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Abstracts

Molecular Mass Growth Processes to Polycyclic Aromatic Hydrocarbons through Radical−Radical Reactions Exploiting Photoionization Reflectron Time-of-Flight Mass Spectrometry

S. J. Goettl, M. Ahmed, A. M. Mebel, R. I. Kaiser

Polycyclic aromatic hydrocarbons (PAHs) represent critical building blocks in molecular mass growth processes to carbonaceous nanoparticles, referred to as interstellar and circumstellar grains along with soot particles in astrophysical environments and combustion systems, respectively. Recent advancements on elucidating elementary steps to PAHs have utilized reactions of aromatic radicals, resonantly stabilized free radicals, and aliphatic radicals with closed shell hydrocarbons. However, the role of radical–radical reactions (RRR) leading to PAHs has remained largely unexplored on the molecular level due to preceding experimental challenges in producing sufficiently high number densities of radical reactants for isomer-selective detection of products from bimolecular and termolecular reactions. This Account offers the latest developments in our knowledge on the mechanisms and pathways to PAHs via RRR probed in a chemical microreactor at temperatures as high as 1600 K. Product preservation in a molecular beam coupled with synchrotron vacuum ultraviolet photoionization reflectron time-of-flight mass spectrometry and photoelectron photoion coincidence spectroscopy enabled isomer-selective detection of PAHs of up to three rings by their photoionization efficiency curves, which were fit with a linear combination of reference curves for identification. Experiments were combined with computational fluid dynamics modeling of the physico-chemical processes in the microreactor, as well as high-level electronic structure calculations to reveal the reaction pathways of each system. Six distinct reaction mechanisms were discovered in this work: Propargyl Addition – BenzAnnulation (PABA), Methyl Addition – Ring Expansion (MARE), CycloPentadienyl Addition – Naphthylization (CPAN), Fulvenallenyl Addition – Cyclization – Aromatization (FACA), Benzyl Addition – Aromatization (BAA), and Phenyl Addition – Pentacyclization (PAP). By systematically varying the number of carbon atoms in the radical reactants, molecular mass growth processes involving reactions between radicals with odd numbers of carbon atoms access aromatics carrying one, two, or three six-membered rings, whereas reactions between even- and odd-carbon-numbered radicals produce aromatics combining five- and six-membered rings. Our investigations reveal unconventional cycloadditions on excited state triplet surfaces, additions of radicals to low spin density carbon-centered radicals, spiroaromatic and fulvene-type intermediates, and highly strained bicyclic reaction intermediates, challenging current perceptions of PAH molecular mass growth processes. All the listed mechanisms, except for FACA, feature endoergic reactions or barriers which lie above the separated reactants and therefore might be central to circumstellar environments of carbon-rich stars and planetary nebulae as their descendants, but they play no role in the gas phase of cold molecular clouds where temperatures as low as 10 K dominate. Overall, this work provides detailed reaction mechanisms of PAH growth processes, advancing our knowledge of the chemistry of carbonaceous matter in the universe

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Formation of thiocarbonic acid (H2CS3) – the sulfur counterpart of carbonic acid (H2CO3) – in interstellar analog ices

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The first experimental formation of thiocarbonic acid (H2CS3) is presented in this work from low-temperature interstellar ice analogs composed of hydrogen sulfide (H2S) and carbon disulfide (CS2) exposed to electron irradiation simulating the impact of galactic cosmic rays (GCRs) on interstellar ices. The recent attention brought to sulfur-bearing molecules, as well as the recent detection of carbonic acid (H2CO3) in the interstellar medium (ISM), invites the study of the interstellar detection of the sulfur counterpart, thiocarbonic acid. However, the interstellar formation pathways of thiocarbonic acid have remained elusive. In this work, thiocarbonic acid was identified in the gas phase during the temperature programmed desorption (TPD) using isomer-selective single photoionization reflectron time-of-flight mass spectrometry (PI-ReToF-MS), suggesting that the hitherto astronomically unobserved thiocarbonic acid represents a promising candidate for future astronomical searches. The formation of H2CS3 isomers was investigated through additional isotopically labeled experiments and the formation mechanisms through quantum chemical studies. These findings unravel a key reaction pathway to thiocarbonic acid and represent a first step toward its possible formation and detection in the ISM, shedding light on the missing sulfur problem.

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Gas-phase synthesis of anthracene and phenanthrene via radical-radical reaction induced ring expansions

S. J. Goettl, A. M. Turner, V. S. Krasnoukhov, V. N. Azyazov, K. Kanayama, P. Hemberger, A. M. Mebel, R. I. Kaiser

Unravelling reaction mechanisms of aromatic and resonance-stabilized radicals is critical to understanding molecular mass growth processes to polycyclic aromatic hydrocarbons (PAHs) and carbonaceous nanoparticles in distinct astrophysical environments (molecular clouds, circumstellar envelopes) and combustion systems. Utilizing photoelectron photoion coincidence spectroscopy (PEPICO), the gas-phase reaction of the methyl radical (CH3) with the aromatic and resonance-stabilized fluorenyl radical (C13H9) was explored under high-temperature conditions in a chemical microreactor. Anthracene and phenanthrene were detected isomer-selectively using photoionization efficiency (PIE) curves and mass-selected threshold photoelectron (ms-TPE) spectra. While phenanthrene is produced through a radical–radical recombination of the carbon-centered radicals, anthracene may plausibly be formed through an unconventional radical addition to a low spin-density fluorenyl carbon. These pathways result in five-membered ring expansion—a critical mechanism crucial to PAH mass growth converting bent PAHs into planar nanostructures.

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Formation of All Three C2H4O Isomers—Ethylene Oxide (c-C2H4O), Acetaldehyde (CH3CHO), and Vinyl Alcohol (CH2CHOH)—in Ethanol-containing Interstellar Analog Ices

Jia Wang , Chaojiang Zhang , Joshua H. Marks , and Ralf I. Kaiser

Oxygen-containing complex organic molecules are key precursors to biorelevant compounds fundamental for the origins of life. However, the untangling of their interstellar formation mechanisms has just scratched the surface, especially for oxygen-containing cyclic molecules. Here, we present the first laboratory simulation experiments featuring the formation of all three C2H4O isomers—ethylene oxide (c–C2H4O), acetaldehyde (CH3CHO), and vinyl alcohol (CH2CHOH)—in low-temperature model interstellar ices composed of carbon monoxide (CO) and ethanol (C2H5OH). Ice mixtures were exposed to galactic cosmic-ray proxies with an irradiation dose equivalent to a cold molecular cloud aged (7 ± 2)e5 yr. These biorelevant species were detected in the gas phase through isomer-selective photoionization reflectron time-of-flight mass spectrometry during temperature-programmed desorption. Isotopic labeling experiments reveal that ethylene oxide is produced from ethanol alone, providing the first experimental evidence to support the hypothesis that ethanol serves as a precursor to the prototype epoxide in interstellar ices. These findings reveal feasible pathways for the formation of all three C2H4O isomers in ethanol-rich interstellar ices, offering valuable constraints on astrochemical models for their formation. Our results suggest that ethanol is a critical precursor to C2H4O isomers in interstellar environments, representing a critical step toward unraveling the formation mechanisms of oxygen-containing cyclic molecules, aldehydes, and their enol tautomers from alcohols in interstellar ices.

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Formation of Lactic Acid (CH3CH(OH)COOH), a Metabolic Keystone for the Molecular Origins of Life, in Interstellar Ice Analogues

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Lactic acid (CH3CH(OH)COOH)−a key biorelevant hydroxycarboxylic acid−is ubiquitous in living organisms and critically linked to the molecular origins of life due to its fundamental role in metabolic pathways. With the anoxic conditions of early Earth, anaerobic metabolic pathways such as lactic acid fermentation may have served as an essential mechanism for primordial cellular metabolisms. Although lactic acid has been detected in high abundances in carbonaceous asteroid Ryugu and various meteorites like Murchison, its formation pathways under extreme conditions of the interstellar medium (low temperature, radiation) have remained elusive. Here, we report the first bottom-up formation of racemic lactic acid via a barrierless radical−radical recombination between the hydroxycarbonyl (HOĊO) radical and the 1-hydroxyethyl (CH3ĊHOH) radical in interstellar analog ices composed of carbon dioxide (CO2) and ethanol (CH3CH2OH). These results provide a first step toward a fundamental understanding of the abiotic formation of biorelevant hydroxycarboxylic acids via nonequilibrium reactions from ubiquitous precursor molecules in extraterrestrial environments. Utilizing isomer-selective vacuum ultraviolet photoionization reflectron time-of-flight mass spectrometry and isotopic substitution experiments, lactic acid and its isomer monoethyl carbonate (CH3CH2OCOOH) were identified in the gas phase during temperature-programmed desorption. These findings suggest that they can likely form in interstellar ices containing carbon dioxide and ethanol in cold molecular clouds via galactic cosmic rays-mediated nonequilibrium chemistries.

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The Aromatic Infrared Bands around the Wolf-Rayet Binary WR140 Revealed by JWST

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We have analyzed the aromatic infrared bands (AIBs) in the 6-11.2 μm range around the Wolf-Rayet binary WR140 (d=1.64 kpc) obtained with the James Webb Space Telescope (JWST) Mid-Infrared Instrument (MIRI) Medium-Resolution Spectrometer (MRS). In WR140's circumstellar environment, we have detected AIBs at 6 μm and 7.7 μm which are attributed to C-C stretching modes. These features have been detected in the innermost dust shell (Shell1; ~2100 au from WR140), the subsequent dust shell (Shell2; ~5200 au), and "off-shell" regions in the MRS coverage. The 11.2 μm AIB, which is associated with the C-H out-of-plane bending mode, has been tentatively detected in Shell2 and the surrounding off-shell positions around Shell2. We compared the AIB features from WR140 to spectra of established AIB feature classes A, B, C, and D. The detected features around WR140 do not agree with these established classes. The peak wavelengths and full width half maxima (FWHMs) of the 6 μm and 7.7 μm features are, however, consistent with those of R Coronae Borealis (RCB) stars with hydrogen-poor conditions. We discuss a possible structure of carbonaceous compounds and environments where they form around WR140. It is proposed that hydrogen-poor carbonaceous compounds initially originate from the carbon-rich WR wind, and the hydrogen-rich stellar wind from the companion O star may provide hydrogen to these carbonaceous compounds.

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Missing interstellar sulfur in inventories of polysulfanes and molecular octasulfur crowns

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The disparity between predicted sulfur abundances and identified reservoirs of sulfur in cold molecular clouds, also known as the sulfur depletion problem, has remained an ongoing debate over decades. Here, we show in laboratory simulation experiments that hydrogen sulfide (H2S) can be converted on ice-coated interstellar grains in cold molecular clouds through galactic cosmic rays processing at 5 K to sulfanes (H2Sn; n = 2–11) and octasulfur (S8). This locks the processed hydrogen sulfide as high-molecular weight sulfur-containing molecules thus providing a plausible rationale for the fate of the missing interstellar sulfur. These sulfuretted molecules may undergo fractionated sublimation once the molecular cloud transforms into star forming regions. The isomeric identification of octasulfur rings (S8) coincides with the recent identification of elementary sulfur in the carbonaceous asteroid (162173) Ryugu, thus providing compelling evidence on the link between sulfur in cold molecular clouds and in our Solar System with, e.g., the Taurus Molecular Cloud (TMC) potentially accumulating an equivalent of 350 Earth masses of octasulfur.

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A fast machine learning tool to predict the composition of interstellar ices from infrared absorption spectra

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Current observations taken by James Webb Space Telescope (JWST) allow us to observe the absorption features of icy mantles that cover interstellar dust grains, which are mainly composed of H2O, CO, and CO2, along with other minor species. Thanks to its sensitivity and spectral resolution, JWST has the potential to observe ice features towards hundreds of sources at different stages along the process of star formation. However, identifying the spectral features of the different species and quantifying the ice composition is not trivial and requires complex spectroscopic analysis. We present Automatic Ice Composition Estimator (AICE), a new tool based on artificial neural networks. Based on the infrared (IR) ice absorption spectrum between 2.5 and 10 μm, AICE predicts the ice fractional composition in terms of H2O, CO, CO2, CH3OH, NH3, and CH4. To train the model, we used hundreds of laboratory experiments of ice mixtures from different databases, which were reprocessed with baseline subtraction and normalisation. Once trained, AICE takes less than one second on a conventional computer to predict the ice composition associated with the observed IR absorption spectrum, with typical errors of ~3% in the species fraction. We tested its performance on two spectra reported towards the NIR38 and J110621 background stars observed within the JWST Ice Age program, demonstrating a good agreement with previous estimations of the ice composition. The fast and accurate performance of AICE enables the systematic analysis of hundreds of different ice spectra with a modest time investment. In addition, this model can be enhanced and re-trained with more laboratory data, improving the precision of the predictions and expanding the list of predicted species.

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Is cosmic dust porous?

Alexey Potapov, Martin R. S. McCoustra, Ryo Tazaki, Edwin A. Bergin, Stefan T. Bromley, Robin T. Garrod, and Albert Rimola

There is a long-standing discussion in the astrophysical/astrochemical community as to the structure and morphology of dust grains in various astrophysical environments (e.g., interstellar clouds, protostellar envelopes, protoplanetary and debris disks, and the atmospheres of exoplanets). Typical grain models assume a compact dust core which becomes covered in a thick ice mantle in cold dense environments. In contrast, less compact cores are likely to exhibit porosity, leading to a pronounced increase in surface area with concomitant much thinner ice films and higher accessibility to the bare grain surface. Several laboratory experimental and theoretical studies have shown that this type of dust structure can have a marked effect on several physico-chemical processes, including adsorption, desorption, mobility, and reactivity of chemical species. Porous grains are thus thought to likely play a particularly important and wide-ranging astrochemical role. Herein, we clarify what is meant by porosity in relation to grains and grain agglomerates, assess the likely astrochemical effects of porosity and ask whether a fractal/porous structural/morphological description of dust grains is appropriate from an astronomical perspective. We provide evidence for high porosity from laboratory experiments and computational simulations of grains and their growth in various astrophysical environments. Finally, we assess the observational constraints and perspectives on cosmic dust porosity. Overall, our paper discusses the effects of including porosity in dust models and the need to use such models for future astrophysical, astrochemical and astrobiological studies involving surface or solid-state processes.

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3D SR-µXCT analysis for lithology detection: Application to Ryugu sample A0159

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Extraterrestrial breccia samples are formed through impact-related processes that combine fragments of distinct lithologies. As such, they are valuable indicators of the complex formation and evolution history of planetesimals in our Solar System. Samples from asteroid (162173) Ryugu, returned to Earth by the Hayabusa2 mission in December 2020, were characterized as breccias. The boundaries of mineralogical assemblages are typically drawn manually based on interpreted results from specific techniques, mostly performed on artificially produced 2D surfaces. This process inherently introduces subjectivity. Here, we present a semi-automated analytical method using Synchrotron Radiation micro X-ray Computed Tomography (SR-µXCT) data, called the Local Histogram method. It enables an unsupervised detection and 3D visualization of few tens to hundreds micrometer-sized lithologies showing sub-micrometer heterogeneities. We developed the method on a millimeter-sized Ryugu sample (A0159) in combination with a more traditional global grayscale threshold segmentation. In A0159, we report five distinct lithologies. They were confirmed and further characterized by an additional Scanning Electron Microscopy (SEM) analysis on Xenon plasma-Focused Ion Beam (Xe-pFIB) produced sections. Some lithologies show specific relationships with large fractures, while one is particularly enriched in sub-micrometer sulfides. A0159 is rich in carbonates and hosts the largest millimeter-scale dolomite vein seen on Ryugu.

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JWST Observations of Young protoStars (JOYS): overview of program and early results

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This paper provides an overview of the JOYS program presenting MIRI-MRS data of 17 low-mass and 6 high-mass protostars. A wide variety of atomic, molecular and ice features are found. Gaseous molecular absorption or emission (CO2, C2H2, HCN, H2O, CH4, SO2, SiO, NH3) is seen toward several sources, but is cool compared with that found in disks, with excitation temperatures of 100–250 K that are determined by non-LTE processes including infrared pumping. Similar gas/ice abundance ratios point to an origin in the warm inner envelopes (“hot cores”) where ice sublimation followed by high temperature chemistry, perhaps stimulated by X-rays, plays a role. Along the outflow, CO2 is often extended. Water is commonly detected on source, even if relatively weak. Off source, water is seen only in the highest density shocks, such as those associated with NGC 1333 IRAS4B, which also shows bright hot C2H2 emission. Deep ice features are seen toward all protostars, revealing not just the major ice components but also ions (as part of salts) and complex organic molecules, with comparable abundances from low- to high-mass sources. We present a second detection of HDO ice in a solar-mass source, with an HDO/H2O ice ratio of 0.4%, thus providing a link with HDO/H2O in disks and comets. A deep search for solid O2 suggests that it is not a significant oxygen reservoir. Only a few embedded Class I disks show the same forest of water lines as Class II disks.

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Fundamental Vibrational Frequencies and Spectroscopic Constants for Additional Tautomers and Conformers of NH2CHCO

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The creation of larger prebiotic molecules in astronomical regions may require aminoketene (NH2CHCO) as an intermediate, and the two conformers of this molecule exhibit infrared vibrational frequencies with intensities larger even than the antisymmetric stretch in CO2. While the present quantum chemically computed frequencies of these fundamentals of ∼4.7 μm are in the same spectroscopic region as features from functionalized polycyclic aromatic hydrocarbons, they provide clear markers for what James Webb Space Telescope IR observations may be able to distinguish. Additionally, the IR and radioastronomical spectral characterization of two additional 2-iminoacetaldehyde, HN=CHC(=O)H, conformers are also computed as are the same data for a new carbene isomer (NH2CC(=O)H). All conformers of aminoketene and 2-iminoacetaldehyde exhibit dipole moments of more than 2.0 D, if not greater than 4.0 D, implying that they would be notable targets for radioastronomical searches. Additionally, the 2-iminoacetaldehyde conformers have a notable mid-IR C=O stretch around 1735 cm−1 slightly below the same fundamental in formaldehyde. This quantum chemical study is providing a more complete set of reference data for the potential observation of these tautomers and conformers of NH2CHCO in the laboratory or even in space.

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Superhydrogenation of indene at low temperatures

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Context. The hydrogenation of polycyclic aromatic hydrocarbons (PAHs) is crucial to understanding molecular hydrogenation formation in the interstellar medium (ISM). This process also helps to elucidate the weakening of the aromatic bonds in PAHs, which may function as a carbon reservoir, facilitating the formation of interstellar complex organic molecules (iCOMs) through top-down chemistry. Tunneling can significantly promote the hydrogenation process in a low-to-moderate temperature range (approximately 10–200 K), which could also be important in warmer regions of the ISM, such as photodissociation regions (PDRs). Aims. We aim to present the hydrogenation sequence of the newly observed PAH molecule, indene, for the first time and clarify the tunneling rule at temperature in PDR and dark molecular-cloud conditions. In addition, we report fit parameters to be utilized in astronomical modeling. Methods. The hydrogenation sequence was studied using simple hydrogenation rules based on tight-binding methods and confirmed by barriers from density functional theory (DFT). The binding energy, activation energies, kinetic rate constants, and tunneling corrections–based on the Bell and Eckart models and supported by the accurate instanton method–were calculated using DFT. To make our kinetic studies useful to modelers, we implemented a Monte Carlo method-based program to generate and optimize random initial fit parameters (α, β, γ, and T0) to achieve the statistically best fit. Results. We find that indene hydrogenation proceeds with saturation of carbon atoms in the pentagonal ring first, followed by hydrogenation of the benzene unit. Indene hydrogenation follows rules similar to those of other PAHs, such as pentacene, coronene, and corannulene, with binding energies for odd-numbered hydrogenation steps ranging from 0.5 to 2 eV and barriers around 0.13 eV for the first, fifth, and seventh hydrogenation steps. The third hydrogenation step is the rate-limiting step, with a barrier of 0.24 eV, similar to what is found for other PAHs. Even-numbered hydrogenation steps have lower barriers and lead to more stable intermediates as a result of radical-radical recombination. The hydrogenation sequence follows a scheme that strongly depends on the PAH's shape, the number of aromatic rings, and the presence of five-membered rings, aiming to preserve the aromaticity as much as possible. Furthermore, we observe that tunneling plays an important role in the hydrogenation of indene at temperatures between 30 and 75 K, which corresponds to the temperatures of dust in PDRs. Finally, our implementation includes fit parameters that reproduce our model with a high degree of accuracy, achieving a static precision of 0.99(R^2) and an RMS error of 1e-2.

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Methyl Isocyanate Formation from Oxygen Insertion in Methyl Cyanide Ices

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In cold molecular clouds, UV photolysis of icy grain mantles generates radicals that lead to new molecule formation. When radical diffusion is limited by low temperatures, oxygen atom addition and insertion reactions, enabled by photolysis of common ice components such as H2O, CO2, CO, and O3, offer an alternative route to chemical complexity through the production of metastable, highly reactive O(1D) atoms. We examine the reactivity of these oxygen atoms generated by UV photolysis of O3 with methyl cyanide (CH3CN). These studies are conducted in an ultra-high vacuum chamber at cryogenic and low-pressure conditions equipped with in situ infrared spectroscopy to monitor destruction and product formation in real time. We conclude that oxygen atoms rapidly insert into CH3CN to produce primarily methyl isocyanate (CH3NCO) in matrix-free ices. Over the range from 10 to 40 K, we observe no temperature dependence to either CH3CN destruction or CH3NCO production. When placing CH3CN:O3 in H2O and CO2 ice matrices, we find that CH3NCO formation remains robust, but that the yield likely decreases due to competing reaction pathways. In the case of the H2O ice, we also observe a shift in product branching ratios toward alternative pathways such as the formation of hydroxyacetonitrile (HOCH2CN). Overall, our results demonstrate that oxygen atom reactivity provides an important channel for generating chemical complexity from nitriles on cold grains where radical mobility is limited.

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Abiotic origin of the citric acid cycle intermediates

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The molecular framework for protometabolism—chemical reactions in a prebiotic environment preceding modern metabolism—has remained unknown in evolutionary biology. Mono-, di-, and tricarboxylic acids that comprise contemporary metabolism, such as the Krebs cycle, are of particular prebiotic relevance and are theorized to predate life on Earth. Researchers have struggled to unravel the molecular origins of respiration, with theories pointing toward abiotic origins later co-opted by the earliest living organisms; however, the molecular network of these molecules has remained elusive. Recent detections of carboxylic acids linked to the Krebs cycle on the Ryugu asteroid and Murchison meteorite rekindled interest in their extraterrestrial origins. Replicating conditions analogous to the environment of dense molecular clouds in laboratory simulation experiments, our work provides compelling evidence on the abiotic synthesis of the complete suite of biorelevant molecules central to the Krebs cycle. The opportunity for these biomolecules forming in deep space could provide molecular origins of protometabolism on early Earth and also provide the molecular feedstock to worlds beyond our own.

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Cosmic dust as a prerequisite for the formation of complex organic molecules in space?

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In cold, dense astrophysical environments dust grains are mixed with molecular ices. Chemistry in those dust/ice mixtures is determined by diffusion and reaction of molecules and radicals. However, investigations of diffusion of astrophysically relevant radicals and molecules across the surface and through the pores of cosmic dust grains and of surface reactions consequent to such diffusion is largely uncharted territory. This paper presents results of a study of a solid-state reaction of two molecular species, CO2 and NH3, separated by a layer of porous silicate grain aggregates, analogues of cosmic dust. The experiments demonstrate that the presence of the dust layer was necessary for a pure thermal CO2 + 2NH3 reaction to proceed, leading to the formation of ammonium carbamate (NH4+NH2COO-), an ionic solid containing a complex organic moiety of prebiotic interest recently detected in a protoplanetary disk. This result speaks for: (i) efficient diffusion of molecules on/within cosmic dust, (ii) an underestimated role for surface catalysis in the astrochemistry of cosmic dust, and (iii) potentially efficient dust-promoted chemistry in warm cosmic environments, such as protostellar envelopes and protoplanetary disks.

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Off-lattice Microscopic Monte Carlo Modeling of Molecular Hydrogen Formation on Carbonaceous Dust Grains

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In this work, we present an off-lattice Monte Carlo model of accretion and migration of hydrogen atoms on a rough surface of carbon dust grain. The migration of physisorbed atoms by means of thermal diffusion and quantum tunnelling through barriers between the surface potential minima is considered. The model is applied to simulations of molecular hydrogen formation in a cold interstellar medium for a temperature range 5—35 K. Eley—Rideal and Langmuir—Hinshelwood mechanisms for the formation of the H2 molecule were taken into account. We found that the surface potential energy minima that hold the accreted hydrogen atoms (binding energy) has wide dispersion of its values. The minimum energy is three times smaller than the maximum energy for the uneven surface of the model grain. The large dispersion of the binding energies results in an extended range of temperatures where H2 formation is efficient: 5—25 K. The dispersion of binding energies also reduces efficiency of diffusion due to tunnelling in comparison to that assumed in kinetic equation codes in which constant values of binding energies are employed. Thus, thermal hopping is the main source for the mobility of the hydrogen atoms in the presented off-lattice model. Finally, the model naturally provides the mean values for the ratio of binding-to-desorption energy. This ratio demonstrates weak dependence on temperature and is in the range of 0.5—0.6.

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Formation of Complex Organic Molecules in Prestellar Cores: The Role of Nondiffusive Grain Chemistry

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We present the results of astrochemical modeling of complex organic molecules (COMs) in the ice and gas of the prestellar

core L1544 with the recently updated MONACO rate equation-based model. The model includes, in particular, nondiffusive processes, new laboratory verified chemical routes for acetaldehyde and methane ice formation, and variations of H and H2 desorption energies depending on the surface coverage by H2 molecules. For the first time, we simultaneously reproduce the abundances of several oxygen-bearing COMs in the gas-phase, the approximate location of the peak of methanol emission, as well as the abundance of methanol in the icy mantles of L1544. Radical–radical reactions on the grain surface between species such as CH3, CH3O, and HCO efficiently proceed nondiffusively. COMs are delivered to the gas-phase via chemical desorption amplified by the loops of H-addition/abstraction surface reactions. However, gas-phase chemical reactions as well provide a noticeable input to the formation of COMs in the gas, but not to the COMs solid-state abundances. This particularly applies for CH3CHO and CH3OCH3. The simulated abundances of COMs in the ice are in the range 1%–2% (for methyl formate ice) or ∼0.1% (for CH3CHO and CH3OCH3) with respect to the abundance of H2O ice. We stress a similarity between the simulated abundances of icy COMs in L1544 and the abundances of COMs in the gas-phase of hot cores/corinos. We compare our nondiffusive model with the diffusive model and provide constraints for the species' diffusion-to-desorption energy ratios.

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Announcements

Icarus Special Issue: Carbon in Planetary Environments (Second announcement)

Icarus is now accepting submissions of manuscripts to be published in a special issue entitled "Carbon in Planetary Environments: Sources and Evolution." Guest editors are Dr. Kelly Miller (SwRI), Dr. Nora Hänni (Univ. of Bern), Dr. Fabian Klenner (Univ. of Washington), Prof. Brett McGuire (MIT) and Prof. Joshua Krissansen-Totton (Univ. of Washington). This cross-disciplinary issue will cover topics related to carbon in the solar system and beyond, including exoplanet and astrochemical environments. Submissions related to space missions, modeling and laboratory work are welcomed. The submission deadline is 30 November 2025. Manuscripts will be published online when they are accepted, and we expect the print issue to be published in the first half of 2026. Submitted manuscripts must be unpublished and should not be under consideration elsewhere. More information is available at the URL, or by contacting the guest editor team (kelly.miller@swri.org).

https://www.sciencedirect.com/special-issue/321476/carbon-in-planetary-environments-sources-and-evolution

Exploring the aromatic universe in the JWST era

We are pleased to announce the conference "Exploring the aromatic universe in the JWST era" to be held from July 6 to 10, 2026 in London, ON, Canada.

Website: https://www.aromaticuniverse.space/

Polycyclic Aromatic Hydrocarbons (PAHs) are a cornerstone of interstellar physics and chemistry. They play a fundamental role in heating the interstellar medium (ISM) through the photoelectric effect, regulating its ionization balance, and contributing to its molecular complexity. Identified as the carriers of the aromatic infrared bands (AIBs), PAHs are detected across a vast range of astrophysical environments—from the ISM of our own Galaxy to the early universe. In addition to their role in the ISM, PAHs serve as critical tracers of star formation in galaxies across cosmic time and as sensitive probes of physical conditions in planet-forming disks. Their detection in a variety of solar system objects has also made them central to discussions of astrobiology and the origin of prebiotic organics.

With JWST's unprecedented combination of spectral resolution, spatial detail, and sensitivity, the study of aromatics has entered a transformative era. JWST enables resolved studies of the evolution of aromatic species in nearby interstellar environments while simultaneously detecting AIBs and the UV attenuation bump at high redshifts, fueling an explosion of extragalactic research using PAHs as tracers of star formation, dust processing, and galaxy evolution.

Yet, many fundamental questions about the life cycle of PAHs and fullerenes remain unanswered: How do these molecules form and survive under the extreme conditions of space? How do their physical and chemical properties transform over cosmic time? What roles do they play in shaping the lifecycle of interstellar matter? Laboratory experiments and quantum chemical calculations are essential to address these questions, enabling robust interpretation of observations and identification of molecular structures and processes. A comprehensive understanding of interstellar aromatics also requires connecting them to other spectral signatures, including the diffuse interstellar bands in the optical and the radio detections of small PAHs in cold molecular clouds.

This symposium will bring together experts from observational astronomy, laboratory astrophysics, theoretical modeling, and quantum chemistry to explore the latest discoveries and future frontiers in PAH and fullerene research. With a special emphasis on extragalactic PAH studies, we will discuss how new observational capabilities (e.g., JWST, SPHEREx) and cutting-edge theoretical and experimental approaches can expand our understanding of these key interstellar species.

The meeting is the fourth installment in a series of international symposia on interstellar PAHs, following previous editions in Toulouse (2010), Noordwijk (2016), and Aarhus (2022).

Scientific Organizing Committee (SOC):
Els Peeters (Western University, Canada, co-chair)
Jan Cami (Western University, Canada, co-chair)
Ewen Campbell (University of Edinburgh, United Kingdom)
Ryan Fortenberry (University of Mississippi, USA)
Sarah Gallagher (Western University, Canada)
Takashi Onaka (The University of Tokyo, Japan)
Jos Oomens (Radboud University, The Netherlands)
Amit Pathak (Banaras Hindu University, India)
Karin Sandstrom (University of California, San Diego, USA)
Irene Shivaei (Centro de Astrobiologia, Spain)
Xander Tielens (University of Maryland, USA)

The Olympian Symposium 2026

We are pleased to announce the upcoming Olympian Symposium 2026, “The evolution of interstellar medium across cosmic times”. This is the 5th in the Olympian Symposium series, and it will take place during 18-22 May, 2026, in Paralia Katerini, Greece, at the Mediterranean Village Hotel, located by the sea at the foot of the world-famous Mount Olympus.

The Olympian Symposia began in 2014 and have since established themselves as a series of focused meetings on star formation and the interstellar medium, promoting collaboration and fruitful discussion in a unique setting that combines science with the inspiring environment of the sea and Mount Olympus.

The 2026 Symposium will continue this tradition, bringing together researchers from around the world to exchange new ideas and results. Further information, including registration, abstract submission, and travel details, will be shared in due course. Please visit the official website: olympiansymposium.org

We encourage you to join the website and enter your email to subscribe to the newsletter to receive all updates regarding the meeting.

We look forward to welcoming you to Mt. Olympus area in 2026 for what promises to be an exciting and stimulating Symposium. We include below the scientific rationale, the list of topics, and the members of the Scientific Organizing Committee.

[via Brandt Gaches]

One Postdoctoral Contract Mid-IR Evolved Stars at the Instituto de Astrofisica de Canarias (IAC)

The IAC (Tenerife) announces ONE postdoctoral contract to work on the project linked to the line of research “Nucleosynthesis and molecular processes in the late stages of stellar evolution”. The contract is funded by the project “The formation of fullerene molecular nanostructures in space” (NanoFullerenes; PID2023-147325NB-I00), led by Dr. Domingo Aníbal García-Hernández.

The successful candidate will pursue research in the following fields:
• Analysis of mid-infrared (IR) spectroscopic observations (Spitzer and James Webb space telescopes) of evolved stars.
• Comparison of laboratory and/or theoretical spectra with astronomical observations for molecular identifications.
• Scientific exploitation of the data provided by the James Webb Space Telescope (JWST) and preparation for data collection in Cycles 6 and 7.
•Preparation for obtaining (and subsequent analysis) of additional IR data on evolved stars.

Particular attention will be given to applicants with experience in the field of mid-IR spectroscopic data with space telescopes (Spitzer and JWST) and IR molecular identifications.

Complete information about this postdoc position and how to apply can be found here:
https://www.iac.es/en/employment/one-postdoctoral-contract-mid-ir-evolved-stars-2025-ps-2025-075
The deadline for applications is 16 November 2025

NanoSpace Training School on Advanced Characterization of Carbon Materials\

When: 20-22 January 2026
Where: Benasque (Pyrenees, Aragon), Spain
Registration Deadline: 30 November 2025
Contact email: arenal@unizar.es, agarcia@iac.es
Website: https://benasque.org/2026nanospace/

We are very happy to announce the “NanoSpace Training School on Advanced Characterization of Carbon Materials”; a COST NanoSpace Winter School on advanced characterization techniques of carbon materials and their potential applications in astrochemistry. The School will be held 20-22 January 2026 in Benasque (Pyrenees, Aragon), Spain.

All detailed information about the NanoSpace Training School on Advanced Characterization of Carbon Materials; i.e.,

programme, organising committee, registration, logistics, etc. can be found on the school's website at: https://benasque.org/2026nanospace/ (also available via the NanoSpace website: https://research.iac.es/proyecto/nanospace/.

The list of confirmed topics and lecturers/trainers is the following:
• Introduction to Carbon Nanomaterials ─ Chris EWELS, CNRS-IMN, France
• Kicking Out Electrons: What Photoemission Tells Us About Carbon Materials ─ Paola AYALA, Vienna Univ., Austria
• Transmission Electron Microscopy (TEM) - Imaging and Spectroscopy on Carbon Nanomaterials ─ Raúl ARENAL, INMA-CSIC-Universidad de Zaragoza, Spain
• Modelling for Experimentalists: The Case of Carbon Defects ─ Chris EWELS, CNRS-IMN, France
• Probing the Matter with infrared and Raman Spectroscopies: from Molecules to Solids ─ Cedric PARDANAUD, CNRS-PIIM, France
• Scanning Probe Microscopy/Spectroscopy (AFM, STM-STS, KPM...) Studies on Carbon Materials ─ José Ángel MARTIN-GAGO, ICMM-CSIC, Spain
• First principles modelling of electronic, structural, and vibrational properties of carbon materials ─ Vincent MEUNIER, Penn State Univ., USA
• Spectral features and Photophysics of Laboratory Analogues of Carbonaceous Nanograins ─ Thomas PINO, CNRS-ISMO, France
• Laboratory IR Spectroscopy of Astrophysically Relevant Molecules and Ions using Fancy Lasers ─ Jos OOMENS, HFML-FELIX, The Netherlands

This NanoSpace Training School on Advanced Characterization of Carbon Materials is organized by the COST Action NanoSpace (CA21126) (https://research.iac.es/proyecto/nanospace/). The main goal of the Advanced Characterization of Carbon Materials Training School is to provide specialized knowledge to PhD students and young researchers, systematically addressing the description of (nano)materials and the principal and advanced methods and techniques for their characterization and study, with a special emphasis on their potential applications in astrochemistry.

The School will be in person with attendance limited to 33 trainees and with priority given to PhD students and Young Researchers, who are strongly encouraged to participate. There is no registration fee and the NanoSpace COST Action will provide financial support (i.e. reimbursement after the event, covering full or partial travel, accommodation, and subsistence costs) for a significant number of participants (at least ~15-20), with high priority to those with a primary affiliation in an institution located in an Inclusiveness Target Country (ITC) / Near Neighbour Country (NNC) participating in the Action. The information requested in the registration form will be used to select the final list of registered participants as well as those eligible for financial support, which will be notified in advance of the Training School (i.e., by 5th December 2025). The attendees are expected to arrange their own travel and accommodation.
[via Anibal García-Hernández, NanoSpace Action Chair on behalf of the Organizing Committee]