AstroChemical Newsletter #109

January 2025

You can access the full abstracts by clicking the paper titles. Submit your abstracts before the 25th of each month for inclusion in the following newsletter.

Abstracts

Ice inventory towards the protostar Ced 110 IRS4 observed with the James Webb Space Telescope. Results from the ERS Ice Age program

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This work focuses on the ice features toward the binary protostellar system Ced 110 IRS 4A and 4B, and observed with JWST as part of the Early Release Science Ice Age collaboration. We aim to explore the JWST observations of the binary protostellar system Ced 110 IRS4A and IRS4B to unveil and quantify the ice inventories toward these sources. We compare the ice abundances with those found for the same molecular cloud. The analysis is performed by fitting or comparing laboratory infrared spectra of ices to the observations. Spectral fits are carried out with the ENIIGMA fitting tool that searches for the best fit. For Ced 110 IRS4B, we detected the major ice species H2O, CO, CO2 and NH3. All species are found in a mixture except for CO and CO2, which have both mixed and pure ice components. In the case of Ced 110 IRS4A, we detected the same major species as in Ced 110 IRS4B, as well as the following minor species CH4, SO2, CH3OH, OCN−, NH+4 and HCOOH. Tentative detection of N2O ice (7.75 microns), forsterite dust (11.2 microns) and CH+3 gas emission (7.18 microns) in the primary source are also presented. Compared with the two lines of sight toward background stars in the Chameleon I molecular cloud, the protostar has similar ice abundances, except in the case of the ions that are higher in IRS4A. The clearest differences are the absence of the 7.2 and 7.4 microns absorption features due to HCOO− and icy complex organic molecules in IRS4A and evidence of thermal processing in both IRS4A and IRS4B as probed by the CO2 ice features. We conclude that the binary protostellar system Ced 110 IRS4A and IRS4B has a large inventory of icy species. The similar ice abundances in comparison to the starless regions in the same molecular cloud suggest that the chemical conditions of the protostar were set at earlier stages in the molecular cloud.

A&A, Accepted for publication
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N-Carbazolyl π-Radical and Its Antiaromatic Nitrenium Ion: A Threshold Photoelectron Spectroscopic Study

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Understanding the structure and properties of heterocyclic radicals and their cations is crucial for elucidating reaction mechanisms as they serve as versatile synthetic intermediates. In this work, the N-carbazolyl radical 1 was generated via pyrolysis and characterized using photoion mass-selected threshold photoelectron spectroscopy coupled with tunable vacuum-ultraviolet synchrotron radiation. The N-centered radical 1 is classified as a π-radical (2B1), with the unpaired electron found to be delocalized over the central five-membered ring of the carbazole. Adiabatic ionization energies corresponding to the transition from radical 1 to its singlet 1+(1A1) and triplet 1+(3B2) cations were determined to be 7.70 ± 0.03 and 8.14 ± 0.03 eV, respectively. The antiaromatic nitrenium ion 1+ exhibits a singlet ground state with an experimental singlet–triplet energy gap (ΔES–T) of −0.44 eV (10.1 kcal/mol), in very good agreement with theory. N-centered radicals are found to have a higher ionization energy than their C-centered analogues due to stabilization of the singly occupied molecular orbital.

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JWST Observations of Young protoStars (JOYS). Overview of gaseous molecular emission and absorption in low-mass protostars

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The MIRI-MRS instrument onboard JWST allows for probing the molecular gas composition at mid-IR wavelengths at unprecedented resolution and sensitivity. It is important to study these features in low-mass embedded protostellar systems since the formation of planets is thought to start in this phase. We present JWST/MIRI-MRS data of 18 low-mass protostellar

systems in the JOYS program, focusing on gas-phase molecular lines in spectra extracted from the central protostellar positions. Besides H2, the most commonly detected molecules are H2O, CO2, CO, and OH. Other molecules such as 13CO2, C2H2, 13CCH, HCN, C4H2, CH4, and SO2 are detected only toward at most three of the sources. The JOYS data also yield the surprising detection of SiO gas toward two sources (BHR71-IRS1, L1448-mm) and for the first time CS and NH3 at mid-IR wavelengths toward a low-mass protostar (B1-c). The temperatures derived for the majority of the molecules are 100-300 K, much lower than what is typically derived toward more evolved Class II sources (>500 K). Toward three sources (e.g., TMC1-W), hot (~1000 K) H2O is detected, indicative of the presence of hot molecular gas in the embedded disks, but such warm emission from other molecules is absent. The agreement in abundance ratios with respect to H2O between ice and gas point toward ice sublimation in a hot core for a few sources (e.g., B1-c) whereas their disagreement and velocity offsets hint at high-temperature (shocked) conditions toward other sources (e.g., L1448-mm, BHR71-IRS1). The typical temperatures of the gas-phase molecules of 100-300 K are consistent with both ice sublimation in hot cores as well as high-temperature gas phase chemistry. Molecular features originating from the inner embedded disks are not commonly detected, likely because they are too extincted even at mid-IR wavelengths by small not-settled dust grains in upper layers of the disk.

2024, A&A 692, A197
DOI: 10.1051/0004-6361/202451967
Full-text URL: https://arxiv.org/abs/2410.01636

A sensitivity analysis of the modeling of Polycyclic Aromatic Hydrocarbon emission in galaxies

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We have conducted a sensitivity analysis on the mid-infrared spectral decomposition of galaxies and the modeling of the PAH emission spectrum with the NASA Ames PAH Infrared Spectroscopic Database (PAHdb) to assess the variance on the average galaxy PAH population properties under a grid of different modeling parameters. We find that the SL and SL+LL Spitzer-IRS decomposition with PAHFIT provides consistent modeling and recovery of the 5-15 μm PAH emission spectrum. For PAHdb modeling, application of a redshift to the calculated spectra to account for anharmonic effects introduces a 15%-20% variance on the derived parameters, while its absence improves the fits by ∼13%. The 4.00-α release of PAHdb achieves the complete modeling of the 6-15 μm PAH spectrum, including the full 6.2 μm band, improving the average fitting uncertainty by a factor of 2. The optimal PAHdb modeling configuration requires selection of pure PAHs without applying a redshift to the bands. Although quantitatively the PAHdb-derived parameters change under different modeling configurations or database versions, their variation follows a linear scaling, with previously reported trends remaining qualitatively valid. PAHdb modeling of JWST observations, and JWST observations smoothed and resampled to the Spitzer-IRS resolution and dispersion have consistent PAHdb derived parameters. Decomposition with different codes, such as PAHFIT and CAFE, produce PAH emission spectra with noticeable variation in the 11-15 μm region, driving a ∼7% difference in the neutral PAH fraction under PAHdb modeling. A new library of galaxy PAH emission templates is delivered to be utilized in galaxy SED modeling.

The Astrophysical Journal, in press.
Full-text URL: https://arxiv.org/abs/2412.01875

Nanosilicates and molecular silicate dust species: properties and observational prospects

Stefan T. Bromley

Silicate dust is found in a wide range of astrophysical environments. Nucleation and growth of silicate dust grains in circumstellar environments likely involves species with diameters ranging from <1 nm (molecular silicates) to a few nanometers (nanosilicates). When fully formed silicate grains with sizes ∼0.1 μm enter the interstellar medium, supernovae shockwaves cause collision-induced shattering which is predicted to redistribute a significant proportion of the silicate dust mass into a huge number of nanosilicates. This presumed population has thus far not been unambiguously confirmed by observation but is one of the main candidates for causing the anomalous microwave emission. By virtue of their extreme small size, nanosilicates and molecular silicates could exhibit significantly different properties to larger silicate grains, which could be of astrochemical and astrophysical importance. Herein, we briefly review the properties of these ultrasmall silicate dust species with a focus on insights arising from bottom-up atomistic computational modelling. Finally, we highlight how such modelling also has the unique potential to predict observationally verifiable spectral features of nanosilicates that may be detectable using the James Webb Space Telescope.

Front. Astron. Space Sci. 11:1523977, 2024.
DOI: 10.3389/fspas.2024.1523977
Full-text URL: https://www.frontiersin.org/journals/astronomy-and-space-sciences/articles/10.3389/fspas.2024.1523977/full

Accurate sticking coefficient calculation for carbonaceous dust growth through accretion and desorption in astrophysical environments

D. Bossion, A. Sarangi, S. Aalto, C. Esmerian, S. R. Hashemi, K. K. Knudsen, W. Vlemmings, G. Nyman

Context. Cosmic dust is ubiquitous in astrophysical environments, where it significantly influences the chemistry and the spectra. Dust grains are likely to grow through the accretion of atoms and molecules from the gas-phase onto them. Despite their importance, only a few studies have computed the sticking coefficients for relevant temperatures and species, along with their direct impact on grain growth. Overall, the formation of dust and its growth are not well understood. Aims. This

study is aimed at calculating the sticking coefficients, binding energies, and grain growth rates over a broad range of temperatures, for various gas species interacting with carbonaceous dust grains. Methods. We performed molecular dynamics simulations with a reactive force field algorithm to compute accurate sticking coefficients and obtain the binding energies. These results were used to build an astrophysical model of nucleation regions to study dust growth. Results. We present, for the first time, the sticking coefficients of H, H2, C, O, and CO on amorphous carbon structures for temperatures ranging from 50 K to 2250 K. In addition, we estimated the binding energies of H, C, and O in carbonaceous dust to calculate the thermal desorption rates. Combining accretion and desorption allows us to determine an effective accretion rate and sublimation temperature for carbonaceous dust. Conclusions. We find that sticking coefficients can differ substantially from what is commonly used in astrophysical models. This offers us new insights into carbonaceous dust grain growth via accretion in dust-forming regions.

2024 A&A, Forthcoming article, accepted: 06 November 2024
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Announcements

Invitation to contribute to EGU GA 2025 PS6.1 – Emergence, chemistry, and evolution of organic matter in the Solar System

The convenor team (Nora Hänni, Niels Ligterink, Kelly Miller, Fabian Klenner, Cécile Engrand) of EGU's session PS6.1 entitled 'Emergence, chemistry, and evolution of organic matter in the Solar System' is inviting your contribution. The EGU General Assembly 2025 will take place in Vienna (Austria) in a hybrid format 27 April – 2 May 2025 and we are aiming to enrich the meeting with a platform for the Solar System organics community.
The scope of our session is the following: We want to bring together scientists with backgrounds in laboratory experimentation, chemical modelling, space exploration, instrumentation, theoretical chemistry, and observations in order to share knowledge and progress our understanding of the evolution of organic chemistry in interplanetary / interstellar dust particles, meteorites, comets, asteroids, KBOs, icy moons, terrestrial planets, and planetary atmospheres and ask how future space exploration missions such as OSIRIS-REx, Hayabusa2, Europa Clipper, JUICE, Dragonfly, and Martian Moons Explorer (MMX) can push the boundaries of our current knowledge.
Key questions of our session are: How did organics in all those environments form? Was this chemical complexity inherited, did it emerge in the Solar System, or a combination of both? What do these molecules tell us about the physical conditions and formational history of planetary bodies and other objects in the Solar System? Is there a link between this organic matter and the emergence of life?
If you are interested in contributing and sharing your research in this session, you can find a more detailed session description here, where you also can submit your abstract to PS6.1:
https://meetingorganizer.copernicus.org/EGU25/session/52089
EGU rules and regulations for abstract submission are compiled here:
https://www.egu25.eu/programme/how_to_submit.html

Abstracts are due Wednesday, 15 January 2025, 13:00 CET.

Postdoctoral Position in Laboratory Astrophysics at Sorbonne Université, MONARIS (Paris, France) : studies of the restructuration of ice analogs under Infrared irradiation.

A postdoctoral fellowship, funded by Emergence CNRS Chimie, is available for a duration of 18 months at Sorbonne Université, MONARIS (de la Molécule aux Nano-Objets: Réactivité, Interactions et Spectroscopies), in Paris, France. The position will take place in the CIRS group (Caracterisations, Interactions and Reactivities : Molecular Spectroscopy), specialized in chemical physics applied to laboratory astrophysics or atmospheric sciences. The fellowship is expected to begin before May 2025.
The project aims to characterize the interactions between low-energy photons and analogs of interstellar ices. Infrared excitations can induce a reorganization of the ice and a desorption of molecules from the ice's surface (infrared photodesorption). In this project, we will study experimentally both the effects of infrared irradiation on the restructuring of ices and molecular desorption, focusing on water ice, a key system in astrophysics. The ultimate goal is to unravel the parameters governing the ice restructuration, and to understand how the injected energy is redistributed within the ice. The results will provide valuable insights for the interpretation of JWST observations and thereby enrich our knowledge of the physical-chemistry of ices.
The postdoctoral fellow will be based at Sorbonne Université, MONARIS (Paris). To perform resonant IR irradiation experiments, the ultra-high vacuum instrument COSPINU2 will be coupled with a tunable IR powerful continuous laser. Ice modifications will be probed with optical diagnostics, high resolution FTIR spectroscopy and mass spectrometry. All the equipments needed to start the project are already available.
The candidate must hold a PhD in Physical Chemistry, Chemistry or Physics, with a maximum of 5-6 years of experience after the PhD.
The ideal candidate must possess a strong background in laboratory astrophysics or a related domain, in molecular physics, spectroscopy, lasers, mass spectrometry. They must speak English fluently and have good communication skills.

Applications should include:
- a cover letter,

- a CV,
- a list of publications,
- Contact information of two potential reference letter writers

Applications should be sent via email to:
Géraldine Féraud : geraldine.feraud@sorbonne-universite.fr
Xavier Michaut : xavier.michaut@sorbonne-universite.fr

Interviews will be conducted until the position is filled. The expected starting date is before May 2025.

42nd URSI sponsored Egyptian National Radio Science Conference

The 42nd URSI sponsored Egyptian National Radio Science Conference #NRSC2025 will be held 6-8 May 2025.

The submitted papers must describe original work and lie in the scope of one of URSI Commissions A-K.
A - Electromagnetic Metrology
B - Fields and Waves
C - Radio Communication Systems and Signal Processing
D - Electronics and Photonics
E - Electromagnetic Environment and Interference
F - Wave Propagation and Remote Sensing
G - Ionospheric Radio and Propagation
H - Waves in Plasmas
J - Radio Astronomy
K - Electromagnetic in Biology and Medicine

Deadline for submission January 11th, 2025
https://nrsc2025.aast.edu