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Abstracts

Revealing SO2 and CO2 adsorption features on forsterite via IR spectroscopy and automated computational approaches

Eric Mates-Torres, Guillermo Escolano Casado, Lorenzo Mino, Nadia Balucani, Piero Ugliengo, Albert Rimola

The interaction between interstellar molecules and silicate dust plays a critical role in the chemical evolution of interstellar and circumstellar environments. In this work, we combine in situ infrared (IR) spectroscopy with automated density functional theory (DFT) calculations to investigate the adsorption and vibrational signatures of CO2 and SO2 on forsterite surfaces. Experimental IR spectra collected under cryogenic conditions reveal coverage- and temperature-dependent features that evolve from physisorbed to chemisorbed regimes. To interpret these observations, we construct theoretical spectra from a large ensemble of adsorption configurations across multiple surface terminations, weighted by their Boltzmann distributions at 100 K and by a per-surface abundance factor. The resulting spectra reproduce key experimental features, enabling the identification of binding trends. For CO2, we predict the transition from weakly bound species to carbonate-like modes at lower frequencies. For SO2, our simulations identify the dominant bands due to bidentate and tridentate chemisorption. This integrative approach highlights the importance of surface morphology and thermodynamic weighting in reconciling theory and experiments providing a framework for the spectroscopic analysis of molecular adsorption on interstellar dust analogs.

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A Fully ab Initio Kinetic Monte Carlo Approach for Modeling Adsorption and Diffusion in Interstellar Icy Grain Mantles: The Case of H2S

Vittorio Bariosco, Stefano Pantaleone, Cecilia Ceccarelli, Piero Ugliengo, Albert Rimola

Understanding diffusion on interstellar ices is key to modeling the chemical evolution of cold molecular clouds, where low temperatures severely limit molecular mobility. In this study, we introduce a robust and fully automated multiscale computational framework to quantify diffusion processes of adsorbates at the surface of amorphous solid water (ASW). Using H2S as a test case, whose binding sites were previously studied at the ab initio level, we constructed a detailed network of 141 adsorption sites connected by over 270 transition states. All density functional energetics were benchmarked against DLPNO−CCSD(T), achieving chemical accuracy in the description of diffusion barriers, which span from 0.1 to 27 kJ mol−1 with a median value of 5.4 kJ mol−1. An off-lattice kinetic Monte Carlo (kMC) model adopting both the ab initio diffusion barriers and binding energies for the desorption processes was carried out to compute temperature-dependent diffusion coefficients and to reconstruct the temperature-programmed desorption (TPD) curve. Our simulations reveal that thermal diffusion of H2S is negligible below 20 K, with diffusion coefficients as low as 10−48 cm2 s−1 at 10 K, thus excluding Langmuir− Hinshelwood surface encounters under typical dense cloud conditions. Moreover, under submonolayer conditions, diffusion was found to have negligible influence on the reconstructed TPD peak position. Furthermore, our results demonstrate that a universal scaling factor f to guess the diffusion barriers (ΔEdiff) from the sole knowledge of BE: f = ΔEdiff/BE does not apply as it exhibits wide variability across the sampled configurations. These findings highlight the need for incorporating statistically meaningful distributions of binding energies and diffusion barriers in astrochemical models to more accurately capture diffusion and surface reactivity on interstellar ices.

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Energy partitioning in H2 formation on interstellar carbonaceous grains. Insights from ab initio molecular dynamics simulations

Léana Jubert, Berta Martínez-Bachs, Gerard Pareras, Albert Rimola

Molecular hydrogen (H2) stands as the most abundant molecule within the interstellar medium (ISM), primarily originating from the coupling of two H atoms on the surfaces of dust grains. The role of dust grains during the H2 formation is of third bodies, dissipating the nascent reaction energy and thereby stabilizing the newly formed molecule and preventing it from dissociating back. Whether the formed H2 remains adsorbed or not on the surface (in this latter case undergoing chemical desorption, CD) largely depends on the type of grain and its capability to absorb the reaction energy excess. In diffuse interstellar clouds, dust grains are typically bare and are composed primarily of silicates or carbonaceous materials, while in denser regions they are covered in ices mostly of water. While water-ice-covered grains have been elucidated to be efficient third bodies, the behavior of carbonaceous grains is still unknown. In this study, ab initio molecular dynamics (AIMD) simulations are employed to analyze how the reaction energy is distributed between the newly formed H2 and a large graphene slab, as a model of carbonaceous grains in diffuse clouds, and assess the feasibility of CD. The results indicate that only a fraction of the reaction energy is absorbed by the surface, leaving the newly formed H2 with sufficient internal energy for CD to occur.

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Predicting accurate binding energies and vibrational spectroscopic features of interstellar icy species. A quantum mechanical study

Alicja Bulik, Berta Martínez-Bachs, Niccolò Bancone, Eric Mates-Torres, Marta Corno, Piero Ugliengo, Albert Rimola

In the coldest, densest regions of the interstellar medium (ISM), dust grains are covered by thick ice mantles dominated mainly by water. Although more than 300 species have been detected in the gas phase of the ISM by their rotational emission lines within the radio frequency range, only a few were found in interstellar ices, e.g. CO, CO2, NH3, CH3OH, CH4 and OCS, by means of infrared (IR) spectroscopy. Observations of ices require a background-illuminating source for absorption, constraining the available sight lines for investigation. Further challenges arise when comparing with laboratory spectra due to the influence of temperature, ice structure and the presence of other species. In the era of IR observations provided by the James Webb space telescope (JWST), it is crucial to provide reference spectral data confirming JWST's assigned features. For this purpose, this study addresses the adsorption of the aforementioned species on water ice surfaces and their IR features by means of quantum chemical computations grounded on the density functional theory (DFT) hybrid B3LYP-D3(BJ) functional, known to give reliable results for binding energy and vibrational frequency calculations, including IR spectra simulation. The calculated binding energies and IR spectral data are presented in the context of experimental spectra of ices and the new findings from the JWST, which have already proven to be insightful thanks to its unmatched sensitivity. We show that quantum chemistry is a powerful tool for accurate frequency calculations of ISM ice interfaces, providing unprecedented insights into their IR signatures.

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The role of the pre-exponential factor on temperature programmed desorption spectra: A computational study of frozen species on interstellar icy grain mantles

S. Pantaleone; L. Tinacci; V. Bariosco; A. Rimola; C. Ceccarelli; P. Ugliengo

Temperature programmed desorption (TPD) is a well-known technique to study gas-surface processes, and it is characterized by two main quantities: the adsorbate binding energy and the pre-exponential factor. While the former has been well addressed in recent years by both experimental and computational methods, the latter remains somewhat ill-defined, and different schemes have been proposed in the literature for its evaluation. In the astrochemistry context, binding energies and pre-exponential factors are key parameters that enter microkinetic models for studying the evolution over time of the chemical species in the universe. In this paper, we studied, by computer simulations, the effect of different pre-exponential factor models using water, ammonia, and methanol adsorbed on amorphous and crystalline ices as test cases: specifically, the one most widely used by the astrochemical community (Herbst–Hasegawa), the models provided by Tait and Campbell, and an extension of the Tait formulation including the calculation of the vibrational partition function. We suggest the methods proposed by Tait and Campbell that provide TPD temperature peaks within 30 K of each other while avoiding demanding quantum mechanical calculations, as they are based on tabulated data. Finally, when the explicit inclusion of the vibrational partition function is needed, we propose a cost-effective strategy to include all the thermal contributions in the partition functions without the need for performing a full vibrational calculation of the whole system.

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Quantum mechanical investigation on the formation of silicate building blocks on interstellar ice mantles

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Silicon monoxide (SiO), a diatomic molecule present in the interstellar medium, probably contributes to the formation of silicate dust grains since orthosilicic acid (Si(OH)4), a SiO derivative, is a precursor of silica and silicates. The formation of Si(OH)4 is investigated here by means of quantum chemical computations, characterizing the interaction and reactivity of SiO with water ice mantles (modelled through different cluster systems) that coat interstellar dust grains in dense clouds. Several reaction pathways involving SiO and H2 O were simulated with the aim of forming Si(OH)2 and subsequently Si(OH)4 . Results highlight that the ice mantle not only supplies a reactant, H2O, but also acts as a chemical catalyst, reducing the energy barrier of the process. The formation of the Si(OH)2 precursor is a crucial step, occurring easily by reaction of SiO with H2O. Subsequently, both the Si(OH)2 + O → OSi(OH)2 + H2O → Si(OH)4 and Si(OH)2 + 2 O → O2Si(OH)2 + 2 H → Si(OH)4 paths have been found to be energetically favourable towards Si(OH)4 formation due to being barrierless, although formation of H2 Si(OH)2 by H addition to Si(OH)2 is a potential competitive channel. This study provides evidence that orthosilicic acid can form due to the addition of H2O, O, and H to SiO on water ice mantles, indicating that silicate grains can potentially form and grow in cold interstellar regions, in addition to originating from material ejected by asymptotic giant branch stars and supernovae remnants. Our results show that grain surface reactions in dense clouds are important not only in the synthesis of volatile molecular species but also in the formation of silicate refractory material precursors.

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Hot Sulfur on the Rocks: The Reaction of Electronically Excited Sulfur Atoms with Water in an Ice-Surface Model

Gabriella Di Genova, Jessica Perrero, Marzio Rosi, Cecilia Ceccarelli, Albert Rimola, Nadia Balucani

In this contribution, we present a theoretical investigation of the reaction involving atomic sulfur in its first electronically excited state, 1D, and H2O on an ice-surface model. This study is motivated by the work of Giustini et al. (ACS Earth Space Chem., 2024, 8, 2318), which indicated a strong effect of the presence of four additional water molecules in the S(1D) + H2O reaction compared to the pure gas-phase case. Our simulation treats the long-range interactions (H-bonds and dispersion forces) with the ice water molecules in a much more realistic way being based on the use of a cluster of 18 water molecules, thus overcoming the limits of the small cluster used by Giustini et al. According to our results, S(1D) reacts via two possible reaction mechanisms: (1) addition to the O atom of a water molecule with the formation of H2OS or (2) insertion into one of the O−H bonds of a water molecule with the formation of HOSH. Both H2OS and HOSH are stabilized on ice by energy dissipation rather than isomerizing or dissociating into two products as seen in the gas-phase reaction. The interaction with surrounding water molecules affects the entire reaction pathway by stabilizing intermediate species, reducing some barriers, and impeding the only twoproduct open channel of the gas-phase reaction. S(1D) can be produced by UV-induced photodissociation of various precursor molecules on the surface of interstellar or cometary ice or by other high-energy processes induced by electrons or cosmic rays also in the ice bulk. Therefore, our results can be of help in elucidating the mysterious sulfur chemistry occurring in the icy mantles of interstellar grains or in cometary nuclei. Furthermore, this study demonstrates that the product branching ratios of gas-phase reactions should not be uncritically used in modeling interstellar ice chemistry.

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Rotational excitation of CO molecules colliding at low energy with a cold graphite surface

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Context. The CO molecule is of interest in various environments because, being IR active, it is often used as a tracer of inactive IR molecules. This is particularly important in the interstellar medium, where CO is the most abundant molecule after H2. Aims. We adopted our computational set-up to obtain insights into the surface elementary processes promoted by the interaction of gaseous CO molecules with graphitic grain surfaces and to resolve the rotational spectra of CO scattered at low collision energies by the cold substrate. Methods. Molecular dynamics simulations are based on a chemical state-to-state treatment,which, by explicitly including the coupling with substrate phonons and the role of long-range interactions, is suitable for controlling the rotational excitation of the incident molecules. Results. Sticking and state-resolved reflection coefficients for CO interacting in its ground roto-vibrational state and two low-lying rotational states with a cold graphite surface are determined. For collision energies lower than 0.01eV, CO adsorbs on a graphitic substrate with high probability, while reflected molecules populate excited rotational states up to level 7. The two atoms in the molecule probe a torque effect, arising from the asymmetric position of the C and O atoms in CO and from the different strengths of their interactions with graphite, influencing the interaction dynamics mainly for extremely low collision energies. In addition, a sort of resonance, more evident at the lowest energies, between the energy of impinging molecules and the phonons of the cold surface that promotes rotational excitation is highlighted for the lowest initial rotational state. Conclusions. Rotational energy transfer undergone by gaseous CO molecules in the ISM is not uniquely induced by CO–H2 collisions but can also be a consequence of the CO–graphitic grain interactions, and hence the amount of H2 inferred from IR spectroscopic measurements is presumably slightly overestimated.

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Exploring Forsterite Surface Catalysis in HCN Polymerization: Computational Insights for Astrobiology and Prebiotic Chemistry

Niccolò Bancone, Stefano Pantaleone, Piero Ugliengo, Albert Rimola, Marta Corno

Understanding the catalytic role of cosmic mineral surfaces is crucial for elucidating the chemical evolution needed for the emergence of life on Earth and other planetary systems. In this study, the catalytic role of silicate forsterite (Mg2SiO4) surfaces in the synthesis of iminoacetonitrile (IAN, HN=CH−CN) from the condensation of two hydrogen cyanide (HCN) molecules is investigated through quantum mechanical simulations. Using density functional theory calculations, the potential energy surfaces alongside the kinetics of various surface-mediated reactions leading to the formation of IAN are characterized. The effectiveness of forsterite as a catalyst is a delicate balance of the surface reactivity: on one side, the deprotonation of HCN is mandatory to trigger the dimerization; on the other side, the species should be weakly bound to the surface, thus allowing for their diffusion to meet with each other. The work reveals interesting counterintuitive results: the (120) and (101) forsterite surfaces (the less reactive ones) exhibit favorable catalytic properties for the reaction, in detriment to the (111) one (one of the most reactive). The implications of these findings in the astrobiology and prebiotic chemistry fields and for laboratory experiments are discussed, highlighting the potential role of cosmic silicates in the synthesis of complex organic molecules.

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Cosmic Silicate Surfaces Catalizing Prebiotic Reactions: Atomistic Modeling on the Polymerization of HCN

Niccolò Bancone, Stefano Pantaleone, Gerard Pareras, Piero Ugliengo, Albert Rimola, Marta Corno

Hydrogen cyanide, HCN, is a fundamental building block in astro- and cosmochemical environments, known for its ability to form prebiotically relevant molecules such as nucleobases. Although its polymerization is inhibited under the cold, dilute conditions of the interstellar medium, the higher temperatures of more evolved rocky bodies, combined with the presence of mineral surfaces, can catalyze the reaction. In this study, we use atomistic simulations grounded on the density functional theory (DFT) to elucidate the complete tetramerization pathway of HCN to diaminomaleonitrile (DAMN) and diaminofumaronitrile (DAFN), catalyzed by the crystalline Mg2SiO4 forsterite (120) surface. Results demonstrate that the intrinsic acid−base properties of the surface facilitate chemical bond formation/cleavage needed for HCN oligomerization, lowering activation barriers by ∼120−220 kJ mol−1 with respect to the gas-phase. Kinetic analyses reveal that the reactions are feasible at temperatures above 300 K, particularly under conditions present in warm, rocky bodies such as asteroids, meteorites, and planetary surfaces. The presence of water further accelerates key steps by assisting proton transfer processes. These findings support a model in which Mg-rich silicate minerals (abundant in the early Solar System) may have directly catalyzed the formation of complex organic molecules, which, in turn, are precursors of more complex biomolecules, thereby contributing to the essential chemical inventory for the emergence of life on early Earth and other primitive planets with propitious conditions.

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Formation of the glycine isomer glycolamide (NH2C(O)CH2OH) on the surfaces of interstellar ice grains: Insights from atomistic simulations

J. Perrero, S. Alessandrini, H. Ye, C. Puzzarini, A. Rimola

Context. Syn-glycolamide, a glycine isomer, has recently been detected in the G+0.693-0.027 molecular cloud. Investigations into its formation in the interstellar medium could offer insights into synthetic routes leading to glycine in prebiotic environments. Aims. Quantum chemical simulations on glycolamide (NH2C(O)CH2OH) formation on interstellar ice mantles, mimicked by a water ice cluster model, are presented. Methods. In this paper, we modeled glycolamide synthesis considering a stepwise process: the coupling between formaldehyde (H2CO) and the radical of formamide (NH2CO•) occurs first, forming the glycolamide precursor NH2C(— O)CH2O•, which is then hydrogenated to give anti-glycolamide. We hypothesize that anti-to-syn interconversion occurs in conjunction with glycolamide desorption from the ice surface. Results. The reaction barrier for NH2C(O)CH2O• formation varies from 9 to 26 kJ mol−1, depending on surface binding sites. Kinetic studies indicate that this reaction step is feasible in environments with a T > 35 K, until desorption of the reactants. The hydrogenation step leading to anti-glycolamide presents almost no energy barrier due to the easy H atom diffusion toward the NH2C(O)CH2O• intermediate. However, it competes with the extraction of an H atom from the formyl group of NH2C(O)CH2O•, which leads to formyl formamide, NH2C(O)CHO, and H2. Nonetheless, according to our results, anti-glycolamide formation is predicted to be the most favored reactive channel.

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Dust Absorption towards Supernova Remnant W44

Tian-Yu Tu, Adwin Boogert, Yang Chen, Wenlang He

Supernova remnants (SNRs) can strongly affect the chemical composition of the interstellar dust. In this paper we investigate to what degree the dust and ices are modified by observing four stars expected to be absorbed by a giant molecular cloud interacting with SNR W44, using medium-resolution spectroscopy in 2-5 μm. Absorption from H2O ice around 3.0 μm and aliphatic hydrocarbon dust around 3.4 μm were detected towards two stars, while probable CO ice at 4.67 μm towards one of them. Millimeter gas-phase CO J = 1-0 lines and three-dimensional dust extinction maps show that the dense molecular gas associated with W44 dominates (> 60%) the total interstellar extinction (A_K ~ 2.6) along these two sightlines. The H2O ice column densities are a factor of 1.5-3 lower than nearby MCs at similar extinctions, possibly because of the destruction of ice by shocks and cosmic rays (CRs) from W44, consistent with the low CO ice abundance relative to H2O (< 12%). One of the sightlines shows an unusually strong 3.4 μm aliphatic hydrocarbon absorption. If the carriers are located in diffuse dust along the sightline, unrelated to W44, its strength is ~ 4 times larger than those typically observed for diffuse dust clouds. Alternatively, the carriers may be enhanced in the W44 environment. We discuss several possible explanations, including shock formation of aliphatic hydrocarbons in diffuse clouds associated with W44, contribution from aliphatic hydrocarbons in shocked and CR-bombarded molecular clouds, and changes in the extinction law due to the SNR interaction.

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Chemistry and ro-vibrational excitation of CH+ in the planetary nebula NGC 7027

Milan Sil, Alexandre Faure, Helmut Wiesemeyer, Pierre Hily-Blant, Tomás González-Lezana, Josh Forer, Jérôme Loreau, François Lique

Small carbon hydride cations, such as the methylidyne ion (CH+), play an important role in the chemistry of the interstellar medium. They participate in gas-phase reaction networks leading to the formation of hydrocarbon species that serve as precursors to more complex organic molecules. CH+ is a highly reactive ion that is rapidly destroyed by H, H2, and free electrons, making its excitation challenging to model. Its level populations depend not only on radiative and inelastic processes but also on chemical formation and destruction rates, a mechanism known as chemical pumping. We investigate this effect using a new set of ab initio state-resolved ro-vibrational (reactive and inelastic) collision data to model the observed CH+ emission. Multiple rotational and ro-vibrational transitions of CH+ detected toward the planetary nebula NGC 7027 are analyzed. The chemical structure of CH+ is modeled with the CLOUDY code using updated reaction rates, providing the temperature and density structure across the nebula. A nonlocal thermodynamic equilibrium analysis is performed using CLOUDY and the single-zone RADEX code with a comprehensive set of spectroscopic and collisional data. In addition, chemical formation and destruction processes are implemented in RADEX and explored via Markov Chain Monte Carlo sampling. The CLOUDY model reproduces the observed CH+ line fluxes within a factor of 1.3 on average. It indicates that rotational and ro-vibrational lines arise from physically distinct regions, primarily differing in temperature. RADEX models show that chemical pumping significantly enhances populations above (υ=0, J=1), strongly increasing ro-vibrational emission, especially in the υ=2→1 band. Single-zone models remain limited, highlighting the need for full 1D modeling including all excitation processes.

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Nondiffusive Formation of Acetaldehyde on Interstellar Ices: An Atomistic Perspective

Berta Martínez-Bachs, Albert Rimola

The detection of interstellar complex organic molecules (iCOMs), such as acetaldehyde (CH3CHO), in cold astrophysical environments challenges standard grain-surface chemistry models, which rely on radical diffusion. At prestellar core temperatures (∼10 K), radical mobility is severely limited, making prevailing formation pathways inefficient. We here present a computational investigation of a nondiffusive, three-body reaction (3BR) mechanism for acetaldehyde formation on interstellar water ices. The mechanism involves the hydrogenation of CO to form HCO near a CH3 radical, enabling immediate reaction without requiring diffusion. We characterize the potential energy surface of the 3BR on a crystalline water ice model by identifying key minima and transition states, as well as evaluating competing pathways such as hydrogen abstraction. To assess the efficiency of this mechanism, ab initio molecular dynamics simulations were performed, with results indicating that CH3CHO can form efficiently at temperatures as low as 10 K. However, the formation of alternative products, such as CH4 and CO, or nonreaction between the newly formed HCO and the nearby CH3, is also observed, leading to an outcome distribution. These findings support the viability of 3BRs as a potential route for iCOM formation in cold interstellar environments.

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Full-text URL: https://iopscience.iop.org/article/10.3847/2041-8213/ae4a8e

Atomistic Modeling of Methyl Formate and Glycolaldehyde Formation on Interstellar Dirty Ice Mantles via a “Radical + Ice” Mechanism

Jessica Perrero, Stefano Pantaleone, Piero Ugliengo, and Albert Rimola

Methylformate (MF) and glycolaldehyde (GA) are two primogenital organic molecules detected in both cold and warm regions of the interstellar medium (ISM). Both gas-phase and grain-surface pathways have been proposed to explain their abundances, yet uncertainties remain, since prevailing grain-surface mechanisms favor the formation of GA over MF, which mismatch observations in different ISM regions. In this work, MF and GA synthetic reactions are atomistically modeled on surfaces containing variable H_2O and CO percentages (interstellar dirty ices), in which one of the reactants coming from the gas phase reacts with an icy CO, thus adopting the following two-step "radical + ice" mechanism: for MF, OCH_3 + CO(ice) -> $COOCH_3$ + H -> $HCOOCH_3$; for GA, CH_2OH + CO(ice) -> $COCH_2OH$ + H -> $HCOCH_2OH$. Calculations show that the first step presents an energy barrier (32–38 kJ/mol for MF and 17–20 kJ/mol for GA), while the second step is nearly barrierless. Although the energetics favor GA formation, the observed abundances are better explained by desorption phenomena rather than reaction barriers are argued. Specifically, the weaker binding energies of MF (16.8–46.1 kJ/mol) than GA (28.4–90.2 kJ/mol) support its higher abundance in the ISM.

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Full-text URL: https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/cplu.202500324

Low-energy glycine formation and spectral masking in star-forming regions

Eric Mates-Torres, Albert Rimola

The presence of amino acids in comets and meteorites has long suggested that prebiotic molecules may have formed in space and contributed to the origins of life on Earth. Glycine, the simplest amino acid, has been identified in several extraterrestrial environments, although its detection in the interstellar medium, including prestellar cores and protostellar regions, remains elusive. Here, we investigate a novel catalytic pathway for glycine formation on silicate grains during relatively warm (> 150 K) stages of star formation. Using atomistic simulations, the feasibility of a Strecker-type synthesis and a direct neutral mechanism involving reactivity between formaldehyde, carbon monoxide and ammonia on forsterite surfaces, the major constituent of interstellar dust, is assessed. Results show that the Strecker pathway is limited by high activation barriers, whereas the proposed direct mechanism proceeds through low-energy surfacestabilized intermediates leading to spontaneous formation of glycine in a single-barrier exoergic process. Additionally, glycine strongly adsorbs onto the mineral surface and is unlikely to desorb under warm conditions. A vibrational analysis reveals that glycine formed through this pathway exhibits spectrally distinct features, including suppression and shifting of characteristic bands, which may account for its persistent non-detection in astronomical observations.

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Experimental investigation of O_2 diffusion and entrapment in interstellar amorphous solid water

L. Coulaud, J. C. Santos, K.-J. Chuang

Context. Interstellar ices are mainly composed of amorphous solid water (ASW) containing small amounts of hypervolatiles, such as O_2, whose diffusion-limited reactions play a key role in space chemistry. Although O_2 is an important precursor molecule present during the early stages of ice formation, its surface diffusion in ASW remains poorly constrained. Aims. In this study, we experimentally investigate the surface diffusion and the entrapment efficiency of O_2 in porous ASW under astrophysically relevant conditions. Methods. Experiments were conducted in an ultrahigh vacuum chamber and monitored using infrared (IR) spectroscopy and quadrupole mass spectrometry. Diffusion coefficients were extracted through a novel approach applicable to IR-inactive molecules, by fitting the mass spectrometer signal during the isothermal phase with a Fickian model. These coefficients were then used to derive the diffusion energy barrier of O_2 in ASW. Entrapment efficiencies were measured by analyzing the subsequent temperature-programmed desorption phase. Results. We measured the surface diffusion coefficients at different temperatures (35K, 40K, 45K) and water ice coverages (40ML, 60 ML, 80 ML), yielding values on the order of $10^{-16}-10^{-15}$ cm^2 s^{-1}. From these values, we derived a diffusion energy barrier of E_{diff} = 10 ± 3 meV (116 ± 35 K), corresponding to a χ ratio of about 0.1. Entrapment measurements revealed that a residual amount of ∼20% of O_2 remains trapped in the ASW matrix at the highest temperatures investigated. Conclusions. This work demonstrates that the surface diffusion of IR-inactive molecules can be experimentally quantified using mass spectrometry. Our findings show that O_2 exhibits a low diffusion barrier, indicating high mobility in interstellar water ices. Moreover, we suggest these water ices likely retain a residual fraction of hypervolatiles entrapped within their structure.

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Announcements

Two PhD fellowships in Astrophysics and Planetary Science

The Niels Bohr Institute/Astrophysics and Planetary Science section invites applicants for two PhD fellowships in the chemistry of planet formation. The project is part of the Villum Young Investigator project “Chemistry meets Astrophysics: pathways to life-enabling ingredients during planet formation”.

Project 1

The PhD project 1 will investigate how the chemical composition of planet-forming disks shapes the volatile inventories of planets. Recent observations with the James Webb Space Telescope (JWST) have revealed a surprising diversity in the chemistry of inner disks, including systems that appear depleted in water but enriched in hydrocarbons. The project will combine infrared spectroscopic observations from JWST with data from the Atacama Large (sub-)Millimeter Array (ALMA) to characterize the chemical composition and physical structure of disks around very low-mass objects. These observations will be complemented by numerical simulations to put firm constraints on the physical and chemical processes responsible for the observed diversity. The project will help establish how variations in disk chemistry influence the building blocks of planets.

Start date is (expected to be) 01.09.2026 or as soon as possible thereafter.

Project 2
The PhD project 2 will focus on characterizing the solid budget of planet-forming disks, including both ices and refractory materials. The student will analyze infrared spectroscopic observations obtained with the James Webb Space Telescope (JWST), targeting a sample of protoplanetary disks. Spectral decomposition will be carried out using state-of-the-art fitting routines in combination with laboratory ice spectra, and the analysis will be complemented by radiative transfer modeling to derive ice column densities. By characterizing disk ices across a statistically significant sample, the project aims to reveal the chemical composition of the solid building blocks available for planet formation.

Start date is (expected to be) 01.01.2027 or as soon as possible thereafter.

Who are we looking for?
We are looking for candidates within the field(s) of physics, chemistry and biology. Applicants can have a background in astrophysics, astrochemistry, planetary science, or related fields, with experience in astronomical data analysis, radiative transfer, or numerical modeling considered an advantage.

Our group and research- and what do we offer?
The position will be hosted in the Astrophysics and Planetary Science section at the Niels Bohr Institute, University of Copenhagen. The group conducts research on star and planet formation, protoplanetary disks, and astrochemistry, with a strong focus on the observational characterization of the physical and chemical conditions in planet-forming environments. Members of the group combine observations from major international facilities, including JWST and the ALMA, with theoretical and numerical modeling to understand the origins of planetary systems and the chemical composition of embedded planets. The research environment is highly collaborative and international, welcoming new ideas. By promoting active engagement and the exchange of diverse perspectives, the research group aims at fostering a dynamic setting where innovative approaches can develop. This inclusive culture will strengthen the quality of the research while empowering team members to pursue novel directions and contribute meaningfully to the project’s goals.

Application deadline:
The deadline for applications is 26 May 2026, 23:59 GMT +2.

Link to job post: here

For specific information about the PhD fellowship, please contact Giulia Perotti (Giulia.perotti@nbi.ku.dk)
[via Giulia Perotti]

Invitation to contribute to EPSC 2026 SB9 – From Primitive Bodies to Rocky Planets: Carbon Chemistry and Chemical Evolution

We are organizing a session entitled ‘From Primitive Bodies to Rocky Planets: Carbon Chemistry and Chemical Evolution’ at this year’s EPSC, which will be run in a fully hybrid format from 6 to 11 September 2026 in The Hague (The Netherlands).

We invite contributions from all disciplines investigating carbon chemistry and its evolution, from primitive bodies to rocky planets and habitable environments. Whether through laboratory studies, observations, in situ measurements, or modeling, all approaches are welcome. You can find a more detailed session description at the following link, where you can also submit your abstract to SB9 (co-organized with EXOA): https://meetingorganizer.copernicus.org/EPSC2026/session/59187
Abstracts are due 13 May 2026, 13:00 CEST.
[via Nora Hänni, Pauline Lévêque, Niels Ligterink, Kelly Miller, Fabian Klenner, Cécile Engrand]

PDRA Position in Laboratory Astrochemistry (3-year STFC-funded post) – The Open University, UK

We are pleased to announce a new Postdoctoral Research Associate position in Laboratory Astrochemistry in the School of Physical Sciences at The Open University, funded by STFC. The post is for three years, based in Milton Keynes, and focuses on laboratory studies of interstellar ices to support the interpretation of JWST mid-infrared observations.

The successful candidate will lead a coordinated programme of experiments investigating how ice composition, thermal evolution, and grain-growth related scattering shape mid-IR ice band profiles. The role involves ultra-high vacuum ice film deposition, cryogenic methods, infrared spectroscopy, and the development of a novel acoustic-levitation system for studying microscopic ice aggregates.

Key details:
– Duration: 3 years
– Location: Milton Keynes, UK (laboratory-based role)
– Closing date: 31 May 2026
– Interviews: 17–18 June 2026 (in person where possible)
– Earliest start date: 1 October 2026
– Minimum education requirement: PhD in experimental physics/physical chemistry, laboratory astrochemistry or a closely related field.

Full job description and application link: here

[via Anita Dawes]