AstroChemical Newsletter #81

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Abstracts

Organic chemistry in the first phases of Solar-type protostars

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Planetary systems such as our own are formed after a long process where matter condenses from diffuse clouds to stars, planets, asteroids, comets and residual dust, undergoing dramatic changes in physical and chemical state in less than a few million years. Several studies have shown that the chemical composition during the early formation of a Solar-type planetary system is a powerful diagnostic to track the history of the system itself. Among the approximately 270 molecules so far detected in the ISM, the so-called interstellar complex organic molecules (iCOMs) are of particular interest both because of their evolutionary diagnostic power and because they might be potential precursors of biomolecules, which are at the basis of terrestrial life. This Chapter focuses on the evolution of organic molecules during the early stages of a Solar-type planetary system, represented by the prestellar, Class 0/I and protoplanetary disk phases, and compares them with what is observed presently in Solar System comets. Our twofold goal is to review the processes at the base of organic chemistry during Solar-type star formation and, in addition, to possibly provide constraints on the early history of our own planetary system.

Chapter on Organic Chemistry in low-mass star forming regions for Protostars & Planets VII
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FAUST VI. VLA 1623--2417 B: a new laboratory for astrochemistry around protostars on 50 au scale

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The ALMA interferometer, with its unprecedented combination of high-sensitivity and high-angular resolution, allows for (sub-)mm wavelength mapping of protostellar systems at Solar System scales. Astrochemistry has benefited from imaging interstellar complex organic molecules in these jet-disk systems. Here we report the first detection of methanol (CH3OH) and methyl formate (HCOOCH3) emission towards the triple protostellar system VLA1623-2417 A1+A2+B, obtained in the context of the ALMA Large Program FAUST. Compact methanol emission is detected in lines from Eu = 45 K up to 61 K and 537 K towards components A1 and B, respectively. LVG analysis of the CH3OH lines towards VLA1623-2417 B indicates a size of 0.11-0.34 arcsec (14-45 au), a column density N(CH3OH) = 1e16-1e17 cm-2, kinetic temperature > 170 K, and volume density > 1e8 cm-3. An LTE approach is used for VLA1623-2417 A1, given the limited Eu range, and yields Trot < 135 K. The methanol emission around both VLA1623--2417 A1 and B shows velocity gradients along the main axis of each disk. Although the axial geometry of the two disks is similar, the observed velocity gradients are reversed. The CH3OH spectra from B shows two broad (4-5 km/s) peaks, which are red- and blue-shifted by about 6-7 km/s from the systemic velocity. Assuming a chemically enriched ring within the accretion disk, close to the centrifugal barrier, its radius is calculated to be 33 au. The methanol spectra towards A1 are somewhat narrower (about 4 km/s), implying a radius of 12-24 au.

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Cosmic rays probed by H2 rovibrational lines: Is chemical modeling important to understand JWST H2 observations?

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Context: It has been proposed that H2 near-infrared lines may be excited by cosmic rays and allow for a determination of the cosmic-ray ionization rate in dense gas. One-dimensional models show that measuring both the H2 gas column density and H2 line intensity enables a constraint on the cosmic-ray ionization rate as well as the spectral slope of low-energy cosmic-ray protons in the interstellar medium (ISM). Aims: We aim to investigate the impact of certain assumptions regarding the H2 chemical models and ISM density distributions on the emission of cosmic-ray induced H2 emission lines. This is of particular importance for utilizing observations of these lines with the James Webb Space Telescope to constrain the cosmic-ray ionization rate. Methods: We compare the predicted emission from cosmic-ray induced, ro-vibrationally excited H2 emission lines for different one- and three-dimensional models with varying assumptions on the gas chemistry and density distribution. Results: We find that the model predictions of the H2 line intensities for the (1-0)S(0), (1-0)Q(2), (1-0)O(2) and (1-0)O(4) transitions at 2.22, 2.41, 2.63 and 3.00 μm, respectively, are relatively independent of the astro-chemical model and the gas density distribution when compared against the H2 column density, making them robust tracer of the cosmic-ray ionization rate. Conclusions: We recommend the use of ro-vibrational H2 line emission in combination with estimation of the cloud's H2 column density, to constrain the ionization rate and the spectrum of low energy cosmic-rays.

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Icy molecule desorption in interstellar grain collisions

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Observations of gaseous complex organic molecules (COMs) in cold starless and prestellar cloud cores require efficient desorption of the COMs and their parent species from icy mantles on interstellar grains. With a simple astrochemical model, we investigate if mechanical removal of ice fragments in oblique collisions between grains in two size bins (0.01 and 0.1 micron) can substantially affect COM abundances. Two grain collision velocities were considered - 10 and 50 meters per second, corresponding to realistic grain relative speeds arising from ambipolar diffusion and turbulence, respectively. From the smaller grains, the collisions are assumed to remove a spherical cap with height equal to 1/3 and 1 ice mantle thickness, respectively. We find that the turbulence-induced desorption can elevate the gas-phase abundances of COMs by several orders of magnitude, reproducing observed COM abundances within an order of magnitude. Importantly, the high gaseous COM abundances are attained for long time-scales of up to 1 Myr and for a rather low methanol ice abundance, common for starless cores. The simple model, considering only two grain size bins and several assumptions, demonstrates a concept that must be tested with a more sophisticated approach.

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Efficiency of Interstellar Nanodust Heating: Accurate Bottom-up Calculations of Nanosilicate Specific Heat Capacities

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Ultrasmall nanosized silicate grains are likely to be highly abundant in the interstellar medium. From sporadically absorbing energy from ultraviolet photons, these nanosilicates are subjected to significant instantaneous temperature fluctuations. These stochastically heated nanograins subsequently emit in the infrared. Previous estimates of the extent of the heating and emission have relied on empirical fits to bulk silicate heat capacities. The heat capacity of a system depends on the range of available vibrational modes, which for nanosized solids is dramatically affected by the constraints of finite size. Although experimental vibrational spectra of nanosilicates is not yet available, we directly take these finite size effects into account by using accurate vibrational spectra of low-energy nanosilicate structures from quantum chemical density functional theory calculations. Our results indicate that the heat capacities of ultrasmall nanosilicates are smaller than previously estimated, which would lead to a higher temperature and more intense infrared emission during stochastic heating. Specifically, we find that stochastically heated grains ultrasmall nanosilicates could be up to 35–80 K hotter than previously predicted. Our results could help to improve the understanding of infrared emission from ultrasmall nanosilicates in the ISM, which could be observed by the James Webb Space Telescope.

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Penetration of Nonenergetic Hydrogen Atoms into Amorphous Solid Water and their Reaction with Embedded Benzene and Naphthalene

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Chemical processes on the surface of icy grains play an important role in the chemical evolution in molecular clouds. In particular, reactions involving nonenergetic hydrogen atoms accreted from the gaseous phase have been extensively studied. These reactions are believed to effectively proceed only on the surface of the icy grains; thus, molecules embedded in the ice mantle are not considered to react with hydrogen atoms. Recently, Tsuge et al. suggested that nonenergetic hydrogen atoms can react with CO molecules even in ice mantles via diffusive hydrogenation. This investigation was extended to benzene and naphthalene molecules embedded in amorphous solid water (ASW) in the present study, which revealed that a portion of these molecules could be fully hydrogenated in astrophysical environments. The penetration depths of nonenergetic hydrogen atoms into porous and nonporous ASW were determined using benzene molecules to be >50 and ∼10 monolayers, respectively (1 monolayer ≈ 0.3 nm).

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Detecting chiral asymmetry in the interstellar medium using propylene-oxide

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(Abridged) Life is distinctly homochiral. The origins of this homochirality are under active debate. Recently, propylene-oxide has been detected in the gas-phase interstellar medium (ISM) (McGuire et al. 2016). The enantiomeric composition of ISM propylene-oxide may be probed through circular polarization measurements, but accurate estimates of the circular dichroism properties of the microwave transitions of propylene-oxide are not available. We develop a model of the circular dichroic activity in torsion-rotation transitions of closed-shell chiral molecules, such as propylene-oxide. With this model, we estimate the viability, and optimize observation strategies, of enantiomeric excess detection in ISM propylene-oxide. We present estimates for the dichroic activity of the torsion-rotation transitions of propylene-oxide, where we predict that the circular polarization fractions of emission lines of enantiopure propylene-oxide relevant to astronomical detection of propylene-oxide are on the order of 1e-6. Due to the low predicted circular polarization fractions, we conclude that enantiomeric characterization of propylene-oxide in the gas phase of the ISM is impossible with current astronomical observation techniques. We suggest that only chiral radical species may be viably employed for enantiomeric excess detection. We estimate that laboratory experiments may be successful in detecting the enantiomeric composition of a mixture of propylene-oxide through microwave dichroism spectroscopy. The theory we present in this paper provides a solid theoretical underpinning for such laboratory circular dichroism measurements in microwave transitions.

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Ice Age : Chemo-dynamical modeling of Cha-MMS1 to predict new solid-phase species for detection with JWST

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Chemical models and experiments indicate that interstellar dust grains and their ice mantles play an important role in the production of complex organic molecules (COMs). To date, the most complex solid-phase molecule detected with certainty in the ISM is methanol, but the James Webb Space Telescope (JWST) may be able to identify still larger organic species. In this study, we use a coupled chemo-dynamical model to predict new candidate species for JWST detection toward the young star-forming core Cha-MMS1, combining the gas-grain chemical kinetic code MAGICKAL with a 1-D radiative hydrodynamics simulation using Athena++. With this model, the relative abundances of the main ice constituents with respect to water toward the core center match well with typical observational values, providing a firm basis to explore the ice chemistry. Six oxygen-bearing COMs (ethanol, dimethyl ether, acetaldehyde, methyl formate, methoxy methanol, and acetic acid), as well as formic acid, show abundances as high as, or exceeding, 0.01% with respect to water ice. Based on the modeled ice composition, the infrared spectrum is synthesized to diagnose the detectability of the new ice species. The contribution of COMs to IR absorption bands is minor compared to the main ice constituents, and the identification of COM ice toward the core center of Cha-MMS1 with the JWST NIRCAM/Wide Field Slitless Spectroscopy (2.4-5.0 micron) may be unlikely. However, MIRI observations (5-28 micron) toward COM-rich environments where solid-phase COM abundances exceed 1% with respect to the water ice column density might reveal the distinctive ice features of COMs.

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Formation of the Simplest Amide in Molecular Clouds: Formamide (NH2CHO) and Its Derivatives in H2O-rich and CO-rich Interstellar Ice Analogs upon VUV Irradiation

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The astronomical detection of formamide (NH2CHO) toward various star-forming regions and in cometary material implies that the simplest amide might have an early origin in dark molecular clouds at low temperatures. Laboratory studies have proven the efficient NH2CHO formation in interstellar CO:NH3 ice analogs upon energetic processing. However, it is still under debate, whether the proposed radical-radical recombination reactions forming complex organic molecules remain valid in an abundant H2O environment. The aim of this work was to investigate the formation of NH2CHO in H2O- and CO-rich ices under conditions prevailing in molecular clouds. Therefore, different ice mixtures composed of H2O:CO:NH3 (10:5:1), CO:NH3 (4:1), and CO:NH3 (0.6:1) were exposed to vacuum ultraviolet photons in an ultra-high vacuum chamber at 10 K. Fourier-transform infrared spectroscopy was utilized to monitor in situ the initial and newly formed species as a function of photon fluence. The infrared spectral identifications are complementarily secured by a temperature-programmed desorption experiment combined with a quadrupole mass spectrometer. The energetic processing of CO:NH3 ice mixtures mainly leads to the NH2CHO formation, along with its chemical derivatives such as isocyanic acid (HNCO) and cyanate ion (OCN−). The formation kinetics of NH2CHO shows an explicit dependency on ice ratios and compositions; the highest yield is found in H2O-rich ice. The astronomical relevance of the resulting reaction network is discussed.

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Erratum "Temperature Spectra of Interstellar Dust Grains Heated by Cosmic Rays. II. Dark Cloud Cores" (2018, ApJS, 239, 6)

J. Kalvans

(No abstract)

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Ozone Production in Electron Irradiated CO2:O2 Ices

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The detection of ozone (O3) in the surface ices of Ganymede, Jupiter's largest moon, and of the Saturnian moons Rhea and Dione, has motivated several studies on the route of formation of this species. Previous studies have successfully quantified trends in the production of O3 as a result of the irradiation of pure molecular ices using ultraviolet photons and charged particles (i.e., ions and electrons), such as the abundances of O3 formed after irradiation at different temperatures or using different charged particles. In this study, we extend such results by quantifying the abundance of O3 as a result of the 1 keV electron irradiation of a series of 14 stoichiometrically distinct CO2:O2 astrophysical ice analogues at 20 K. By using mid-infrared spectroscopy as our primary analytical tool, we have also been able to perform a spectral analysis of the asymmetric stretching mode of solid O3 and the variation in its observed shape and profile among the investigated ice mixtures. Our results are important in the context of better understanding the surface composition and chemistry of icy outer Solar System objects, and may thus be of use to future interplanetary space missions such as the ESA Jupiter Icy Moons Explorer and the NASA Europa Clipper missions, as well as the recently launched NASA James Webb Space Telescope.

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Predicting binding energies of astrochemically relevant molecules via machine learning

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The behaviour of molecules in space is to a large extent governed by where they freeze out or sublimate. The molecular binding energy is thus an important parameter for many astrochemical studies. This parameter is usually determined with time-consuming experiments, computationally expensive quantum chemical calculations, or the inexpensive, but inaccurate, linear addition method. In this work we propose a new method based on machine learning for predicting binding energies that is accurate, yet computationally inexpensive. A machine learning model based on Gaussian Process Regression is created and trained on a database of binding energies of molecules collected from laboratory experiments presented in the literature. The molecules in the database are categorized by their features, such as mono- or multilayer coverage, binding surface, functional groups, valence electrons, and H-bond acceptors and donors. The performance of the model is assessed with five-fold and leave-one-molecule-out cross validation. Predictions are generally accurate, with differences between predicted and literature binding energies values of less than ±20%. The validated model is used to predict the binding energies of twenty one molecules that have recently been detected in the interstellar medium, but for which binding energy values are not known. A simplified model is used to visualize where the snowlines of these molecules would be located in a protoplanetary disk. This work demonstrates that machine learning can be employed to accurately and rapidly predict binding energies of molecules. Machine learning complements current laboratory experiments and quantum chemical computational studies. The predicted binding energies will find use in the modelling of astrochemical and planet-forming environments.

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Low-temperature nitrogen-bearing polycyclic aromatic hydrocarbon formation routes validated by infrared spectroscopy

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Polycyclic aromatic hydrocarbons (PAHs) are abundant in many regions of the Universe, representing a major reservoir for cosmic carbon. However, their formation pathways in cold regions of space remain elusive. Recent astronomical detections show that current astrochemical models drastically underestimate the abundance of aromatic molecules and suggest that additional formation pathways such as ion–molecule reactions need to be considered. Here we reveal efficient low-temperature formation pathways towards nitrogen-containing PAHs via exothermic pyridine+ and acetylene ion–molecule reactions. The experimental approach combines kinetics with spectroscopic probing and unambiguously identifies key reaction intermediates and the final nitrogen-containing PAH product quinolizinium+, a structure that is thought to contribute to the 6.2 μm interstellar emission feature. This study not only provides competing formation pathways relevant in the chemistry of the interstellar medium and Titan's atmosphere, but also delivers information to verify in-silico potential energy surfaces, astrochemical models and infrared observations.

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