is determined by analyzing archival spectra and literature data. Information on the cation population is obtained from published characteristics of the main diffuse interstellar bands attributed to C_{60}^+ and absorption cross sections already reported for the vibronic bands of the cation. The population of neutral molecules is described in terms of upper limits because the relevant vibronic bands of C_{60} are not brought out by observations. We revise the oscillator strengths reported for C_{60} and measure the spectrum of the molecule isolated in Ne ice to complete them.

Results. We scale down the oscillator strengths for absorption bands of C_{60} and find an upper limit of approximately 1.3 for the C_{60}:C_{60}^+ ratio.

Conclusions. We conclude that the fraction of neutral molecules in the buckminsterfullerene population of diffuse and translucent interstellar clouds may be notable despite the non-detection of the expected vibronic bands. More certainty will require improved laboratory data and observations.

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Dark cloud-type chemistry in PDRs with moderate UV field

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We present a study of emission lines of small hydrocarbons C_2H and c-C_3H_2, and COMs precursors H_2CO and CH_3OH in order to better understand the possible chemical link between the molecular abundances and UV radiation field in photodissociation regions (PDRs). We study two PDRs around extended and compact H II regions with $G \leq 50$ Habings in the S235 star-forming complex. We find the highest abundances of both hydrocarbons on the edges of molecular clumps, while c-C_3H_2 is also abundant in the low-density expanding PDR around compact H II region S235 A. We see the highest methanol column density towards the positions with the UV field $G \approx 20$–30 Habings and explain them by reactive desorption from the dust grains. The N_{C_2H}/N_{CH_3OH} ratio is lower by a factor of few or the order of magnitude in comparison with the Horsehead and Orion Bar PDRs. The ratio is similar to the value observed in hot corinos in the Perseus cloud. We conclude that ion-molecular and grain surface chemical routes rule the molecular abundances in the PDRs, and the PDRs inherit molecular abundances from the previous dark stage of molecular cloud evolution in spite of massive stars already emitting in optics.

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MNRAS, **507**:3810 (2021)

https://doi.org/10.1093/mnras/stab2361
https://arxiv.org/abs/2108.05387

Discovery of benzyne, c-C_6H_4, in TMC-1 with the QUIJOTE line survey

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We report the detection for the first time in space, in the direction of TMC-1, of a new non-functionalized hydrocarbon cycle: c-C_6H_4 (ortho-benzyne). We derive a column density for this hydrocarbon cycle of $(5.0\pm1.0)\times10^{11}$ cm^{-2}. The abundance of this species is around 30 times lower than that of the cycles cyclopentadiene and indene (Cernicharo et al. 2021, A&A, 647, L2). We compare the abundance of benzyne with that of other pure hydrocarbons, cycles or chains, and find that it could be formed from neutral-radical reactions such as C_2H + CH_2CHCCH and C + C_5H_5, and possibly through C_4H + C_2H_4, C_3H + CH_2CCH_2, and C_3H_2 + C_3H_3. Hence, the rich content of hydrocarbon cycles observed in TMC-1 could arise through a bottom-up scenario involving reactions of a few radicals with the abundant hydrocarbons recently revealed by the QUIJOTE line survey.

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https://arxiv.org/pdf/2108.02308.pdf

Fundamental Vibrational Frequencies and Spectroscopic Constants of Substituted Cyclopropenylidene (c-C_3HX, X = F, Cl, CN)

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The recent detection of ethynyl-functionalized cyclopropenylidene (c-C_3HC_2H) has initiated the search for other functional forms of cyclopropenylidene (c-C_3H_2) in space. There is existing gas-phase rotational spectroscopic data for cyano-cyclopropenylidene (c-C_3HCN), but the present work provides the first anharmonic vibrational spectral data for that molecule, as well as the first full set of both rotational and vibrational spectroscopic data for fluoro- and chloro-cyclopropenylidene (c-C_3HF and c-C_3HCl). All three molecules have fundamental vibrational frequencies with substantial infrared intensities. Namely, c-C_3HCN has a moderately intense fundamental frequency at 1244.4 cm^{-1}, while c-C_3HF has two large intensity modes at 1765.4 and 1125.3 cm^{-1}, and c-C_3HCl again has two large intensity modes at 1692.0 and 1062.5 cm^{-1}. All of these frequencies are well within the spectral range covered by the high-resolution EXES instrument on NASA's *Stratospheric Observatory for Infrared Astronomy* (SOFIA). Further, all three molecules have dipole moments of around 3.0 D in line with c-C_3H_2, enabling them to be observed by pure rotational spectroscopy, as well. Thus, the rovibrational spectral data presented herein should assist with future laboratory studies of functionalized cyclopropenylidenes and may lead to their interstellar or circumstellar detection.

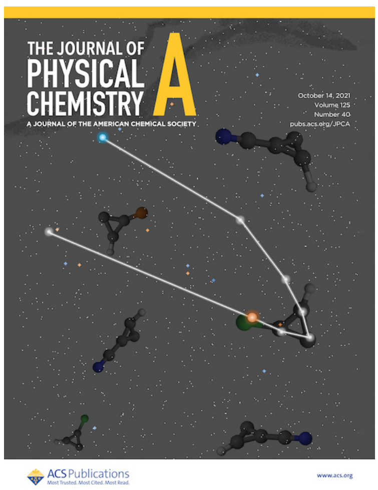

Figure 5 *– Cover art*

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https://pubs.acs.org/doi/10.1021/acs.jpca.1c06576

Understanding dehydrogenation sequence in fluorene$^+$ by multiphoton ionisation-excitation processes

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The dehydrogenation sequence in fluorene$^+$ up to a loss of 3 hydrogen (H) atoms, is explored using a kinetic energy (KE) correlated time of flight mass spectrometer (ToFMS). Four dehydrogenation reactions are identified for the internal energy ranging between 8.5 and 9.0 eV. A dichotomy is observed in fluorene$^+$ in the H-loss channel processed within the studied internal energy. This is explained with the help of a hydrogen migration process leading to post-ionisation isomerization, which is explored using DFT calculations. Presence of two modes of molecular hydrogen (H_2) loss is also noted in the dehydrogenation sequence, including observation of direct elimination of H_2 from fluorene$^+$.

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The vibrational properties of benzene on an ordered water ice surface

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We present a hybrid CCSD(T)+PBE-D3 approach to calculating the vibrational signatures for gas phase benzene and benzene adsorbed on an ordered water-ice surface. We compare the results of our method against experimentally recorded spectra and calculations performed using PBE-D3-only approaches (harmonic and anharmonic). Calculations use a proton ordered XIh water-ice surface consisting of 288 water molecules, and results are compared against experimental spectra recorded for an ASW ice surface. We show the importance of including a water ice surface into spectroscopic calculations, owing to the resulting differences in vibrational modes, frequencies and intensities of transitions seen in the IR spectrum. The overall intensity pattern shifts from a dominating ν_{11} band in the gas-phase to several high-intensity carriers for an IR spectrum of adsorbed benzene. When used for adsorbed benzene, the hybrid approach presented here achieves an RMSD for IR active modes of 21 cm^{-1}, compared to 72 cm^{-1} and 49 cm^{-1} for the anharmonic and harmonic PBE-D3 approaches, respectively. Our hybrid model for gaseous benzene also achieves the best results when compared to experiment, with an RMSD for IR active modes of 24 cm^{-1}, compared to 55 cm^{-1} and 31 cm^{-1} for the anharmonic and harmonic PBE-D3 approaches, respectively. To facilitate assignment, we generate and provide a correspondence graph between the normal modes of the gaseous and adsorbed benzene molecules. Finally, we calculate the frequency shifts, $\Delta\nu$, of adsorbed benzene relative to its gas phase to highlight the effects of surface interactions on vibrational bands and evaluate the suitability of our chosen dispersion-corrected density functional theory.

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Evolved Stars and their Circumstellar Environments

Online
14–17 December, 2021

https://sofia-science-series.constantcontactsites.com/

The upcoming online workshop ‘Evolved Stars and their Circumstellar Environments’, happening on December 14–17, will be an exciting platform for discussions about the current main questions in the field of evolved stars, and the next observational opportunities. The event will explore how theoretical and observational studies of evolved stellar objects can contribute to the understanding of a critical part of stellar evolution. It will feature discussions on synergies between infrared observations and other techniques, and how laboratory work can contribute to the advancement of the field. Invited talks by J. Cernicharo, C. Kemper, H. Linnartz, G. Sloan, M. Lugaro and L. Ziurys are confirmed. We encourage community members to submit an abstract for a contributed talk (submission deadline is November 22nd). There is no registration deadline or fee, and we strongly support participation from all interested scientists, in particular early-career.

Addressed topics will include:

- Gas chemistry in different regions of stellar objects / different star types
- Connection to the ISM
- Elemental enrichment
- Dust formation theory
- Dust observations: chemical composition and polarimetric properties
- Temporal evolution

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Announcements

Two Postdoctoral Contracts at the Instituto de Astrofisica de Canarias (IAC)

Advertised by Domingo Aníbal García Hernández

The IAC (Tenerife) announces TWO postdoctoral contracts to work on topics within the projects NanoFull (PROID2020010051) financed by the ACIISI with funds from the Operational Program FEDER Canarias and COSJWST (PID2020-115758GB-I00) financed by MICINN, led by Dr. Domingo Aníbal García-Hernández.

Research topics at the IAC include most areas of astrophysics: Solar Physics (FS), Exoplanetary System and Solar System (SEYSS), Stellar and Interstellar Physics (FEEI), The Milky Way and The Local Group (MWLG), Formation and Evolution of Galaxies (FYEG), and Cosmology and Astroparticles (CYA-CTA). All of these are supported by an ambitious instrumentation programme. In 2020, the IAC was granted by the Spanish Government the status of Severo Ochoa Center of Excellence, a prestigious recognition awarded for the third time to the IAC as a leading research institute in Spain. Further information about the IAC's research programme, its Observatories and the 10.4m GTC is available at the IAC's web page: https://www.iac.es/.

Postdoc 1: "Multi-wavelength astronomical observations of complex organic species"

Tasks: The successful candidate will pursue research in one or more of the following fields:

- Analysis of multi-wavelength spectroscopic observations (from the UV to the far-IR) of fullerene-rich circumstellar envelopes.
- Comparison of laboratory and/or theoretical spectra with astronomical observations.
- Scientific exploitation of the data provided by the James Webb telescope and preparation for data collection in cycle 2.
- Preparation for obtaining (and subsequent analysis) of additional data on circumstellar envelopes in the IR and radio wavelength ranges.

Particular attention will be given to applicants with experience in the field of multi-wavelength spectroscopic data (from the UV to the far-IR) with space telescopes.

Complete information about this postdoc position can be found here: https://www.iac.es/en/employment/one-postdoctoral-contract-nanofull-cosjwst-2021-ps-2021-081

Postdoc 2: "Quantum chemistry simulations of complex organic species"

Tasks: The successful candidate will pursue research in the following fields:

- Computational quantum-chemical simulations of complex organic species (fullerene and graphene compounds as well as large aromatic/aliphatic species).
- Identification of the nature of the vibrational modes seen in the laboratory/astronomical data.
- Exploration of the footprints of fullerene/graphene derivatives and larger molecules in the radio wavelength range.

Particular attention will be given to applicants with experience and good knowledge in the fields of quantum mechanics and chemistry, group theory and spectroscopy, and electronic structure theory (especially when applied to fullerene/graphene derivatives and/or other large organic species).

Complete information about this postdoc position can be found here: https://www.iac.es/en/employment/one-postdoctoral-contract-cosjwst-quimica-cuantica-2021-ps-2021-080

Deadline: November 15, 2021

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Webpage: https://www.iac.es/index.php/en/employment

AstroPAH Newsletter

http://astropah-news.strw.leidenuniv.nl Next issue: 18 November 2021

astropah@strw.leidenuniv.nl Submission deadline: 5 November 2021