AstroChemical Newsletter #121

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Abstracts

Cryogenic Infrared Action Spectroscopy of $[H_2NCO]^+$ and $[H_2NCS]^+$, Protonated Forms of Interstellar HNCO and HNCS

M. Gerlach, N. R. Schneider, S. Petrić, H. Kaur, P. B. Changala, B. Redlich, S. Brünken

HNCS, isothiocyanic acid, and HNCO, isocyanic acid, are important molecules in the interstellar medium due to their composition of the essential atoms for organic life and their possible prebiotic role. They are assumed to be formed by dissociative recombination of their protonated versions, $[H_2NCO]^+$ and $[H_2NCS]^+$, where protonation may occur either on the N- or the O/S-atom. Here, we report the investigation of $[H_2NCO]^+$ and $[H_2NCS]^+$ by broadband infrared (IR) spectroscopy in a cryogenic 22-pole ion trap instrument via tag-free leak-out spectroscopy. Infrared radiation in the range of 450–3500 cm–1 was provided by the infrared free-electron laser FELIX-2 at HFML–FELIX. We predominantly observe the N-protonated isomers, H_2NCS^+ and H_2NCO^+, with potentially a small contribution of $HNCOH^+$. Five fundamental transitions in the range of 450–3500 cm–1 were observed of H_2NCO^+ and eight fundamental and overtone/combination bands of H_2NCS^+. The transitions are assigned with the help of quantum-chemical calculations using a combination of CCSD(T)/cc-pCVTZ for anharmonic transition energies and ωB97XD/cc-pVQZ for anharmonic transition intensities. Several modes show a rotational substructure, which is discussed in detail for the $\nu_5(b_1)$ bending vibrational mode of H_2NCS^+. The data presented in this paper is the first experimental study investigating the IR spectra of these ions and also the first experimental investigation of $[H_2NCS]^+$. This work provides important reference data for upcoming studies of formation mechanisms of HNCO and HNCS at cryogenic conditions.

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An interstellar energetic and non-aqueous pathway to peptide formation

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The origin of the molecular building blocks of life is a central question in science. A few α-amino acids, such as glycine, the simplest proteinogenic amino acid, have been detected in meteorites and comets, indicating an extraterrestrial origin for some prebiotic molecules. However, the formation of peptides, short chains of α-amino acids linked by peptide bonds, has remained unresolved under astrophysical conditions. Here we show that the building blocks of proteins can form in interstellar ice analogues exposed to ionizing radiation without the presence of liquid water. Using isotopically labelled glycine irradiated with protons at cryogenic temperatures, we detect the formation of glycylglycine, the simplest dipeptide, along with deuterated and undeuterated water as by-products. The formation of peptide bonds is confirmed by infrared spectroscopy and high-resolution mass spectrometry, which also reveal the production of other complex organic species. These findings demonstrate a non-aqueous route to peptide formation under space-like conditions and suggest that such molecules could form in the cold interstellar medium and be incorporated into forming planetary systems. Our results challenge aqueous-centric models of early biochemical evolution and broaden potential settings for the origins of life.

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Discovery of propadienone. Study of the chemistry of linear and cyclic H2C3O and H2C3S in TMC-1

G. Esplugues, J. C. Loison, M. Agúndez, G. Molpeceres, N. Marcelino, B. Tercero, and J. Cernicharo

We report the first detection in space of propadienone, the linear isomer (l-H2C3O) of cyclopropenone (c-H2C3O). We also report the first detection of the isotopologues c-H213CCCO and c-HDCCCO of c-H2C3O. The astronomical observations are part of QUIJOTE, a line survey of TMC-1 in the frequency range 31.0–50.3 GHz, complemented with data between 71.6–116.0 GHz, and carried out with Yebes-40 m and IRAM-30 m telescopes, respectively. We obtain a total column density of 3.7e10 cm−2 for l-H2C3O at an excitation temperature of 4.8 K. We find that the isomer is about eight times less abundant than the cyclic one. We also report a detailed line-by-line study of cyclopropenethione (c-H2C3S) to compare the abundance of the O and S isomers. We find that cyclic O-isomers are more abundant than cyclic S-isomers; however, the opposite trend is found for the most stable linear isomers, with l-H2C3S being more than one order of magnitude more abundant than l-H2C3O. A comprehensive theoretical chemical analysis shows that the abundances of the H2C3O and H2C3S isomers are controlled by different formation pathways. In particular, while l-H2C3O is potentially produced by dissociative electron recombination reactions, ion-neutral chemistry is more effective at producing l-H2C3S and c-H2C3S.

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Spectral survey of the diffuse gas toward BL Lac in the Q band

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The chemical composition of diffuse interstellar clouds is not fully established. They host an active chemistry despite their relatively low density and the ubiquitous presence of far-UV radiation. To further explore the chemical composition of diffuse clouds, we performed a spectral scan toward the bright radio source BL Lac in the Q band (from 32 to 50 GHz) using the Yebes 40 m telescope. Yebes observations were performed interleaving frequency switching and position switching integrations toward BL Lac, using a spectral resolution of 38 kHz. We achieved an unprecedented sensitivity on the continuum of 0.02–0.07%, allowing for the detection of very faint absorption features. We confirm previous detections of HCS+, C3H, C3H+, CH3CN, and HC3N in diffuse clouds and report new detections of CCS, C4H, CH3CHO, H2CCO, HNCO, and H2CS along the line of sight to BL Lac, with abundances relative to H2 from a few 1e-11 to a few 1e-10. We compiled molecular detections toward diffuse clouds to obtain the chemical inventory of a typical diffuse interstellar cloud. The chemical inventory of diffuse interstellar clouds includes complex organic species with up to four heavy atoms. These species are efficiently formed in the diffuse interstellar gas and reach abundances similar to those measured in dense photodissociation regions, pointing to similar gas-phase chemical processes.

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IR-Action Spectroscopy of the Astrochemically Relevant HCCS+ Cation

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The thioketenyl cation (HCCS+) has been recently detected in the dark cloud TMC-1 by radioastronomical observations within the QUIJOTE survey. However, the experimental infrared (IR) spectrum of this ion is yet to be reported in the literature. In this work, we demonstrate a method for the selective generation of the HCCS+ ion in the ground state and use this to obtain IR band positions. To do this, the IR (450–1850 and 3000–3350 cm–1) spectrum of H2-tagged HCCS+ has been measured in a cryogenic 22-pole ion trap via IR photodissociation (IR-PD) spectroscopy with the FELIX light source. The assignment of the experimental HCCS+ vibrational bands is aided by comparison with ab initio computed values. These findings will facilitate new reactivity investigations and spectroscopic measurements to be conducted, enabling HCCS+ to be included in astrochemical models and databases.

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Interstellar medium phases and abundances in the central parsec : JWST MIRI/MRS view of the Galactic center

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The Galactic center (GC) is a unique and extreme astrophysical laboratory for studying the interplay between gas, stars, and a supermassive black hole (SMBH). The circumnuclear disk (CND) and its central cavity (CC) present two contrasting environments in terms of gas content, density, and stellar activity. These regions are suited to study the multiphase structure and chemical composition of the interstellar medium (ISM). We aim to determine the temperature, density, abundances, and spatial distribution of the ISM phases in the central parsec of the GC, with focus on the ionized medium. We used new observations from the Mid-Infrared Instrument (MIRI) with the Medium Resolution Spectrometer (MRS) on the James Webb Space Telescope (JWST) to extract spectra from 5 to 27 microns in the CND and the CC. We used the photoionization code CLOUDY to generate synthetic spectra with the same coverage and resolution across a wide range of gas phases and abundances. We determined the contribution of each phase to the spectra. After estimating abundances and phase contributions, we identified four dominant phases and performed spatial analysis to determine their contribution to each spaxel in the datacubes. We find that in both the CND and the CC, most emission comes from warm ionized gas with temperatures between 10^4 and 10^4.8 K. In the CND, molecular gas contributes strongly and is spatially structured. In the CC, molecular gas is minimal, as expected. Coronal gas is detected in both regions at the interface between molecular and warm ionized gas. The hottest coronal phase is faint and patchy in the CC and elongated in the CND. Abundance fitting (solar-normalized logarithmic units) is constrained mainly by relative abundances. We measure depletion of Fe relative to alpha elements with log(Fe/alpha) = -0.78 ± 0.20 (CC) and -0.84 ± 0.26 (CND). CNO is mildly enhanced relative to alpha with log(CNO/alpha) = 0.27 ± 0.20 (CC) and 0.05 ± 0.26 (CND). Absolute abundances are supersolar but degenerate. Best-fit models give (log alpha, log CNO, log Fe) = (1.4, 1.4, 0.4) in the CC and (2.0, 1.8, 1.2) in the CND. The abundance pattern (enhanced CNO and alpha elements with suppressed Fe) indicates a chemically young environment enriched by core-collapse supernovae and stellar winds with limited Type Ia supernova input. This favors recent massive star formation over long-term enrichment. The orientation of the elongated hot coronal feature in the CND, perpendicular to the direction toward the SMBH, suggests a large-scale shock likely produced by past energetic outflows.

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Electric Fields Can Assist Prebiotic Reactivity on Hydrogen Cyanide

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Hydrogen cyanide (HCN) is present in many astrochemical environments, including interstellar clouds and comets. On Saturn's moon Titan, large amounts of HCN ice are present in the atmosphere and, following surface deposition, may influence both chemical and geological evolution. However, despite HCN's relevance to origin of life chemistry, the physiochemical properties of its solid state remain poorly characterized. For example, the crystals of HCN exhibit a range of rare properties, including pyroelectricity, and the ability to glow and jump under certain conditions. Here we use quantum chemical methods to predict HCN crystal surface energies, from which we derive the needle-like, high-aspect-ratio morphology of HCN nanocrystals. The predicted tips expose high-energy polar facets imbued with strong electric fields. We suggest that the combination of tips of opposite polarity helps to explain the cobweb-structure of solid HCN, and that fracture can transiently expose energetic surfaces, capable of catalysis at low temperature. One such process is predicted to be the near-barrierless formation of isocyanide (HNC) on HCN crystals, following proton addition or abstraction, for example, via radiation or acid/base-chemistry. Such field-assisted surface mechanisms may contribute to HCN-to-HNC isomerization under relevant conditions, and are suggested to explain part of the out-of-equilibrium abundance of HNC in cold environments such as Titan's atmosphere, and, potentially, in cometary comae.

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Binding Energies of Interstellar Complex Organic Molecules on Water Ice Surfaces: A Quantum Chemical Investigation

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Interstellar dust grains are enveloped by ices of frozen molecules in cold, dense regions of the interstellar medium (ISM), which are also observed in the gas phase. Whether a species is in the solid or gaseous state is governed by its binding energy (BE) on the grains. Hence, BEs are crucial in the solid-to-gas transition and are key input parameters for astrochemical models that simulate the physicochemical processes leading to the evolution of chemistry in the ISM. About 40% of the currently detected interstellar molecules belong to the category of interstellar complex organic molecules (iCOMs). This work aims to accurately evaluate the BEs of 19 iCOMs by means of quantum chemical calculations. Atomistic surface models simulating the structures of both crystalline and amorphous water ice were employed adopting a periodic approach, thereby accounting for the hydrogen bond (H-bond) cooperativity imparted by the extensive network present in the surfaces. A cost-effective but reliable procedure based on density functional theory was used to predict the structures of the adsorption complexes and calculate their BEs, which are mainly driven by H-bond and dispersion interactions, the latter presenting a fair contribution. A final discussion on the astrophysical implications of the computed BEs and the importance of obtaining reliable BEs on realistic interstellar ice surfaces in relation to the snow lines of iCOMs in hot cores/corinos and protoplanetary disks is provided.

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PDRs4All XVII: Formation and excitation of HD in photodissociation regions. Application to the Orion Bar.

Marion Zannese, Jacques Le Bourlot, Evelyne Roueff, Emeric Bron, Franck Le Petit, Dries Van De Putte, Maryvonne Gerin, Naslim Neelamkodan, Javier R. Goicoechea, John H. Black, Ryan Chown, Ameek Sidhu, Emilie Habart, Els Peeters and Olivier Berné

The James Webb Space Telescope enabled the first detection of several rovibrational emission lines of HD in the Orion Bar, a prototypical photodissociation region. This provides an incentive to examine the physics of HD in dense and strong PDRs. Using the latest data available on HD excitation by collisional, radiative and chemical processes, our goal is to unveil HD formation and excitation processes in PDRs by comparing our state-of-the-art PDR model with observations made in the Orion Bar and discuss if and how HD can be used as a complementary tracer of physical parameters in the emitting region. We compute detailed PDR models, using an upgraded version of the Meudon PDR code, which are compared to NIRSpec data using excitation diagrams and synthetic emission spectra. The models predict that HD is mainly produced in the gas phase via the reaction D + H2 = H + HD at the front edge of the PDR and that the D/HD transition is located slightly closer to the edge than the H/H2 transition. Rovibrational levels are excited by UV pumping. In the observations, HD rovibrational

emission is detected close to the H/H2 dissociation fronts of the Orion Bar and peaks where vibrationally excited H2 peaks, rather than at the maximum emission of pure rotational H2 levels. We derive an excitation temperature around Tex ~ 480 - 710 K. Due to high continuum in the Orion Bar, fringes lead to high noise levels beyond 15 μm, no pure rotational lines of HD are detected. The comparison to PDR models shows that a range of thermal pressure P = (3-9)e7 K cm−3 with no strong constraints on the intensity of the UV field are compatible with HD observations. This range of pressure is compatible with previous estimates from H2 observations with JWST. This is the first time that observations of HD emission lines in the near-infrared are used to put constraints on the thermal pressure in the PDR.

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JWST observations of photodissociation regions: II. Warm molecular hydrogen spectroscopy in the Horsehead nebula.

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H2 is the most abundant molecule in the interstellar medium and is a useful tool to study photodissociation regions, where radiative feedback from massive stars on molecular clouds is dominant. The James Webb Space Telescope, with its high spatial resolution, sensitivity, and wavelength coverage provides unique access to the detection of most of H2 lines and the analysis of its spatial morphology. Our goal is to use H2 line emission detected with the JWST in the Horsehead nebula to constrain the physical parameters (e.g., extinction, gas temperature, thermal pressure) throughout the PDR and its geometry. The study of H2 morphology reveals that FUV-pumped lines peak closer to the edge of the PDR than thermalized lines. From H2 lines, we estimate the value of extinction throughout the PDR. We find that AV is increasing from the edge of the PDR to the second and third H2 filaments. Then, we study the H2 excitation in different regions across the PDR. The temperature profile shows that the observed gas temperature is quite constant throughout the PDR, with a slight decline in each of the dissociation fronts. This study also reveals that the OPR is far from equilibrium. We observe a spatial separation of para and ortho rovibrational levels, indicating that efficient ortho-para conversion and preferential ortho self-shielding are driving the spatial variations of the OPR. Finally, we derive a thermal pressure in the first filament around P > 6x10^6 K cm−3, about ten times higher than that of the ionized gas. We highlight that template stationary 1D PDR models cannot account for the intrinsic 2D structure and the very high temperature observed in the Horsehead nebula. We argue the highly excited, over-pressurized H2 gas at the edge of the PDR interface could originate from the mixing between the cold and hot phase induced by the photo-evaporation of the cloud.

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Expanding the C3H6O2 Isomeric Interstellar Inventory: Discovery of Lactaldehyde and Methoxyacetaldehyde in G+0.693-0.027

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The tentative detection of 3-hydroxypropanal (HO(CH2)2C(O)H) toward the Galactic center molecular cloud G+0.693-0.027 prompts a systematic survey in this source aimed at detecting all C3H6O2 isomers with available spectroscopy. We use an ultra-deep broadband spectral survey of G+0.693-0.027, carried out with the Yebes 40 m and IRAM 30 m telescopes, to conduct the astronomical search. We report the first interstellar detection of lactaldehyde (CH3CH(OH)C(O)H) and methoxyacetaldehyde (CH3OCH2C(O)H), together with the second detections (i.e., confirmation) of methyl acetate (CH3C(O)OCH3) and hydroxyacetone (CH3C(O)CH2OH), and new detections in this source of both anti- and gauche-conformers of ethyl formate (CH3CH2OC(O)H), the latter tentatively. In contrast, neither propionic acid, CH3CH2C(O)OH, nor glycidol, c-CH2OCHCH2OH (i.e., the most and the least stable species within the C3H6O2 family, respectively) were detected, and we provide upper limits on their fractional abundances of ≤1.5e-10 and ≤3.7e-11. Interestingly, all C3H6O2 isomers can be synthesized through radical-radical reactions on the surface of dust grains, ultimately tracing back to CO as the parent molecule. We suggest that formation of the detected isomers is mainly driven by successive hydrogenation of CO, producing CH3OH and CH3CH2OH as the primary parent species. Conversely, propionic acid is thought to originate from the oxygenation of CO via the HOCO intermediate, which help us rationalize its non-detection. Overall, our findings notably expand the known chemical inventory of the interstellar medium and provide direct observational evidence that increasingly complex chemistry involving O-bearing species occurs in space.

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Abiotic Formation of Nitrile Precursors to Amino Acids and Nucleobases in Interstellar Ice Analogues

Jia Wang, Shiori Inada, Chaojiang Zhang, Joshua H. Marks, Zesen Wang, Alexandre Bergantini, Mason McAnally, André K. Eckhardt and Ralf I. Kaiser

Amino acids and the five canonical nucleobases have been identified in carbonaceous meteorites such as Murchison and Murray; however, their formation mechanisms under interstellar conditions have remained largely elusive. Here, we report the synthesis of biorelevant nitriles, key precursors to amino acids and nucleobases, in low-temperature interstellar model ices composed of hydrogen cyanide (HCN) irradiated with galactic cosmic ray proxies in the form of energetic electrons. Ammonia (NH3), trans-diazene (HNNH), methylamine (CH3NH2), ammonium cyanide (NH4CN), ethanimine (CH3CHNH), and nitriles including isocyanogen (CNCN), cyanamide (NH2CN), iminoacetonitrile (HNCHCN), N-cyanomethanimine (H2CNCN), and methyl cyanamide (CH3NHCN) were identified utilizing vacuum ultraviolet photoionization reflectron time-of-flight mass spectrometry combined with Fourier-transform infrared spectroscopy and quadrupole mass spectrometry. These results suggest that previously astronomically undetected trans-diazene, ammonium cyanide, and methyl cyanamide represent suitable targets for future astronomical searches. Furthermore, our findings provide fundamental insights into the non-equilibrium formation pathways leading to nitrogen-bearing molecules including complex nitriles in HCN-rich interstellar ices, thereby advancing our understanding of the abiotic origins of amino acids and nucleobases in extraterrestrial environments.

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Quantum chemical rovibrational spectroscopic data for possible observation of thiocarbonic acid (H2CS3) in interstellar environments

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The second-lowest conformer of thiocarbonic acid (cis–trans-H2CS3) lies 0.64 kcal mol−1 above the global minimum and possesses a 2.17 D dipole moment compared to the 0.75 D dipole moment of the cis–cis global minimum. While these properties are qualitatively similar to those of standard carbonic acid (H2CO3), the relative energy is lower, and the dipole moment of cis–cis-H2CS3 is higher than in cis–cis-H2CO3. As such, the quantum chemically computed spectroscopic constants and fundamental vibrational frequencies of these two conformers of thiocarbonic acid are provided in this work as well as those for the trans–trans conformer. Previous quantum chemical work has highlighted that the provided rotational constants should be within 3.5 MHz, if not 1.5 MHz, of experiment, and prior experimental work implies that this molecule can form on interstellar ices and be easily desorbed into the gas phase thereafter. Hence, these data will be able to assist in laboratory characterization or even potential interstellar searches for thiocarbonic acid.

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Broadband Vibrational Spectroscopy of Protonated and Radical Cationic Forms of Interstellar Formamide, [HCONH2]H+ and [HCONH2]+

Hunarpreet Kaur, Sara Petrić, Marius Gerlach, Britta Redlich, and Sandra Brünken

Formamide (HCONH2), the simplest organic molecule with a peptide bond, has been detected in various interstellar environments and is regarded as a potential precursor to essential biomolecules, such as amino acids and nucleic acids. Many of the proposed synthetic routes involve its ionized and protonated forms in the interstellar medium, where ion–molecule gas-phase reactions are predominant. However, spectroscopic data on cationic and protonated formamide is limited. In this work, we report the first bare-ion and Ne-tagged broadband vibrational spectra of isomeric forms of the formamide cation [HCONH2]+ (m/z 45) and protonated formamide [HCONH2]H+ (m/z 46). The vibrational spectra were obtained using two techniques, leak-out spectroscopy and Ne-tagging infrared predissociation spectroscopy, in a cryogenic 22-pole ion trap at the infrared free-electron laser facility HFML-FELIX. The measured spectra within the fingerprint region 650–1800 cm–1 are compared to anharmonic vibrational frequency calculations at the B2PLYP-D3/aug-cc-pVTZ level of theory for structural identification and band assignments. For the formamide cation, spectral signatures of both the low-energy aminohydroxycarbene isomer (NH2–C•+–OH) and the higher-energy canonical cation (HCONH2•+) were detected, while protonated formamide was observed exclusively as the more stable O-protonated isomer with no indication of N-protonation. Additionally, a comparative analysis of the two spectroscopic techniques, supported by potential energy surface and vibrational frequency calculations, highlights how the weakly bound Ne tag subtly affects the vibrational signatures of the ions.

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Isomer effects on neutral-loss dissociation channels of nitrogen-substituted PAH dications

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We investigate two nitrogen-containing isomers of PAHs, quinoline (Q) and isoquinoline (IQ), of composition C9H7N in collisions with keV energy O+ and O6+ ions. Employing ion-ion coincidence mass spectrometry, we find that loss of H, C2H2, and HCN are primary decay channels of Q2+ and IQ2+ dications, where HCN-loss is found to be the dominant decay channel. Moreover, a parallel experiment on naphthalene, the simplest PAH, reveals that HCN-loss in both isomers has a higher propensity than the analogous C2H2 loss of naphthalene. In PES calculation, Q2+ and IQ2+ are further identified to isomerize via seven-membered ring structures before emission of C2H2 and HCN. Also HCN and HCNH+ are the highest contributing fragments observed in fragmentation of both dications. The dominance of neutral HCN and HCNH+ cation in ion-induced dissociation of PANHs indeed can be one of reasons for the abundant detection of these species in Titan’s atmosphere.

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The Nucleated Atomistic Grain Growth Simulator (NAGGS): application to the size-dependent structural and physical properties of nanosilicate dust

Joan Mariñoso Guiu, Antoni Macià Escatllar, Stefan T. Bromley

We report the Nucleated Atomistic Grain Growth Simulator (NAGGS) as a new tool to model the growth of realistic nanosized dust grains through the progressive accretion of monomers onto a nucleated seed. NAGGS can be used with open source molecular dynamics codes, allowing for the modelling of grains that have different chemical compositions and are grown under a range of astrophysical conditions. To demonstrate how NAGGS works, we use it to produce 40 nanosilicate grain models with diameters of approx. 3.5 nm and consisting of approx. 1500 atoms. We consider Mg-rich olivinic and pyroxenic grains, and growth under two circumstellar dust-producing conditions. We calculate properties from the atomistically detailed nanograin structures (e.g. morphology, surface area, density, dipole moments) with respect to the size, chemical composition, and growth temperature of the grains. Our simulations reveal detailed new insights into the complex interacting degrees of freedom during grain growth and how they affect the resultant physicochemical properties. For example, we find that surface roughness depends on the Mg:Si ratio during this growth. We also find also find that nanosilicates have very high dipole moments, which depend on the growth temperature. Such findings could have important consequences (e.g. astrochemistry, microwave emission). In summary, our bottom-up physically motivated approach offers a detailed understanding of nanograins that could help in both interpreting observations and improving dust models.

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Quantification of abundance uncertainties in chemical models of exoplanet atmospheres

Marcelino Agúndez

Chemical models are routinely used to predict the atmospheric composition of exoplanets and compare it with the composition retrieved from observations, but little is known about the reliability of the calculated composition. We carried out a sensitivity analysis to quantify the uncertainties in the abundances calculated by a state-of-the-art chemical atmosphere model of the widely observed planets WASP-33b, HD209458b, HD189733b, WASP-39b, GJ436b, and GJ1214b. We found that the abundance uncertainties in the observable atmosphere are relatively small, below one order of magnitude and in many cases below a factor of two, where vertical mixing is a comparable or even larger source of uncertainty than (photo)chemical kinetics. In general, planets with a composition close to chemical equilibrium have smaller abundance uncertainties than planets whose composition is dominated by photochemistry. Some molecules, such as H2O, CO, CO2, and SiO, show low abundance uncertainties, while others such as HCN, SO2, PH3, and TiO have more uncertain abundances. We identified several critical albeit poorly constrained processes involving S-, P-, Si-, and Ti-bearing species whose better characterization should lead to a global improvement in the accuracy of models. Some of these key processes are the three-body association reactions S + H2, Si + O, NH + N, and N2H2 + H; the chemical reactions S + OH --> SO + H, NS + NH2 --> H2S + N2, P + PH --> P2 + H, and N + NH3 --> N2H + H2; and the photodissociation of molecules such as P2, PH2, SiS, CH, and TiO.

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Full-text URL: https://arxiv.org/abs/2512.02587

Announcements

PhD position in computational astrochemistry at University College Dublin

We invite applications for a PhD position in computational astrochemistry at the School of Physics at University College Dublin, Ireland. You will work with Dr Marie Van de Sande on the ERC Starting Grant ASHES on dust formation in the outflows of asymptotic giant branch (AGB) stars.

Most stars will go through an AGB phase near the end of their lives, losing their outer layers by means of a stellar outflow and enriching the interstellar medium (ISM) with the building blocks for the next generation of stars and planets. This outflow is driven by dust formation. Despite the importance of dust, we still do not know exactly how it is formed.

You will extend a large chemical reaction network to include dust nucleation, using the results of quantum chemical

calculations, and calculate the first 1D bottom-up dust growth models. As a next step, you will create 3D chemical models by post-processing hydrodynamical models, helping to close the gap between theory and observations. As part of the ERC Starting Grant ASHES, there are ample opportunities for attending conferences, workshops, and research stays.
This project would be suitable for a student with a degree in chemistry, physics or astronomy who wants to build on their skills in coding (python and Fortran), data analysis and visualisation, and would like to work in chemical kinetics modelling.

Application instructions
Applications should include a CV (including personal data, education, skills, and expertise), a one-page motivation letter, and the names and contact details of two references. Please send the documents to mvdsande@strw.leidenuniv.nl before 15 March 2026.

Inquiries
If you have any questions, contact Dr Marie Van de Sande at mvdsande@strw.leidenuniv.nl

Conference "Unifying Galactic and Extragalactic Views of Star Formation - Spectroscopic studies & Data Science", April 20-24, 2026, Paris (France)

https://daoism2026.sciencesconf.org

We have the pleasure to announce the upcoming workshop “Unifying Galactic and Extragalactic Views of Star Formation - Spectroscopic Studies & Data Science” . This workshop will take place at Institut d’Astrophysique de Paris from April 20th to April 24th. We will also broadcast the conference for registered participants through zoom.

The objectives of this workshop, at the interface between astronomy and data science, are to discuss spectroscopic studies of molecular clouds both locally in the Milky Way and in nearby galaxies. A focus will be put on the challenges posed by the analysis of large spectroscopic data sets, thanks to interdisciplinary discussions between data scientists and astronomers.

Research topics to be discussed at the conference will include:
- Multi-line observations of the Milky Way and nearby galaxies;
- Chemistry, magnetic field and star formation;
- Inverse problems, regularization and information theory;
- Statistical & Bayesian inference, machine learning and neural networks.

We welcome submission for oral contributions before 2026 February 27th in the evening.

Second Announcement — Exploring the aromatic universe in the JWST era

We are pleased to announce that abstract submission is now open for “Exploring the aromatic universe in the JWST era”, which will take place at Western University (London, Ontario, Canada) on 6–10 July 2026.

Important dates:
- Mon February 2, 2026: Abstract submission opens
- Spring 2026: Registration opens
- Sun March 15, 2026: Abstract submission deadline
- Wed April 15, 2026: Regular registration closes
- Mon June 15, 2026: Late registration closes

A list of confirmed invited speakers and additional details are available at: https://www.aromaticuniverse.space

Nautilus and KIDA training school

22 – 23 September 2026
Bordeaux (France)

Nautilus is a gas–grain astrochemical model. It is a three-phase model, which means that in addition to the gas phase, it treats ices as two separate phases: a surface and a bulk. It can be used in a variety of interstellar environments. Associated with Nautilus, the KIDA astrochemical database provides kinetic data for Nautilus based on laboratory and theoretical studies. Both Nautilus and KIDA are open to the public and available online here: https://astrochem-tools.org
Considering the number of new users each year, we propose a two-day training course on these tools. The program will include one day of lectures presenting the tools, followed by a hands-on session and time to work on users’ specific problems on the second day.
The number of participants is limited to 20 and registrations will be accepted on a first come, first served basis.

You can register through the link below before September 14th.

https://nautilus.sciencesconf.org

Atelier "Données de physique de référence pour la matière interstellaire et les atmosphères"

8-11 Juin 2026 Saint Florent (France)

Nous sommes heureux d'annoncer la tenue de l'atelier "Données de physique de référence pour la matière interstellaire et les atmosphères", qui aura lieu à Saint Florent (Corse, France) du 8 au 11 Juin 2026. Cet atelier vise à réunir physiciens, chimistes et astrophysiciens autour de la thématique des bases de données physico-chimiques nécessaires à l'interprétation des observations astrophysiques.

Les observations obtenues par les grands observatoires actuels (ALMA, JWST, IRAM, précurseurs de SKA) mettent en évidence une grande richesse moléculaire et facilitent l'accès aux états quantiques excités et aux raies de recombinaison, permettant une compréhension plus poussée des processus physiques et chimiques de nombreux objets astrophysiques. L'interprétation de ces observations n'est possible qu'en disposant de données physico-chimiques (spectroscopie, constantes de réactions, taux de collisions,...) et d'outils spécifiques mis à la disposition de la communauté dans le cadre des services nationaux d'observations.

Le but de l'atelier est de dresser un état des besoins des données physico-chimiques, et de coordonner les efforts de production de nouvelles données ainsi que de leur diffusion.

Les inscriptions sont ouvertes à l'adresse suivante: https://data-ism-2026.sciencesconf.org/

Date limite d'inscription: 10 mars 2026
Le nombre de places est limité à 40.