AstroChemical Newsletter #114

June 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

Reexploring Molecular Complexity with ALMA: Insights into chemical differentiation from the molecular composition of hot cores in Sgr B2(N2)

A. Belloche, R. T. Garrod, H. S. P. Müller, N. J. Morin, S. A. Willis, K. M. Menten

We used ALMA to perform a line survey of the high-mass star forming region Sgr B2(N), called ReMoCA. We modeled under the assumption of LTE the spectra obtained toward the sources embedded in the secondary hot core Sgr B2(N2). We compared the chemical composition of these sources to that of sources from the literature and to predictions of the chemical kinetics model MAGICKAL. We detected up to 58 molecules toward Sgr B2(N2)'s hot cores, including up to 24 COMs, as well as many less abundant isotopologs. The compositions of some pairs of sources are well correlated, but differences also exist in particular for HNCO and NH2CHO. The abundances of series of homologous molecules drop by about one order of magnitude at each further step in complexity. The nondetection of radicals yields stringent constraints on the models. The comparison to the chemical models confirms previous evidence of a high cosmic-ray ionization rate in Sgr B2(N). The comparison to sources from the literature gives new insight into chemical differentiation. The composition of most hot cores of Sgr B2(N2) is tightly correlated to that of the hot core G31.41+0.31 and the hot corino IRAS 16293-2422B after normalizing the abundances by classes of molecules (O-, N-, O+N-, and S-bearing). There is no overall correlation between Sgr B2(N2) and the shocked region G+0.693-0.027 also located in Sgr B2, and even less with the cold starless core TMC-1. The class of N-bearing species reveals the largest variance among the four classes of molecules. The S-bearing class shows in contrast the smallest variance. These results imply that the class of N-bearing molecules reacts more sensitively to shocks, low-temperature gas phase chemistry after non-thermal desorption, or density. The abundance shifts observed between the N- and O-bearing molecules may indicate how violently and completely the ice mantles are desorbed. [abridged]

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DOI: 10.1051/0004-6361/202554411
Full-text URL: https://arxiv.org/abs/2505.03262

CoCCoA: Complex Chemistry in hot Cores with ALMA. The chemical evolution of acetone from ice to gas

Y. Chen, R. T. Garrod, M. Rachid, E. F. van Dishoeck, C. L. Brogan, R. Loomis, A. Lipnicky, and B. A. McGuire

Acetone (CH3COCH3) is one of the most abundant three-carbon oxygen-bearing complex organic molecules (O-COMs) that have been detected in space. Recently, acetone ice has been reported as (tentatively) detected toward B1-c, which enables the gas-to-ice comparison of its abundances. The detection of acetone ice warrants a more systematic study of its gaseous abundances which is currently lacking. Therefore, we conducted systematic measurements of acetone gas in a dozen hot cores observed by the CoCCoA survey and investigate the chemical evolution from ice to gas of acetone in protostellar systems. We fit the ALMA spectra to determined the column density, excitation temperature, and line width of acetone, along with propanal (C2H5CHO), ketene (CH2CO), and propyne (CH3CCH), which might be chemically linked with acetone. We found that the observed gas abundances of acetone are surprisingly high compared to those of two-carbon O-COMs, while aldehydes are overall less abundant than other O-COMs (e.g., alcohols, ethers, and esters). This may suggest specific formation or destruction mechanisms that favor the production of ethers, esters, and ketones over aldehydes. The derived physical properties suggest that acetone, propanal, and ketene have the same origin from hot cores as other O-COMs, while propyne tends to trace the more extended outflows. The acetone-to-methanol ratios are higher in ice than in gas by one order of magnitude, hinting at gas-phase reprocessing after sublimation. There are several suggested formation pathways of acetone (in both ice and gas) from acetaldehyde (CH3CHO), ketene, and propylene (C3H6). The observed ratios between acetone and the relevant species are rather constant across the sample, and can be well reproduced by astrochemical simulations, but more investigations are needed to draw solid conclusions.

A&A, 696, A198 (2025)
DOI: 10.1051/0004-6361/202453389
Full-text URL: https://arxiv.org/abs/2503.13770

Origin and transport of water in the Universe

Kirsanova, M. S., Baklanov, P. V., Vasiliev, E. O., Vasyunin, A. I.,Wiebe, D. S., Drozdov, S. A., Larchenkova, T. I., Likhachev, S. F., Moiseev, A. V., Pavlyuchenkov, Ya. N.; Sozinova, P. S.; Topchieva, A. P.; Tret'yakov, I. V., Fedoseev, G. S., Khudchenko, A. V., Shakhvorostova, N. N.

The origin and transport of water in the Universe are two of the key scientific programs for the Millimetron Space Observatory. This paper covers several astrochemical problems, from the formation of water in the local Universe to protoplanetary disks and comets. We discuss how to solve these problems with the Millimetron Space Observatory.

Physics Uspekhi, 68 278–293 (2025)
DOI: 10.3367/UFNe.2024.08.039744
Full-text URL: https://ufn.ru/en/articles/2025/3/e/

Polycyclic (anti)aromatic hydrocarbons: interstellar formation and spectroscopic characterization of biphenylene and benzopentalene

Athena R. Flint, Vincent J. Esposito, Ryan C. Fortenberry

Formation of biphenylene (C6H4)2 and its isomer benzopentalene, C12H8, may act as a consumption route for ortho-benzyne (o-C6H4) in interstellar clouds such as TMC-1. MRCI-F12 and CCSD(T)-F12 potential energy surfaces show that o-C6H4 dimerization is possible through a C2h-symmetry single-bond association to a (C6H4)2 precursor before isomerization to (C6H4)2 and subsequently C12H8. Formation of a bimolecular product set from either species is energetically hindered, allowing (C6H4)2 and C12H8 to stabilize radiatively. To remedy the dearth of spectroscopic data for these species, anharmonic frequencies from explicitly-correlated quartic force fields (QFFs) for o-C6H4 and c-C4H4 are employed to reparameterize the semiempirical method PM6 for use in lower-cost QFFs for (C6H4)2 and C12H8. In both cases, at least one reparameterized PM6-QFF spectrum results in the prominent C–H stretch and symmetric C–H out-of-plane-bend features to be accurately predicted with respect to gas-phase experiment or the B3LYP/N07D anharmonic absorption spectrum. B3LYP/N07D accurately recreates the experimental infrared spectrum of (C6H4)2, showing the utility of this method for spectral prediction of small and midsize polycyclic hydrocarbons on the whole. For larger systems, reparameterized PM6-QFF spectra can reproduce the most important infrared features for a species. B3LYP/N07D cascade emission spectra show that the 730 cm−1 C–H symmetric out-of-plane bending feature dominates the emission spectrum of (C6H4)2, while the spectrum of C12H8 becomes characterized by the collective set of C–H out-of-plane bends. As such, infrared emission spectra of (C6H4)2 will likely be overshadowed by C2H2. Derivatives such as cyanobiphenylene are likely better targets for infrared observation.

PCCP 2025 (Advance Article)
DOI: 10.1039/D5CP00630A
Full-text URL: https://pubs.rsc.org/en/content/articlelanding/2025/cp/d5cp00630a

Electron irradiation of crystalline nitrous oxide ice at low temperatures: Applications to outer Solar System planetary science

Duncan V. Mifsud, Sándor Góbi, Péter Herczku, Béla Sulik, Zoltán Juhász, Sergio Ioppolo, Nigel J. Mason, and György Tarczay

The radiation chemistry and physics of solid N2O have been increasingly studied due to its potential presence on the surfaces of cold, outer Solar System bodies. However, to date, no study has investigated systematically the influence of temperature on this chemistry and physics. In this present study, crystalline N2O ices were irradiated using 2 keV electrons at five different temperatures in the 20–60 K range and the radiolytic dissociation of the molecular solid (as well as the radiolytic formation of seven product molecules) was quantified through the G-value. Our results indicate that temperature does indeed play a role in the radiolytic destruction of crystalline N2O, with higher temperatures being associated with higher destruction G-values. The formation G-values of NO, NO2, N2O2, N2O3, N2O4, N2O5, and O3 were also noted to vary with temperature, with each product molecule exhibiting a distinct trend. The applications of our experimental results to further understanding solid-phase radiation chemistry in the outer Solar System are discussed.

2025, Low Temperature Physics, 51, 412-425
DOI: 10.1063/10.0036117
Full-text URL: https://arxiv.org/abs/2411.11936

Cosmic Ray Irradiation of Interstellar Ices on Sulfur-Rich Grains: A Possible Source of Sulfur-Bearing Molecules

Duncan V. Mifsud, Zuzana Kaňuchová, Olivier Auriacombe, Péter Herczku, Danna Qasim, Sándor T. S. Kovács, Richárd Rácz, Béla Sulik, Zoltán Juhász, István Rajta, István Vajda, Sándor Biri, Robert W. McCullough, Sergio Ioppolo, Ujjwal Raut, and Nigel J. Mason

The major reservoir of sulfur in dense interstellar clouds is still largely unknown, although a growing body of evidence suggests that it may exist in a refractory form (i.e., as minerals or allotropes of the element). Therefore, it is possible that the irradiation of sulfur-free interstellar ices on top of sulfur-rich refractory grain components by cosmic rays or stellar winds may result in the formation of simple inorganic sulfur molecules that could be readily detected by ground- or space-borne telescopes. In this study, we have irradiated neat ices of O2, CO, CO2, and H2O on top of layers of allotropic sulfur at 20 K using 1 MeV He+ ions as a mimic of space radiation. Experiments with CO2 and H2O ices were also repeated at 70 K to provide data obtained under conditions more relevant to icy bodies in the outer solar system for comparative purposes. We have found qualitative mid-infrared spectroscopic evidence for the synthesis of SO2, CS2, OCS, and H2SO4 hydrates, but not H2S, in our experiments and have quantified the efficiency of their formation by calculating the G-value (i.e., the number of molecules formed per 100 eV of energy deposited) for each ice-refractory system. Overall, SO_2 and CS_2 are the most commonly observed products in our experiments, although the highest G-value was that for H_2SO_4 hydrates formed as a result of the irradiation of H_2O ice on top of sulfur at 70 K. An important outcome of our study is that our experimental results are consistent with recent observational surveys that suggest SO_2 formation in interstellar ices proceeds primarily via an “energetic” route involving radiolytic processes, while OCS forms as a result of “nonenergetic” processes such as atom or radical addition reactions.

2025, ACS Earth and Space Chemistry, 9, 1227-1242
DOI: 10.1021/acsearthspacechem.5c00036
Full-text URL: https://pubs.acs.org/doi/10.1021/acsearthspacechem.5c00036

The AstroPAH 10 Years of Science Review

H. R. Hróðmarsson, I. Aleman, A. Candian, S. Wiersma, J. Palotás, D. Dubois, A. Sidhu, D. Loru, P. Sundarajan, E. Sciamma-O’Brien, A.G.G.M. Tielens

We celebrate the first ten years of the AstroPAH Newsletter by giving an overview of the scientific advances in the field of polycyclic aromatic hydrocarbons (PAHs) in astronomical environments that have been disseminated through the AstroPAH newsletter. This overview comprises ten chapters – each of which comprising subsections focused on observations, experiments, theory, and modeling – dedicated to subjects such as infrared emission, ultraviolet processing, dust, H_2 formation, galaxies, dark molecular clouds, Herbig Ae/Be stars and protoplanetary disks, solar system objects, the diffuse interstellar bands, and the anomalous microwave emission.

Space Sci. Rev., 221, 42 (2025)
DOI: 10.1007/s11214-025-01161-x
Full-text URL: https://doi.org/10.1007/s11214-025-011

APE: An analytical protostellar environment to provide physical conditions to chemical models and synthetic observations

Pierre Marchand, Audrey Coutens, Antoine Espagnet, Fernando Cruz-Sáenz de Miera, Jean-Christophe Loison, Valentine Wakelam

Chemical modeling and synthetic observations are powerful methods to interpret observations, both requiring a knowledge of the physical conditions. In this paper, we present the Analytical Protostellar Environment (APE) code, which aims at making chemical simulations and synthetic observations accessible. APE contains a physical model of protostellar evolution (including the central object, the envelope, the protoplanetary disk and the outflow) as well as interfaces to publicly available codes to perform chemical simulations, radiative transfer calculations, and synthetic interferometry imaging. APE produces density and temperature maps of protostellar systems. The code can also follow individual particles throughout their journey in a collapsing core. APE includes a treatment of the dust grain size-distribution to compute opacities self-consistently for subsequent radiative transfer. We show an example of application of APE by computing chemical abundance maps of CO, CN, CS, H_2CO, and CH_3OH in a Class I protostellar system. We also performed synthetic ALMA observations of their molecular emission assuming an edge-on source inclination. The moment 0 maps of CO, CS, and H_2CO display an X-shaped emission similar to what is observed toward the Class I source IRAS 04302+2247.

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Full-text URL: https://arxiv.org/abs/2505.11364

More π, please: What drives the formation of unsaturated molecules in the interstellar medium?

Jhoan Londoño-Restrepo, Santiago Gómez, Heidy M. Quitián-Lara, Felipe Fantuzzi and Albeiro Restrepo

We present a computational investigation into the fragmentation pathways of ethanolamine (C_2H_7NO, EtA), propanol (C_3H_8O, PrO), butanenitrile (C_4H_7N, BuN), and glycolamide ($C_2H_5NO_2$, GlA) — saturated organic molecules detected in the interstellar medium (ISM), particularly in the molecular cloud complex Sagittarius B2 (Sgr B2) and its molecular cloud G+0.693-0.027. Using electron-impact ionization data and Born-Oppenheimer molecular dynamics simulations, we investigate how cosmic rays, cosmic-ray-induced UV fields, and shock-induced heating can induce the fragmentation of these molecules, resulting in the formation of unsaturated species with extended pi-bond networks. Despite the attenuation of external UV radiation in G+0.693-0.027, these energetic processes are capable of driving partial transformations of saturated into unsaturated molecules, supporting the coexistence of species like EtA and GlA alongside unsaturated nitriles such as cyanoacetylene (HC_3N), cyanopropyne (CH_3C_3N), and cyanoallene (CH_2CCHCN). Our findings underscore the significance of high-energy mechanisms in enhancing chemical complexity within molecular clouds and offer insights into the pathways that govern the evolution of organic molecules in the ISM.

Chem. Sci., 2025, 16, 3051-3065
DOI: 10.1039/D4SC07986H
Full-text URL: https://pubs.rsc.org/en/content/articlehtml/2025/sc/d4sc07986h

Photodissociation of ethanolamine in interstellar clouds driven by UV and soft X-ray irradiation

Heidy M Quitián-Lara , Jhoan Londoño-Restrepo , Santiago Gómez , Kelly V García-González , Albeiro Restrepo ,

Nigel J Mason , Paola Caselli , Heloisa M Boechat-Roberty , Felipe Fantuzzi

We investigate the photoinduced fragmentation of ethanolamine (EtA, CH5NO), a prebiotically relevant amino alcohol detected in G+0.693–0.027, under ultraviolet (UV) and soft X-ray irradiation (12–310 eV) to explore its stability and chemical pathways in astrophysical environments. Experimental data were combined with Born–Oppenheimer molecular dynamics simulations, which revealed dominant fragmentation pathways and identified nitrogen-containing species as the major ionic products. Notably, CH2NH2+, a highly stable cation formed via C–C bond cleavage and charge localization on the nitrogen centre, emerged as a key fragment. While CH2NH2+ has not yet been detected in the interstellar medium, our results indicate it as a promising candidate for future astronomical searches. Calculated photoionization and photodissociation cross-sections enabled the estimation of photodissociation rates and half-lives for EtA under the X-ray conditions of Sgr B2. EtA exhibited a half-life on the order of 1e3 yr, comparable to other complex organic molecules like methyl formate (HCOOCH3) and acetic acid (CH3COOH), but shorter than simpler molecules such as formic acid (HCOOH). These findings reinforce EtA as a key astrochemical molecule with significant potential for astrobiological implications.

Monthly Notices of the Royal Astronomical Society, Volume 539, Issue 4, June 2025, Pages 3778–3788,
DOI: 10.1093/mnras/staf595
Full-text URL: https://academic.oup.com/mnras/article/539/4/3778/8128843

Binding Energies of Small Interstellar Molecules on Neutral and Charged Amorphous Solid Water Surfaces

T. Vorsselmans, E. Neyts

The interstellar medium (ISM) is all but empty. To date, more than 300 molecules have already been discovered. Because of the extremely low temperature, the gas-phase chemistry is dominated by barrierless exothermic reactions of radicals and ions. However, several abundant molecules and organic molecules cannot be produced efficiently by gas-phase reactions. To explain the existence of such molecules in the ISM, gas-surface interactions between small molecules and dust particles covered with amorphous solid water (ASW) mantles must be considered. In general, surface processes such as adsorption, diffusion, desorption, and chemical reactions can be linked to the binding energy of molecules to the surface. Hence, a lot of studies have been performed to identify the binding energies of interstellar molecules on ASW surfaces. Cosmic radiation and free electrons may induce a negative charge on the dust particles, and the binding energies may be affected by this charge. In this study, we calculate the binding energies of CO, CH4, and NH3, on neutral and charged ASW surfaces using DFTdensity functional theory calculations. Our results indicate that CO can interact with the surface charge, increasing its binding energy. In contrast, the binding energy of CH4 remains unchanged in the presence of surface charge, and that of NH3 typically decreases.

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DOI: 10.3847/1538-4357/add145
Full-text URL: https://arxiv.org/abs/2506.01431

A Catalytic Pathway for the Formation of Cyanobenzene in Nitrogen-rich Environments and the Spectroscopy of the Reactive Intermediates

V.J. Esposito, S. Alessandrini, D. Dubois, R.C. Fortenberry

The catalytic reaction of isocyanobenzene (C6H5NC) with NCN− produces cyanobenzene (C6H5CN) through various highly stable reactive intermediate species. Nitrogen-rich environments such as Titan's atmosphere serve as favorable locations to study reaction pathways involving nitrogenated species contributing to organic growth. Formation pathways of cyanobenzene have been characterized, but none with the contribution of anions or phenyl groups. In regions with a high abundance of nitrogen anions, such as Titan's atmosphere, reactions with species such as NCN− may play a role in the formation of cyanobenzene. Highly accurate computational methods are used to compute the rotational and vibrational spectroscopic properties of five thermodynamically stable reactive intermediate anions. Further, immense permanent dipole moments (∼10 D) make these five intermediates, and INT1 (phenyl–NCNCN−) in particular, highly detectable with radio astronomy, and searches with facilities such as the Atacama Large Millimeter/submillimeter Array and the Green Bank Telescope may lead to their discovery. Four of the reactive intermediates possess intense CN stretching transitions in the 2100–2200 cm−1 region that may produce a uniquely identifiable signal in high spatial and spectral resolution JWST spectra. Based on these reaction pathways, a future nondetection of isocyanobenzene in the atmosphere of Titan may point to cyanobenzene as a possible reservoir for this isomeric family of molecules.

Vincent J. Esposito et al 2025 Planet. Sci. J. 6 113
DOI: 10.3847/PSJ/adcf17
Full-text URL: https://iopscience.iop.org/article/10.3847/PSJ/adcf17/meta

Rotational Excitation of Vinyl Cyanide by Collisions with Helium Atoms at a Low Temperature

K. Sogomonyan; M. Ben Khalifa, J. Loreau

Among the numerous molecular systems found in the interstellar medium (ISM), vinyl cyanide is the first identified olephinic nitrile. While it has been observed in various sources, its detection in Sgr B2 is notable as the 2_11–2_12 rotational transition exhibits maser features. This indicates that local thermodynamic equilibrium conditions are not fulfilled, and an

accurate estimation of the molecular abundance in such conditions involves solving the statistical equilibrium equations, taking into account the competition between the radiative and collisional processes. This, in turn, requires the knowledge of rotational excitation data for collisions with the most abundant species, He or H2. In this paper, the first three-dimensional CH2CHCN–He potential energy surface is computed using the explicitly correlated coupled-cluster theory [(CCSD(T)-F12] with a combination of two basis sets. Scattering calculations of the rotational (de-)excitation of CH2CHCN induced by He atoms are performed with the quantum mechanical close-coupling method in the low-energy regime. Rotational state-to-state cross sections derived from these calculations are used to compute the corresponding rate coefficients. The interaction potential exhibits a high anisotropy, with a global minimum of −53.5 cm–1 and multiple local minima. Collisional cross sections are calculated for total energies up to 100 cm–1. When the cross sections are thermally averaged, collisional rate coefficients are determined for temperatures up to 20 K. A propensity favoring the transitions with Δka = 0 is observed.

ACS Earth Space Chem. 2025, 9, 2, 394–402
DOI: 10.1021/acsearthspacechem.4c00387
Full-text URL: https://arxiv.org/abs/2501.17679

Toward Unraveling Cyanopolyyne Surface Chemistry: A Preview on Isolated Systems from HC3N to Ethyl Cyanide and Propylamine

M. Raaphorst, J. Enrique-Romero, T. Lamberts

Cyanopolyynes, a family of nitrogen-containing carbon chains, are common in the interstellar medium and possibly form the backbone of species relevant to prebiotic chemistry. Following their gas-phase formation, they are expected to freeze out on ice grains in cold interstellar regions. In this work, we present the hydrogenation reaction network of isolated HC3N, the smallest cyanopolyyne, that consists of over-a-barrier radical–neutral reactions and barrierless radical–radical reactions. We employ density functional theory, coupled cluster, and multiconfigurational methods to obtain activation and reaction energies for the hydrogenation network of HC3N. This work explores the reaction network of the isolated molecule and constitutes a preview of the reactions occurring on the ice grain surface. We find that the reactions where the hydrogen atom adds to the carbon chain at the carbon atom opposite of the cyano group give the lowest and narrowest barriers. Subsequent hydrogenation leads to the astrochemically relevant vinyl cyanide and ethyl cyanide. Alternatively, the cyano group can hydrogenate via radical–radical reactions, leading to the fully saturated propylamine. These results can be extrapolated to give insight into the general reactivity of carbon chains on interstellar ices.

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DOI: 10.1021/acsearthspacechem.5c00021
Full-text URL: https://arxiv.org/abs/2505.19908

Can thermodynamic equilibrium be established in planet-forming disks?

Jayatee Kanwar, Peter Woitke, Inga Kamp, Paul Rimmer, Christiane Helling

The inner regions of planet-forming disks are warm and dense. The chemical networks used for disk modelling so far were developed for a cold and dilute medium and do not include a complete set of pressure-dependent reactions. The chemical networks developed for planetary atmospheres include such reactions along with the inverse reactions related to the Gibb's free energies of the molecules. The chemical networks used for disk modelling are thus incomplete in this respect. We want to study whether thermodynamic equilibrium can be established in a planet-forming disk. We identify the regions in the disk most likely to reach thermodynamic equilibrium and determine the timescale over which this occurs. We employ the theoretical concepts used in exoplanet atmosphere chemistry for the disk modelling with PROtoplanetary DIsk MOdel (ProDiMo). We develop a chemical network called CHemistry Assembled from exoplanets and dIsks for Thermodynamic EquilibriA (ChaiTea) that is based on the UMIST 2022, STAND, and large DIscANAlysis (DIANA) chemical networks. It consists of 239 species. From the STAND network, we adopt the concept of reversing all gas-phase reactions based on thermodynamic data. We use single-point models for a range of gas densities and gas temperatures to verify that the implemented concepts work and thermodynamic equilibrium is achieved in the absence of cosmic rays and photoreactions including radiative associations and direct recombinations. We then study the impact of photoreactions and cosmic rays that lead to deviations from thermodynamic equilibrium. We explore the chemical relaxation timescales towards thermodynamic equilibrium. Lastly, we study the predicted 2D chemical structure of a typical T\,Tauri disk when using the new {\sc ChaiTea} network instead of the large DIANA standard network, including photorates, cosmic rays, X-rays, and ice....

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Full-text URL: https://arxiv.org/abs/2505.13705

Can Implicit Solvation Methods Capture Temperature Effects on the Infrared Features of Astrophysical Ices?

D. A. B. Oliveira, V. S. A. Bonfim, F. Fantuzzi, S. Pilling

Astrophysical ices play a crucial role in the chemistry of cold interstellar environments. However, their diverse compositions, temperatures, and grain morphologies pose significant challenges for molecular identification and quantification through infrared observations. We investigate the ability of implicit solvation approaches to capture temperature-dependent infrared spectral features of CO2 molecules embedded in astrophysical ice analogues, comparing their performance to that of explicit ice models and experimental data. Using DFT calculations and vibrational frequency scaling, we model CO2 trapped in both amorphous (cold) and crystalline (warm) H2O ice clusters. The implicit model qualitatively identifies certain trends but fails to reliably capture the magnitude of frequency shifts and band strengths. Explicit models correctly reproduce the gas-to-solid redshifts for both the asymmetric stretch and bending modes; however, neither approach successfully replicates the experimentally observed temperature-dependent trend in the bending mode. While continuum-like methods may be useful as first-order approximations, explicit modelling of the molecular environment is essential for accurately simulating the infrared spectral behaviour of CO2 in astrophysical ices and for interpreting observational data on ice composition and evolution.

Photochem 2025, 5(1), 5.
DOI: [10.3390/photochem5010005](https://doi.org/10.3390/photochem5010005)
Full-text URL: https://www.mdpi.com/2673-7256/5/1/5

Hidden under a warm blanket: If planets existed in protostellar disks, they would hardly produce observable substructures

P. Nazari, A. D. Sellek, G. P. Rosotti

The onset of planet formation is actively under debate. Recent mass measurements of disks around protostars suggest an early start for planet formation in class 0/I disks. However, dust substructures, one possible signature of forming planets, are rarely observed in the young class 0/I disks, while they are ubiquitous in the mature class II disks. It is not clear whether the lack of dust substructures in class 0/I disks indicates an absence of planets or whether it is due to other physical effects such as temperature and dust opacity. Here, we consider the effect of temperature on the ability of planets to produce dust substructures. We prescribed the evolution of the disk and the protostar from class 0 to the class II phase and calculated the disk temperature using radiative transfer models at various stages of the evolution. We used the mid-plane temperature to calculate the disk scale height and the minimum planet mass needed to open observable dust gaps using the thermal criterion. We find that this minimum planet mass decreases as a function of time. In particular, we find that if a planet up to ∼5 M⊕ in the inner ∼5 au or up to ∼10-50 M⊕ at radii ≳5 au were already formed in the early protostellar phase (t < 2e5 yr), it would barely produce any dust substructures. We conclude that a major contribution to the observed lack of substructures (if produced by planets) in the early protostellar phase – lowering their frequency by ∼50% – could be elevated temperatures rather than the absence of planets.

Astronomy & Astrophysics, Volume 697, id.A84, 14 pp.
DOI: [10.1051/0004-6361/202451116](https://doi.org/10.1051/0004-6361/202451116)
Full-text URL: https://arxiv.org/abs/2410.09042

Announcements

ASI Symposium 004 on Genesis and Evolution of Organics in Space (2 Symposium of Organics in Space consortium) | Bangalore India | 16-18 July 2025

We are delighted to invite you to participate in the ASI Symposium 004 on "Genesis and Evolution of Organics in Space" (the 2nd Symposium of the Organics in Space consortium), to be held at GITAM University, Bengaluru, India, from 16th to 18th July 2025. This event is part of the Astronomical Society of India (ASI) symposium series for this year.

This multidisciplinary symposium aims to bring together researchers from chemistry, astrophysics, planetary science, astrobiology, and related fields to explore the formation, transformation, and detection of organic molecules in diverse astrophysical environments. The presented talks and posters will be peer-reviewed, and selected contributions will be published in a conference proceedings in the form of an article. There are Best Poster Prizes for outstanding contributions by students and post-docs.

Building on the success of the inaugural symposium held at the Indian Institute of Space Science and Technology (IIST) in January 2024, this edition will further strengthen collaborative efforts, showcase cutting-edge research, and highlight the significance of organics in shaping future space missions.

We look forward to your participation in this exciting scientific gathering!

Key Details:
Dates: 16–18 July 2025

Venue: GITAM University, Bengaluru
NH 207, Nagadenehalli, Doddaballapura Taluk,
Bengaluru, Karnataka 561203 India, [Location: https://maps.app.goo.gl/eZx3BYJZoBCEp3hn7]

Organized by: Department of Chemistry, School of Science, GITAM University, Bengaluru

For detailed information about registration, deadlines, confirmed speakers etc, please visit:
https://organicsinspace.in/second-symposium/
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Icarus Special Issue: Carbon in Planetary Environments

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

Funded PDRA position: 'Exploring the fundamentals of impact capture to maximize future dust collections’

The Centre for Astrophysics and Planetary Science at the University of Kent is pleased to announce that we have an STFC funded PDRA position available within the Impact Group.

The project is titled 'Exploring the fundamentals of impact capture to maximize future dust collections' and will make use of the Impact Groups two-stage light gas gun facility to explore the most appropriate methods to collect cosmic dust for three mission scenarios relating to space mission/experiment concepts currently in development. These are:
- The collection of dust from the volcanic plumes of Io
- The collection of dust from icy plumes of Enceladus
- The opportunistic collection of dust in the Near-Earth environment by space hardware.

The successful candidate will work with an interdisciplinary team led by Dr Penny Wozniakiewicz, which covers physics, planetary science, chemistry and biosciences. They will use a range of analytical instrumentation including optical and electron microscopes, GC-MS, MP-AES and Raman spectroscopy to assess the performance of different available capture media. They will also join our active external collaborations with members of Io and Enceladus dust sampling mission concept teams, providing key underpinning data for these, and future, mission concepts.

The closing date for applications is Monday 9th June, with interviews to be held the week of the 16th June.

For further information and details on how to apply please go to: https://jobs.kent.ac.uk/vacancy.aspx?ref=EMP-001-25-R

Alternatively, if you have any questions please don't hesitate to contact Penny Wozniakiewicz at pjw@kent.ac.uk