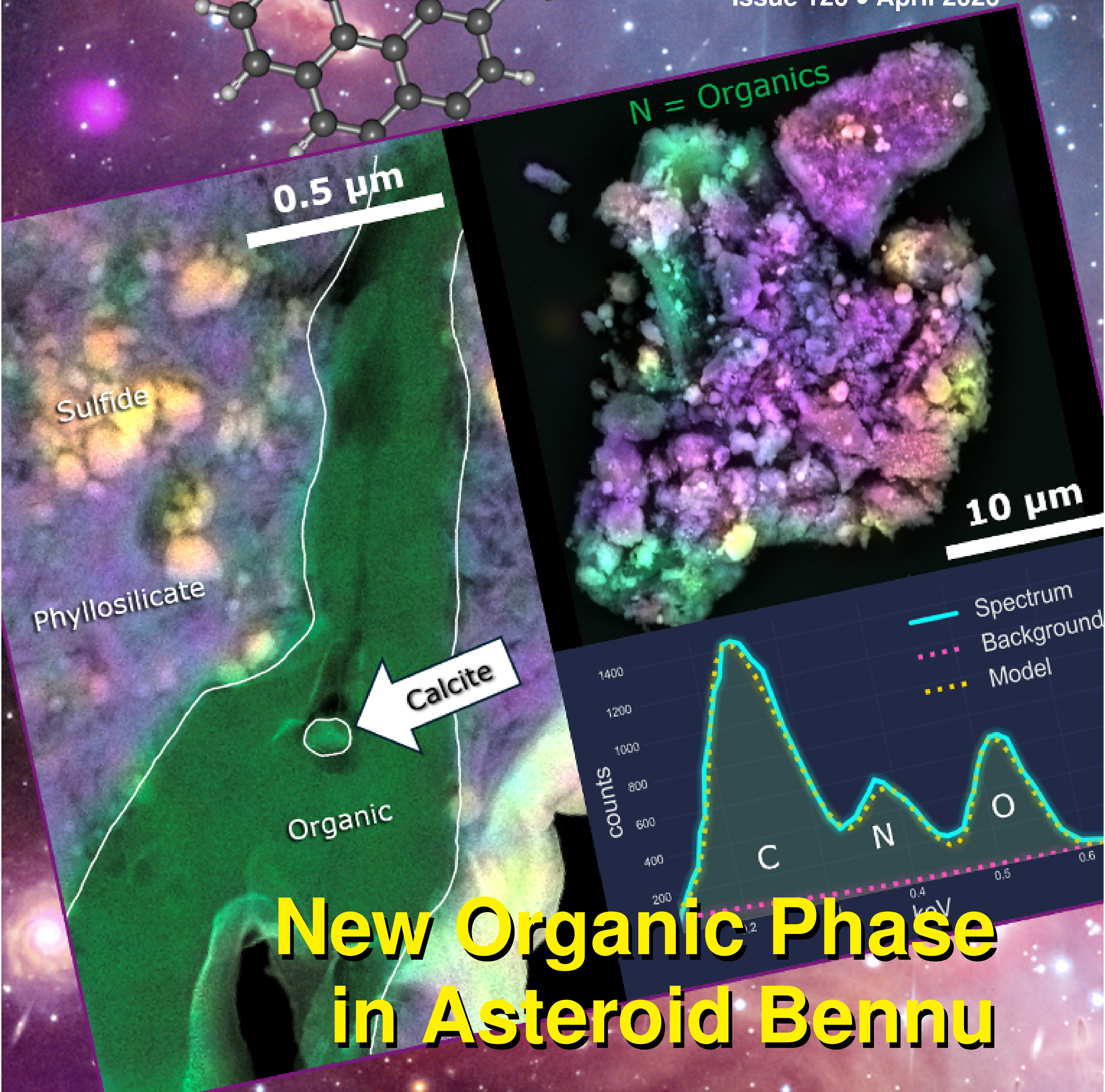
AstroPAH

A Newsletter on Astronomical PAHs

Issue 126 • April 2026



New Organic Phase in Asteroid Bennu

Editorial

Dear Colleagues,

In this 126th volume of AstroPAH, the Picture of the Month and In Focus are dedicated to the discovery of a new organic phase in samples from asteroid Bennu collected by NASA's mission *OSIRIS-REx*. In the In Focus, Scott Sanford (NASA, USA), Zack Gainsforth (Berkeley, USA) and Michel Nuevo (NASA, USA) discuss this new phase, which consists of a polymer-like material rich in nitrogen and oxygen.

This issue's *Abstracts* section features two new perspectives on the bottom-up formation of the PAH precursors phenol and pyrrole. A study on the impact ionization of polypyrrole looks at potential top-down PAH destruction products, with additional insight into polypyrrole's impact on mass spectra as a common coating in dust acceleration studies. In the theme of PANHs, new UV-Vis spectral data has been computed for PANHs derived from anthracene and phenanthrene. Observational work featured in this issue reveals the source of unusually strong CO emission in some galaxies relative to the intensity of coupled PAH features. A nondetection for the 1.05 µm band tied to PAH cations is also reported. Finally, a new recurrent fluorescence model shows the potential for the contribution of "forbidden" electronic transitions to the radiative cooling of PAH cations, with promising applicability to more PAH-related species.

A PhD position to study the photochemistry of icy clouds in Neptune's atmosphere is open at CIMAP/GANIL to work with David Dubois (our dear former editor!) and Alicja Domaracka.

AstroPAH can help you promote your research. Please send your contributions to our email address.

Thank you all for your contributions!

The Editorial Team

Next issue: 21 May 2026.
Submission deadline: 8 May 2026.

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PAH Picture of the Month

A new organic phase has been discovered in samples from asteroid Bennu collected by NASA's *OSIRIS-REx*. This phase consists of a polymer-like material rich in nitrogen and oxygen. Details of this discovery can be found in Sandford & Gainsforth et al. (2025) and are introduced in this month's In Focus section!

Credits: Zack Gainsforth for the electron microscopy image of a Bennu particle FIB section (Left), the SEM backscatter + EDS view of the larger particle before FIB (Top Right), and the EDS spectrum of the CNO peaks of the organic phase (Bottom Right).

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In Focus

Synopsis of

“Nitrogen- and Oxygen-Rich Organic Material Indicative of Polymerization in Pre-Aqueous Cryochemistry on Bennu’s Parent Body”

(Nature Astronomy, 2025, https://doi.org/10.1038/s41550-025-02694-5)

by Scott A. Sandford[1], Zack Gainsforth[2], and Michel Nuevo[1]

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Abstract

This article provides a condensed synopsis of the information that appeared in Sandford & Gainsforth et al. (2025) and its associated Supporting Online Materials. In this work, it was shown that pristine samples returned from asteroid Bennu by NASA’s *Origins, Spectral Interpretation, Resource Identification, and Security–Regolith Explorer* (*OSIRIS-REx*) mission contain polymeric organics that are exceptionally rich in nitrogen and oxygen. These polymers are seen in multilayered organic sheets and contain a variety of functional groups including amines, amides, N-heterocycles, as well as aliphatic and aromatic hydrocarbons, among others. Their morphology and composition indicate formation from cryogenic, pre-aqueous N-rich precursors, and later modification during aqueous alteration.

Background

NASA’s *OSIRIS-REx* spacecraft returned 121.6 g of pristine regolith from the C-rich asteroid (101955) Bennu to Earth (Lauretta & Connolly Jr. et al. 2024). Analyses of the returned samples have confirmed that they have been extensively altered by interactions with aqueous fluids and are similar to the Ivuna-type (CI) carbonaceous chondrites (Connolly Jr. & Lauretta et al. 2025), with a bulk C/N ratio of 20. Ammonia (NH_3) and N-rich organic compounds including amines, amino acids, and N-heterocycles were found in the Bennu soluble organic fraction (Glavin & Dworkin et al. 2025).

During an effort to obtain infrared (IR) spectra of individual 5–50-µm grains from the Bennu samples, we discovered a category of materials whose spectra contained a strong N–H stretching absorption band together with a family of other absorption features associated with multiple organic functional groups (see below).

Using multiple analytical techniques, namely Fourier-transform infrared (FTIR) spectroscopy, scanning transmission X-ray microscopy (STXM), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and secondary ionization mass spectroscopy (SIMS), we were able to characterize this remarkable carbonaceous material and demonstrate that it consists of a polymeric organic materials with exceptionally high O/C and N/C ratios, as described in detail in Sandford & Gainsforth et al. (2025) and its supporting online material.

Results

Infrared Spectroscopy

The IR spectra of most powdered Bennu particles are dominated by phyllosilicate-carbonate mixtures. Many particles contain traces of organics, as evidenced by weak C–H stretching bands in the 3000–2820 cm^{-1} range. The dominant C–H stretching modes are from aliphatic functional groups, although weak aromatic C–H stretching features around 3065 cm^{-1} are occasionally seen. The aliphatic features show the presence of $–CH_3$ and $–CH_2–$ groups, with $–CH_2–$ groups dominating.

N-rich organic polymer-containing particles (like Particles 2, 26, and 33 in **Figure 1**) show atypical spectra that exhibit a strong N–H absorption band (3285 cm^{-1}), strong aromatic and aliphatic C–H stretching bands, as well as absorption features associated with modes involving C=O stretching in amides ($R(C{=}O)NH_xR$), N–H bending, CH_2 and CH_3 bending, C–N stretching, and C–O stretching in aromatic ethers and carbonates (**Figure 1**). A weak band present near 2145 cm^{-1} in the spectra of Particles 2 and 33 may be due to the CN stretching in S–C≡N, O–C≡N, or N=C=N. A band near 1740 cm^{-1} in Particle 26 may be esters or lactones. A band around 1575 cm^{-1} in Particles 26 and 33 could be aromatic C=C modes. A 1515 cm^{-1} shoulder on the 1540 cm^{-1} N–H peak is assigned to molecular carbonates.

Peak heights of the bands associated with $–CH_3$ and $–CH_2–$ groups have ratios larger than those typically seen in the spectra of CI and CM meteorites and the diffuse interstellar medium, but that fall in the range measured for interplanetary dust particles (IDPs), CR2 meteorites, and comet Wild 2. Measurements of the areas of the individual aliphatic C–H stretching bands yields $–CH_2–/–CH_3$ group ratios of 3.1, 4.4, and 5.5 for Particle 33, Particle 2, and Particle 26, respectively. The high abundance of $–CH_2–$ groups implies longer, less-branched carbon chains, but may also reflect the presence of terminal functional groups such as NH_2, COOH, OH, or C≡N, which decrease the number of terminal CH_3 groups in carbon chains and result in higher $–CH_2–/–CH_3$ ratios.

Electron Microscopy

A focused ion beam (FIB) was used to place Particles 2 and 33 onto Si substrates and prepare electron-transparent FIB lamella for TEM and STXM analysis (**Figure 2**).

Particle 2 contains a carbonaceous vein sandwiched between phyllosilicates (**Figures 3A** and **3B**) which does not otherwise penetrate the phyllosilicate pores. A calcite crystal

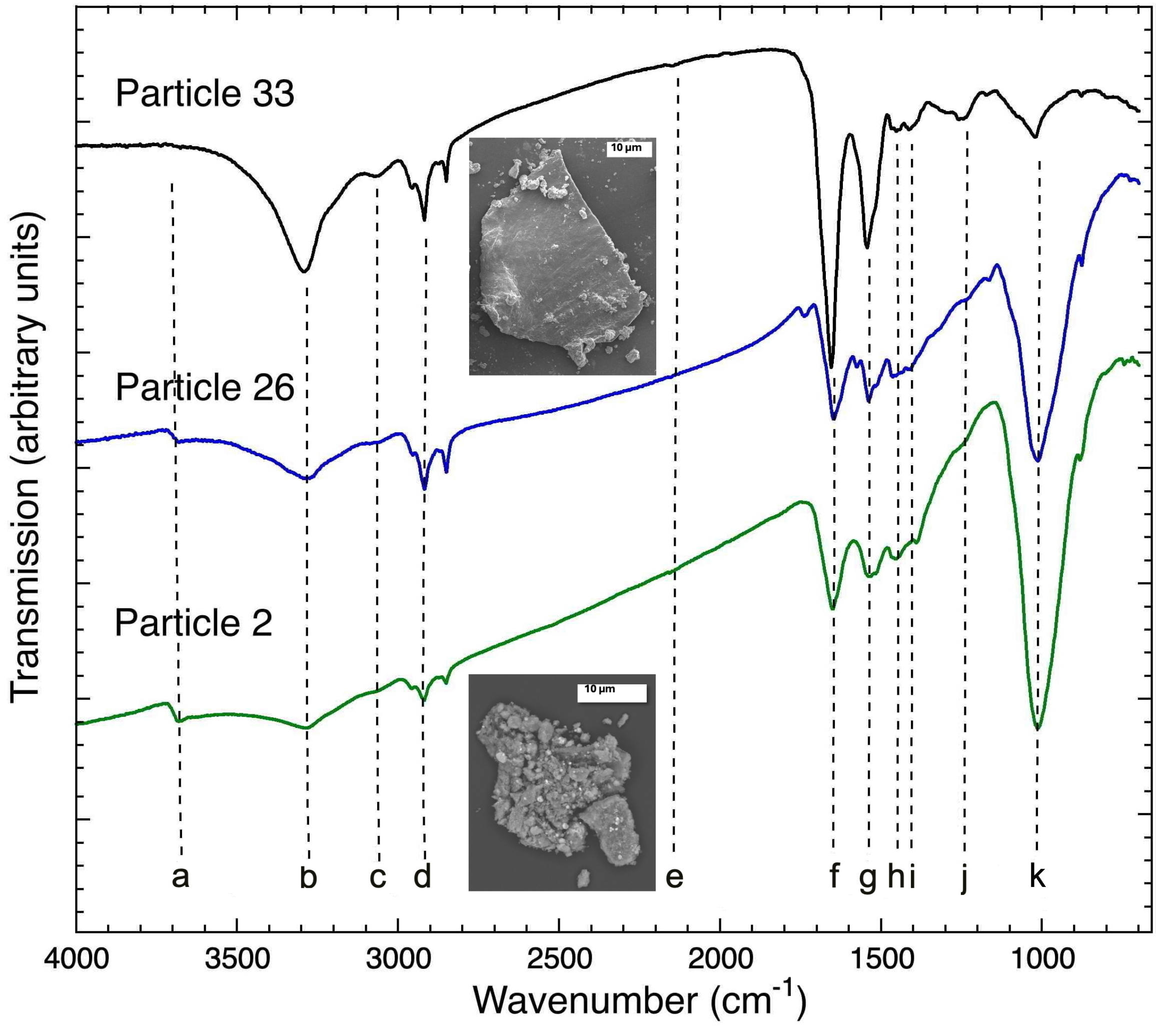

***Figure 1** – **The mid-IR spectra of particles that contain nitrogen-rich organics.** The bottom two spectra are from particles that contained associated phyllosilicate and carbonate minerals. The top spectrum contains very little phyllosilicate material. The labeled vertical dashed lines correspond to specific bands summarized in Table 1 of Sandford & Gainsforth et al. (2025).*

($CaCO_3$) is in the middle of the vein, and vesicles are present. Scanning transmission electron microscopy (STEM)/energy-dispersive spectroscopy (EDS) analysis of the carbon vein in shows a composition of C:N:O = 3:1:1, indicating extraordinary N and O enrichment (**Figure 3C**) compared to insoluble organics in CI and CM meteorites, which typically contain atomic N/C and O/C ratios in the 2.5–3.7% and 10–22% ranges, respectively. Selected area electron diffraction (SAED)(**Figure 3D**) shows that the carbon is amorphous.

In contrast, Particle 33 appears as a separate sheet of carbonaceous material on the diamond window after crushing. Some phyllosilicates were associated with it but were not directly adhering as they were in Particle 2 (**Figure 2**). Optical imaging of Particle 33 exhibits interference fringes, indicating it is transparent in the optical wavelengths. SEM images show features characteristic of plastic deformation. SEM-EDS analysis was performed on one corner of Particle 33 to avoid heavily irradiating the entire object. A 10×10×2 µm region of Particle 33 was sectioned using slice-and-view in the FIB to observe its 3D structure. The reconstructed data show that the film is $\sim$2 µm thick and has at least three CNO layers sandwiching two carbonate inclusion layers (see the original paper for figures and

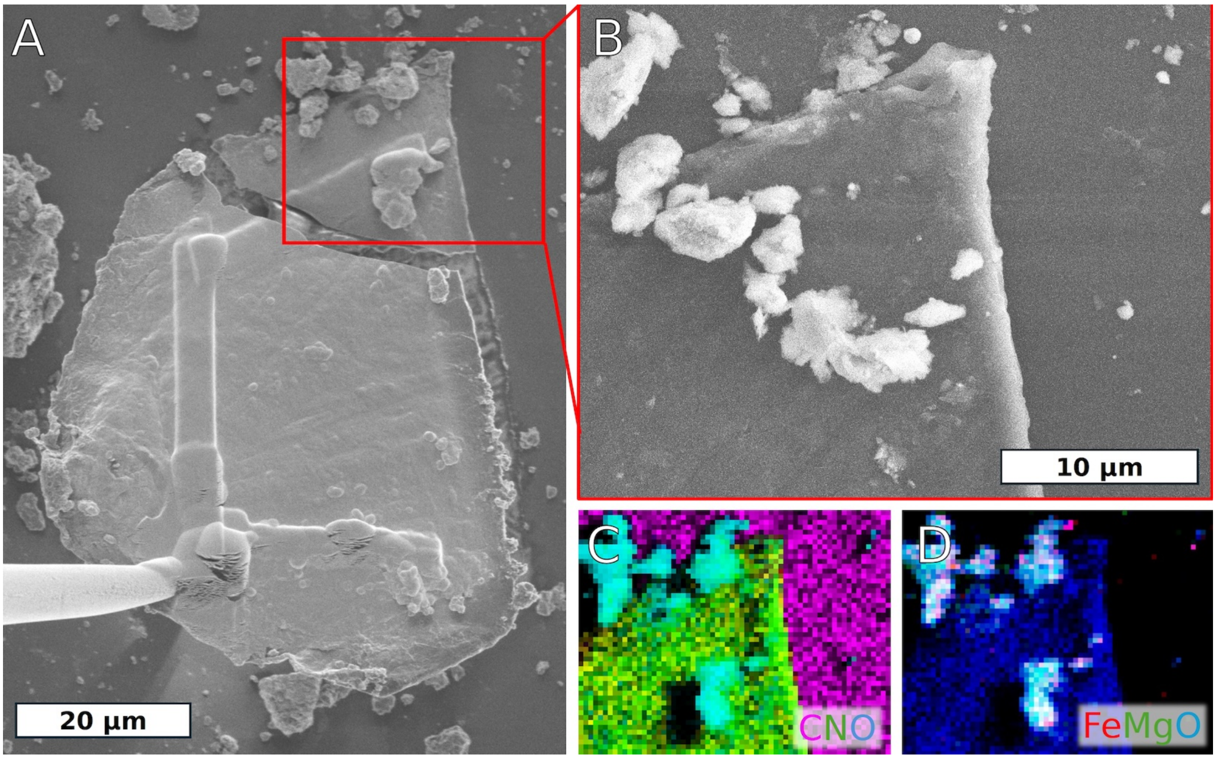

***Figure 2** – **Electron microscopy of Particle 33.** **(A)** Image of Particle 33 immediately after lifting from diamond substrate. The upper right corner measured using SEM/EDS shattered. **(B)** SEM image of the region analyzed by EDS. Some phyllosilicates sitting on the surface mobilized during scanning. **(C)** C-K (red), N-K (green), and O-K (blue) map showing nitrogen is abundant in Particle 33 but not in the phyllosilicates or diamond substrate. **(D)** Fe-L (red), Mg-K (green), O-K (blue) map showing the location of the phyllosilicates (light blue/white), and that Particle 33 contains O, but the diamond substrate does not.*

a supplemental video). The inclusion layers contain varying kinds of crystals; at least one grain is calcite, and Ca enrichment is present throughout the inclusion layer. Particle 33's composition as determined by STEM/EDS is C:N:O = 5:1:1. Electron diffraction shows that Particle 33 is amorphous.

X-ray Spectroscopy, Nitrogen Isotopes, and Water Solubility

STXM analysis of Particles 2 and 33 shows functional groups in the C-K, N-K, and O-K edges that complement the IR analysis (see Table 1 of Sandford & Gainsforth et al. 2025) and show evidence for bonding associated with C=C, CHx, pyridine, amides (R(C=O)NHxR) and aminated heterocycles, C=N, C=O, urea, alcohol, or ether groups, and possible some C≡N. Repeated line scans over the same locations showed a reduced overall intensity of N, and the amide peak disappeared. We ascribe this to beam sensitivity of the N–H bonds in amines and amides.

SIMS nitrogen isotopic measurements of Particle 33 yielded $\delta^{15}N_{air}$ = –28 ± 7 ‰ (2σ). Negative δ^{15}N values are not as commonly seen in extraterrestrial organics as positive δ^{15}N anomalies. Nitrogen in soluble Bennu extracts show positive δ^{15}N values (Glavin & Dworkin et al. 2025). Since the N-rich polymeric organic materials contain negative δ^{15}N, different chemical processes may have been involved in their formation compared to the soluble organics. Various processes have been suggested to produce positive δ^{15}N

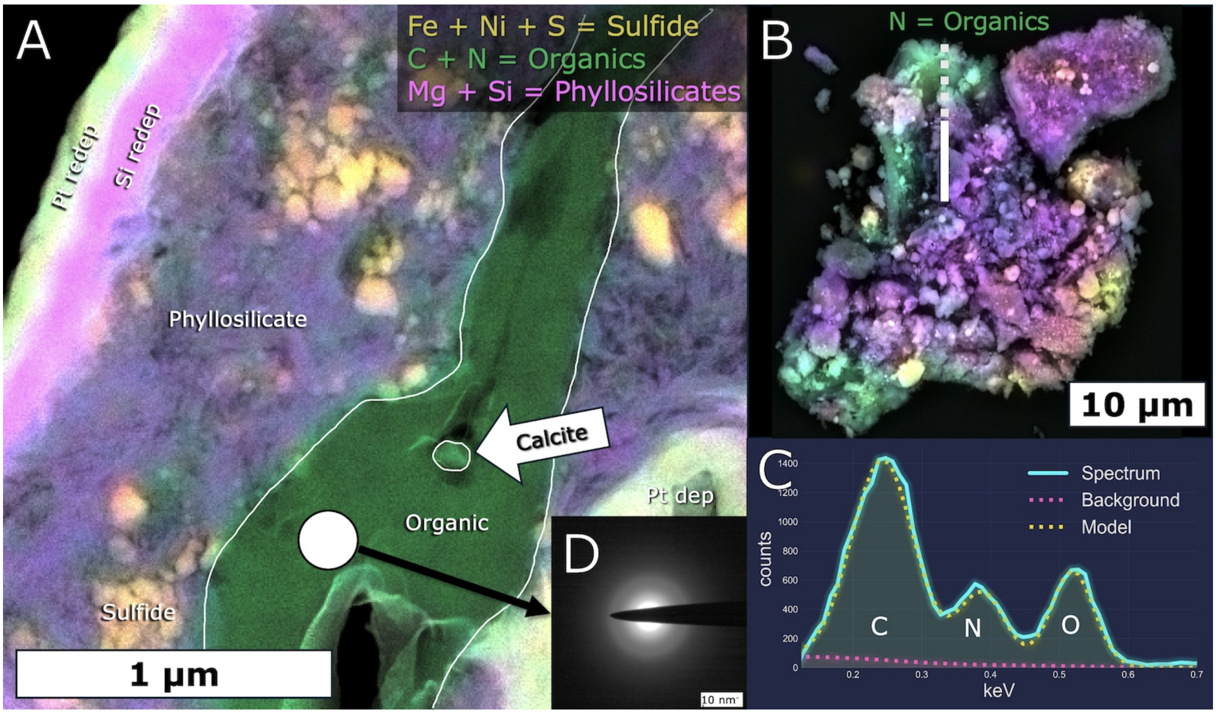

***Figure 3** – **Electron microscopy of Particle 2.** **(A)** STEM high-angle annular dark field (HAADF) + EDS image of a FIB section extracted from Particle 2 showing the nitrogenous vein (green) sandwiched between phyllosilicate regions (purple). The Pt (light green) and Si (pink) deposition ('dep') and redeposition ('redep') layers were created during the FIB processing. The white circle shows the location where SAED acquisition was conducted (see D). **(B)** SEM backscatter + EDS view of Particle 2 before extracting the FIB section. The line shows the location of the FIB liftout; the dashed portion of the line is outside the field of view in A. **(C)** EDS spectrum of the CNO peaks of the organic phase along with the fit used for quantification. **(D)** SAED acquisition showing the nitrogenous vein is amorphous.*

values in extraterrestrial materials, including ion–molecule reactions and aqueous parent-body chemistry involving heavy δ^{15}N precursors. In contrast, the observed negative δ^{15}N in the materials studied here is more consistent with kinetic fractionation chemistry at cryogenic temperatures, which favors light isotopes in the chemical products (Watkins & Antonelli 2021).

To determine whether the N-rich organic is water-soluble, another N-rich organic grain (Particle 64) was placed on an Au-coated Si chip. After it was imaged, it was immersed under a droplet of deionized water from a hypodermic syringe. After the water evaporated, the grain was observed to be unchanged.

Discussion

Organic Formation

Based on the N-rich chemistry reported in Bennu sample soluble organics, components of Bennu's parent body accreted beyond the ammonia ice line (Glavin & Dworkin et al. 2025). Thus, Bennu's original parent body likely accreted ices that contained both H_2O and more volatile species like NH_3 and CO_2. In the earliest stages of the parent body's existence, radioisotope decay produced heat, which caused an increase in temperature.

Under these conditions, NH_3- and CO_2- dominated ices would melt or sublime before H_2O. A mixture of NH_3 and CO_2 with excess NH_3 would have produced ammonium carbamate (NH_4COONH_2) at 75 K (Noble et al. 2014). As the temperature increased above 150 K, the carbamate converted to carbamic acid until H_2O melts, at which point the carbamic acid would decompose into ammonium (NH_4^+) and carbonate (CO_3^{2-}). Carbamate is a known polymerization precursor for amine and amide polymers (Maisonneuve et al. 2015) and may be a key monomer of the observed N-rich organic polymeric material. Indeed, experimental evidence under relevant conditions suggests that the presence of small amounts of H_2O ice can catalyze carbamate formation (Rodríguez-Lazcano et al. 2013). Once H_2O ice melted and any unpolymerized carbamate decomposed, NH_4^+ would have diffused throughout the parent body, and it would have been difficult or impossible to reach the high concentration of N relative to C necessary to produce the observed N-rich organic materials. Therefore, initial polymerization of carbamate to produce Particles 2 and 33 likely occurred at temperatures below the melting of H_2O ice, and any unpolymerized monomer decomposed into NH_4^+ and CO_3^{2-} after H_2O ice melted. These ions could have subsequently participated in the creation of other organics and carbonates.

Emplacement Evidence and Formation Scenario

The particles we studied place constraints on the physical emplacement processes of the organic sheets that complement the chemical sequence described above.

The structure of Particle 33 (**Figure 2**) suggests layering that could have formed via deposition. The physical and chemical heterogeneity of the inclusions in the middle layer of Particle 33 is consistent with the idea of particulates decorating organic coatings on pre-existing grains. Subsequent movement of coated grains caused some of them to adhere to each other and sandwich the carbonates between organic sheets. Such reworking could also detach sheets and allow them to fold or stack to produce multilayered structures. The convoluted shape of the organic vein in Particle 2 with a carbonate and void inclusions could be explained by such folding (**Figure 3**).

In light of the above observations, a multistep chemical process is proposed to explain the observed compositions and morphologies of the newly discovered N-rich polymeric materials in Bennu samples. These steps are shown and described in **Figure 4**.

Implications to Prebiotic Chemistry

The observation of the N- and O-rich phases reported here, combined with the detection of N-rich soluble organic compounds (Glavin & Dworkin et al. 2025), demonstrates that asteroids like Bennu's parent body could have been a significant source of N-rich volatiles and compounds of biological importance, including ammonia, amino acids, nucleobases, and other chemical precursors that contributed to the prebiotic inventory that led to the emergence of life on Earth. The observation of polymeric N-rich organics that contain abundant amine and amide functional groups adds a new dimension to this asteroidal prebiotic inventory.

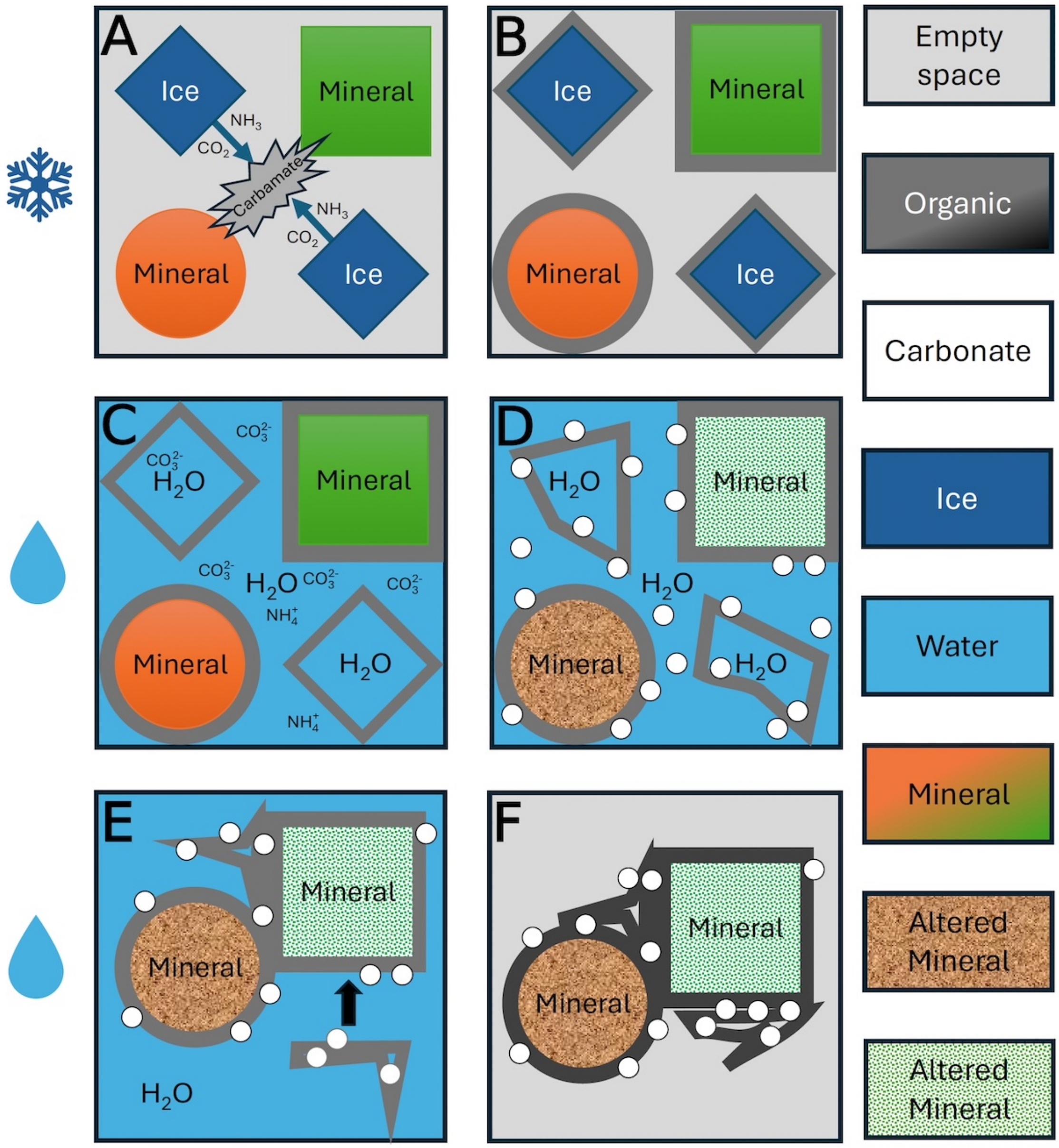

***Figure 4** – **Proposed multistep formation process of the new organic phase. (A)** As the parent body warmed, NH_3 and CO_2 from ices reacted to form carbamate via gas–grain or solid-state reactions before H_2O ice melted. **B** Carbamate underwent partial polymerization to produce a water-insoluble organic phase at low temperatures that formed or was deposited on grain surfaces (gray). **(C)** Further warming melted H_2O ice and decomposed any unpolymerized carbamate into NH_4^+ and CO_3^{2-} dissolved in water (blue). **(D)** Aqueous alteration led to the precipitation of some calcites (white circles) and initiated conversion of anhydrous silicates to phyllosilicates (textured fills of the circle and square). Calcites precipitated as either isolated grains or grains that stuck to or nucleated on the organic surfaces. **(E)** Organic coatings from adjacent grains adhered, producing a layered structure with embedded carbonates and voids. Any mantles around ice grains would collapse or fold. **(F)** Further aqueous alteration may have then folded the polymer sheets to produce more complicated structures, triggered additional chemistry, and set the final morphology (dark gray). Panels **A** and **B** occur at cryogenic temperatures below the melting of the H_2O–NH_3 eutectic, whereas panels **C–F** occur after the melting of H_2O ice.*

Scott Sandford has worked as a research laboratory astrophysicist/astrochemist/astrobiology at NASA's Ames Research Center since 1986. Much of his work addresses scientific issues associated with the formation and evolution of organic materials in astrophysical environments through the combined use of infrared astronomy, laboratory simulations, and the study of actual extraterrestrial materials. The extraterrestrial materials he has studied include interplanetary dust collected in the stratosphere by NASA high-altitude aircraft, meteorites, and samples returned to Earth by sample return missions. He has played a major role in sample return missions that have returned materials from comets (NASA's Stardust mission) and asteroids (NASA's *OSIRIS-REx* mission and JAXA's *Hayabusa* and *Hayabusa2* missions).

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Zack Gainsforth has worked at the University of California's Space Sciences Laboratory for the last two decades. He studies the early history of the solar system using interstellar, cometary, and asteroidal samples returned by NASA and JAXA missions. He is especially interested in connecting the dots between different epochs of solar system formation. His work on NASA's Stardust mission included characterizing some of the first interstellar dust returned to Earth and determining the formation history of comet Wild 2. His work on NASA's *OSIRIS-REx* and JAXA's *Hayabusa2* missions has included determining the petrography of asteroids Bennu and Ryugu, and the relationship of organic species to their mineral environment. He primarily uses a suite of electron and X-ray microscopy techniques that reveal the structures of extraterrestrial rocks at multiple scales from the atomic to the macro.

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Michel Nuevo has worked as a research scientist in the Astrophysics & Astrochemistry Laboratory at NASA Ames since 2007. His research interests focus on the study of the formation and evolution of organic materials in cold astrophysical objects (comets, asteroids, icy moons, dwarf planets) and environments (molecular clouds, protoplanetary disks). In particular, he performs laboratory simulations in which organic compounds are formed from the energetic processing of ices, and he studies extraterrestrial materials (meteorites, asteroids) to search for the presence of organic compounds. These studies are performed using Fourier-transform infrared (FTIR) spectroscopy and microscopy, gas chromatography coupled to mass spectrometry (GC-MS), and X-ray absorption near-edge structure (XANES) spectroscopy. More recently, he has been involved in the study of samples from asteroids Ryugu and Bennu, collected and returned by JAXA's *Hayabusa2* and NASA's *OSIRIS-REx* missions, respectively.

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Bottom-up Formation of Phenol (C_6H_5OH) in Interstellar Analog Ices of Acetylene and Water Exposed to Ionizing Radiation

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Although oxygenated benzene derivatives are key precursors in the abiotic synthesis of biorelevant molecules and fundamental building blocks of functionalized polycyclic aromatic hydrocarbons, their formation mechanisms under interstellar conditions have remained largely unexplored. Here, we report the first bottom-up formation of phenol (C_6H_5OH) in low-temperature interstellar ice analogs composed of acetylene and water (C_2H_2–H_2O). Utilizing vacuum ultraviolet photoionization reflectron time-of-flight mass spectrometry and resonance-enhanced multiphoton ionization, phenol, along with aromatic hydrocarbons including benzene (C_6H_6), phenylacetylene (C_6H_5CCH), styrene ($C_6H_5CHCH_2$), naphthalene ($C_{10}H_8$), and phenanthrene ($C_{14}H_{10}$), were identified in the gas phase during temperature-programmed desorption. Among these species, styrene, naphthalene, and phenanthrene have not yet been detected in the interstellar medium, suggesting that they are suitable targets for future astronomical searches. These findings reveal viable low-temperature formation pathways for phenol through nonequilibrium chemistry in acetylene-containing interstellar ices, thereby advancing our understanding of the abiotic formation of oxygenated benzene derivatives in extraterrestrial environments.

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The Astrophysical Journal, **1000**, 76 (2026)

https://iopscience.iop.org/article/10.3847/1538-4357/ae48fa

Localized Deviations from the CO–PAH Relation in PHANGS-JWST Galaxies: Faint PAH Emission or Elevated CO Emissivity?

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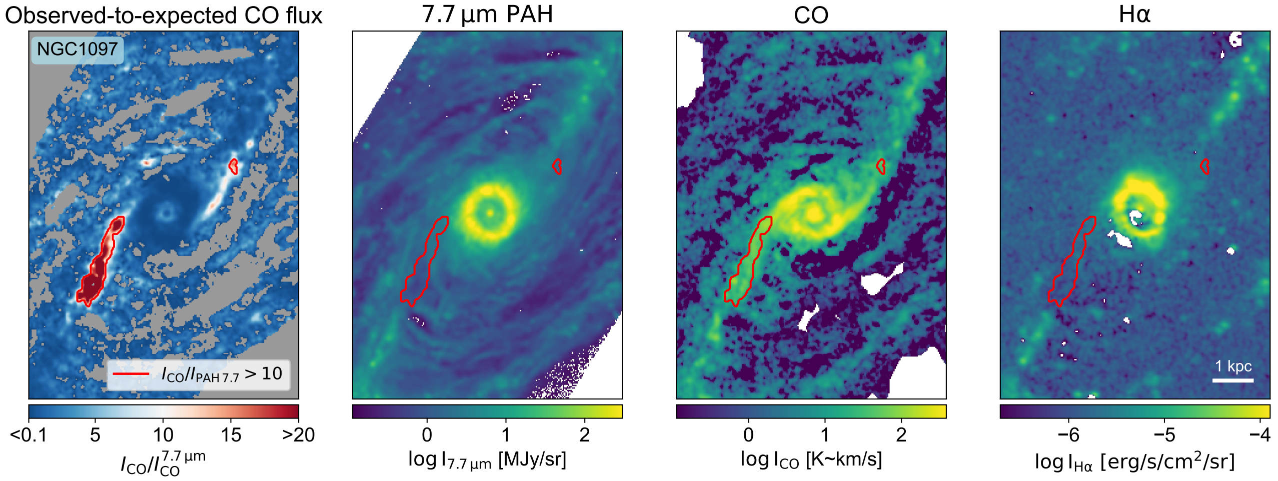
Polycyclic aromatic hydrocarbon (PAH) emission is widely used to trace the distribution of molecular gas in the interstellar medium, exhibiting a tight correlation with CO(2–1) emission across nearby galaxies. Using PHANGS-JWST and PHANGS-ALMA data, we identify localized regions where this correlation fails, with CO flux exceeding that predicted from 7.7 µm PAH emission by more than an order of magnitude. These outlier regions are found in 20 out of 70 galaxies and are located in galaxy centers and bars, without signs of massive star formation. We explore two scenarios to explain the elevated CO-to-PAH ratios, which can either be due to suppressed PAH emission or enhanced CO emissivity. We examine PAH emission in other bands (3.3 µm and 11.3 µm) and the dust continuum dominated bands (10 µm and 21 µm), finding consistently high CO-to-PAH (or CO-to-dust continuum) emission ratios, suggesting that 7.7 µm PAH emission is not particularly suppressed. In some outlier regions, PAH sizes and spectral energy distribution of the radiation differ slightly from nearby control regions with normal CO-to-PAH ratios, though without a consistent trend. We find that the outlier regions show higher CO velocity dispersions ($\Delta v_{\rm CO}$). This increase in $\Delta v_{\rm CO}$ lowers CO optical depth and raises its emissivity for a given gas mass. Our results favor a scenario where shear along the bar lanes and shocks at the bar ends elevate CO emissivity, leading to the breakdown of the CO–PAH correlation. Future JWST spectroscopy and deep ALMA observations of CO isotopologues will provide critical tests of this scenario.



An example galaxy (NGC 1097) hosting outlier regions with abnormally high CO-to-PAH ratios (red contours). The first column shows the ratio of CO flux to that expected from 7.7 µm PAH emission. Subsequent columns show the 7.7 µm PAH, CO, and Hα observations. These outlier regions are spatially localized along bar lanes and show no signs of massive star formation in Hα.

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The Astrophysical Journal, **1001**, 67 (2026)

https://iopscience.iop.org/article/10.3847/1538-4357/ae4599

Impact Ionization Properties of Polypyrrole Nanoparticles

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Upcoming space missions flying dust impact ionization mass spectrometers will detect and analyze dust grains that are partially organic in composition. These organic components are expected to include mixtures of polycyclic aromatic hydrocarbons, heterocyclic compounds (containing oxygen, sulfur, and nitrogen), and additional functionalized condensed species. Dust impact ionization is a strongly velocity-dependent process that produces atomic and molecular ions reflective of the composition of the impacting particle. In this work, we characterize the impact ionization response of the nitrogen-bearing heterocyclic polymer polypyrrole (PPy). Because of its electrical conductivity, PPy is commonly used as a coating material for both mineral and organic dust particles in electrostatic dust accelerator studies. PPy nanoparticles were accelerated to velocities of 2–30 km s^{-1}, and the resulting time-of-flight mass spectra were analyzed as a function of impact velocity with additional care paid to spectral variations with particle mass. The resultant mass spectra produced by impacts under roughly 8 km s^{-1} are dominated by smaller PPy-derived molecular fragments at masses 27, 28, 56, and 63u, in addition to common contaminants such as Na^{+} (23u) and K^{+} (39u). Some of these molecular fragments can be understood as originating from pyrrole, i.e., the species from which PPy is derived, while others appear to be unique to PPy. At higher velocities, the impact ionization of PPy produces two homologous series of fragment ions with the general form $C_nH_m{}^+$ and $C_nNH_m{}^+$, alongside the molecular fragments. This study refines our understanding of impact ionization processes for organic heterocyclic compounds and provides essential reference data for interpreting dust spectra from upcoming interstellar and interplanetary missions.

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ACS Earth and Space Chemistry, **10**, 3 (2026)

https://doi.org/10.1021/acsearthspacechem.5c00370

Pyrrole without Life: Reaction of Aminomethylene with the Propargyl Radical

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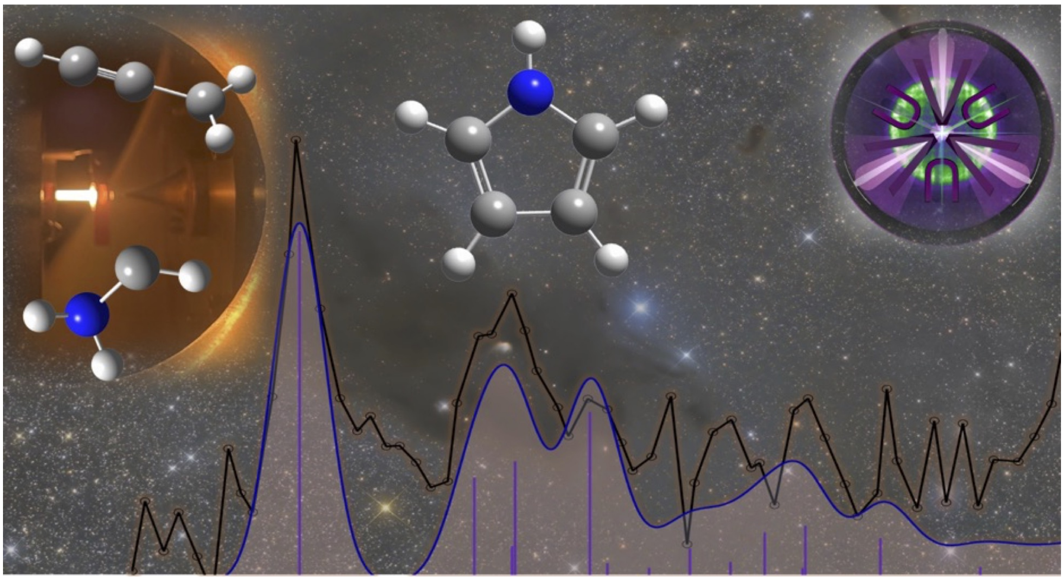
Carbenes are reactive species found across gas-phase environments, from combustion to planetary atmospheres and interstellar space. Their reactions with radicals represent a compelling path to increasing chemical complexity, in which the formation of the first aromatic ring is a foundational step. To date, no selective gas-phase, bottom-up route to the smallest nitrogen-bearing aromatic ring, pyrrole, is known. We investigated the reaction of the simplest aminocarbene, aminomethylene, with the prototypical resonance stabilized propargyl radical. Photoelectron photoion coincidence spectroscopy and semi-automated electronic structure calculations reveal a barrierless, addition–elimination mechanism producing pyrrole + H. The reaction path depends on the orientation of propargyl during the association, in which the allenyl resonance form ($H_2C{=}C{=}CH^\bullet$) of propargyl leads to pyrrole formation. This selective pathway highlights the promise of carbene–radical chemistry to fill important gaps in chemical reaction networks.



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The Journal of Physical Chemistry Letters, **17**, 2078 (2026)

https://pubs.acs.org/doi/10.1021/acs.jpclett.5c03948

Modeling the emission spectra of polycyclic aromatic hydrocarbons by recurrent fluorescence

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Recurrent fluorescence (RF) is an important relaxation mechanism in polycyclic aromatic hydrocarbons (PAHs), which could stabilize them and contribute to the production of aromatic infrared bands that are observed in the infrared spectra of the interstellar medium (ISM). In this theoretical work, a statistical model of relaxation by recurrent fluorescence is formally developed, including Herzberg-Teller and Duschinsky rotation effects as well as a full account of vibrational progressions. Using canonical and harmonic approximations, the RF rate constants can be determined from the transition dipole moment time autocorrelation functions. Application to the naphthalene, anthracene, and pyrene cations is presented based on quantum chemical inputs obtained from time-dependent density-functional theory. For these highly symmetric molecules, the low-lying, symmetry-forbidden electronic transitions are predicted to contribute possibly even more than higher energy, non-forbidden transitions. Such an unexpected contribution could increase the cooling efficiency of PAHs and, in turn, stabilize them further under the highly ionized environments of the ISM.

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The Journal of Chemical Physics, **164**, 134106 (2026)

https://doi.org/10.1063/5.0318065
https://arxiv.org/abs/2601.02173

Impact of spatial topology and nitrogen atoms embedding in π-conjugated chromophores on their UV-Vis and IR spectra

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A comparative study of π-conjugated chromophores of interest in astrochemistry is carried out by using density functional theory (DFT) and time-dependent DFT. The point of the study is the simultaneous systematic evaluation of both UV/Visible and IR spectra by usage of the same B3LYP functional and the same basis set of polarized triple-zeta quality. The most attention is paid to the impact of spatial topology and the number of substituted nitrogen atoms in the simplest polycyclic aromatic hydrocarbons and their N-heteroaromatic analogues with one and two nitrogen atoms, e.g. anthracene (acridine and phenazine) and phenanthrene (7,8-benzoquinoline and 1,10-phenanthroline) on relative energies and radiative properties of their lowest singlet and triplet $\pi\pi^*$ and $n\pi^*$ states as well as wavenumbers and intensities of vibrational transitions in the mid-frequency IR region. The estimated eigenvalues of the lowest singlet $n\pi^*$ state in nitrogen-substituted polycyclic aromatic hydrocarbons are a valuable contribution to data available in the literature since they are usually unobserved if they are located above the lowest singlet $\pi\pi^*$ state. The evaluated energies and transition probabilities of both PAHs and PANHs help to make assignment of the unidentified IR emission and UV absorption bands in the interstellar medium.

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Journal of Quantitative Spectroscopy and Radiative Transfer, **347**, 109646 (2025)

https://doi.org/10.1016/j.jqsrt.2025.109646

Searching for the Shortest-wavelength Aromatic Infrared Bands: No Evidence for the Predicted 1.05 µm Polycyclic Aromatic Hydrocarbon Feature

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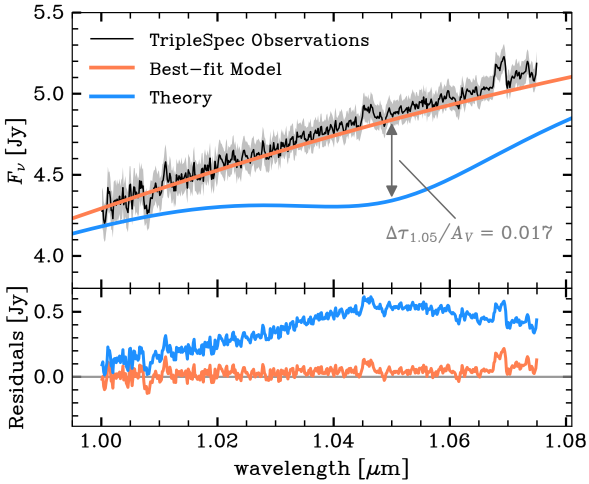
Polycyclic aromatic hydrocarbons (PAHs) are responsible for a variety of near- and mid-infrared spectral features in Galactic and extragalactic sources. A feature at 1.05 µm arising from electronic transitions in PAH cations is predicted by laboratory experiments but has never been observationally confirmed. We conduct a dedicated search for this feature in absorption on a highly-extinguished sight line toward BD+40 4223, a blue supergiant in Cyg OB2, using the TripleSpec spectrograph at Palomar Observatory. We place a 5σ upper limit on the feature strength of $\Delta\tau_{1.05}/A_V < 5.6 \times 10^{-3}$, ruling out theoretical estimates with $> 10\sigma$ significance. We constrain the effective temperature of BD+40 4223 to be $\log_{10}(T_{\rm eff}) = 4.41 \pm 0.03$ and infer that it is veiled by 6.39 ± 0.05 magnitudes of visual extinction, consistent with but more constraining than previous determinations. As dust on the sight line toward BD+40 4223 appears typical of the diffuse interstellar medium, this non-detection challenges existing models of PAH material properties and/or charge distribution.



TripleSpec observations, shown in black with 1σ uncertainties shown in gray. Best-fit model spectrum, fit to the TripleSpec observations, is shown as the orange line. Blue curve indicates a model sharing the same extinction and stellar parameters as our best fit model spectrum, but with the depth of the 1.05 µm feature set to the theoretical model from Hensley & Draine (2023). Residuals are shown in the lower panel.

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The Astrophysical Journal, **1001**, 6 (2026)

https://arxiv.org/abs/2602.12331
https://doi.org/10.3847/1538-4357/ae4ed8

PhD Position

Photochemical evolution study of the clouds in Neptune's atmosphere under the influence of cosmic rays

Advertised by David Dubois & Alicja Domaracka

Scientific background: Neptune is the outermost planet in the solar system. Alongside Uranus, the other so-called "ice giant," it is among the least understood bodies orbiting our sun. Neptune's mass is composed of roughly 10-20% hydrogen and helium, with the remaining 80-90% consisting of heavier elements. Its atmosphere, extending hundreds of kilometers, includes a troposphere in the deepest layers and a thermosphere at the uppermost reaches. Despite being located 30 astronomical units away, Neptune receives UV and cosmic radiation that affects its atmosphere, primarily composed of dihydrogen (H_2), helium (He), and methane (CH_4) [1]. Photochemical products such as acetylene (C_2H_2), ethylene (C2H4), hydrogen cyanide (HCN), carbon monosulfide (CS), and aromatics have been detected in its atmosphere or inferred by models. However, the atmospheric chemistry and photochemical evolution of the organic haze clouds (below 200 K) remain largely unknown [1,2]. Laboratory simulation studies will help investigate this chemistry in preparation for future space missions.

Objectives: The main objective will be to study the photochemistry of the icy clouds in Neptune's atmosphere and to understand the physicochemical processes leading to the formation of complex molecules under the influence of ionizing radiation. Special attention will be given to molecules already detected on Neptune, aiming to better understand their photochemical evolution as well as to investigate molecules not yet observed that may be present.

Methodology: The student will use the experimental platform MIRRPLA (Multiple-beam IRRadiation PLAtform) at the Centre de Recherche sur les Ions, les Matériaux et la Photonique (CIMAP), located at the Grand Accélérateur National d'Ions Lourds (GANIL) in Caen, France. The heavy ion beams delivered by the GANIL particle accelerator aim to simulate the chemistry induced by cosmic rays and heavy energetic nuclei. MIRRPLA is a unique versatile instrument that enables the formation of planetary and astrophysical ice mixtures and their irradiation by combining a UV lamp, an electron gun, and heavy ions [3]. The simultaneous effect of heavy ions, UV photons, and electrons will be taken into account to reproduce the more realistic radiation field found in space. Coupled with the irradiation of ices simulating Neptunian clouds, the analysis of complex organic molecules will be performed using infrared and mass spectrometry. To understand the role of organic aerosols, ices will also be deposited on aerosol analogs called tholins, which act as condensation nuclei. Theoretical support for the experimental measurements is also planned.

Details:
Supervisors: David Dubois, Alicja Domaracka
Laboratory: CIMAP/GANIL
Starting date: October 2026
Length: 3 years

References:

[1] Moses, J. I., Cavalié, T., Fletcher, L. N., & Roman, M. T. (2020). Atmospheric chemistry on Uranus and Neptune. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, **378**(2187), 20190477.

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[3] Domaracka, A., & Danger, G. (2023). Multiple beam irradiation platform MIRRPLA: origin and evolution of organic matter in the solar system. *Nuclear Physics Newsletter*, **33**(4), 36.

Application deadline: 15 May 2026

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AstroPAH Newsletter

http://astropah-news.strw.leidenuniv.nl — Next issue: 21 May 2026

astropah@strw.leidenuniv.nl — Submission deadline: 8 May 2026