AstroChemical Newsletter #69

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You can access the full abstracts by clicking the paper titles. Submit your abstracts before the 25th of each month for inclusion in the following newsletter.

Abstracts

Chemical analysis of prestellar cores in Ophiuchus yields short timescales and rapid collapse

Stefano Bovino, Alessandro Lupi, Andrea Giannetti, Giovanni Sabatini, Dominik R. G. Schleicher, Friedrich Wyrowski, Karl M. Menten

Sun-like stars form from the contraction of cold and dense interstellar clouds. How the collapse proceeds and the main physical processes driving it, however, are still under debate and a final consensus on the timescale of the process has not been reached. Does this contraction proceed slowly, sustained by strong magnetic fields and ambipolar diffusion, or is it driven by fast collapse with gravity dominating the entire process? One way to answer this question is to measure the age of prestellar cores through statistical methods based on observations or via reliable chemical chronometers, which should better reflect the physical conditions of the cores. Here we report APEX observations of ortho-H2D+ and para-D2H+ for six cores in the Ophiuchus complex and combine them with detailed three-dimensional magneto-hydrodynamical simulations including chemistry, providing a range of ages for the observed cores of 100-200 kyr. The outcome of our simulations and subsequent analysis provides a good matching with the observational results in terms of physical (core masses and volume densities) and dynamical parameters such as the Mach number and the virial parameter. We show that models of fast collapse successfully reproduce the observed range of chemical abundance ratios as the timescales to reach the observed stages is shorter than the free-fall time of the cores and much shorter than the ambipolar diffusion time, measured from the electron fraction in the simulations. Our work establishes the ortho-H2D+/para-D2H+ ratio as a reliable chemical clock and opens up to the possibility of exploring the star formation process in a statistically relevant sample through observations of these tracers.

A&A, Forthcoming article
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Which molecule traces what: chemical diagnostics of protostellar sources

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The physical and chemical conditions in Class 0/I protostars are fundamental in unlocking the protostellar accretion process and its impact on planet formation. The aim is to determine which physical components are traced by different molecules at sub-arcsecond scales (100 - 400 au). We use a suite of Atacama Large Millimeter/submillimeter Array (ALMA) datasets in Band 6 (1 mm), Band 5 (1.8 mm) and Band 3 (3 mm) at spatial resolutions 0.5 - 3" for 16 protostellar sources. The protostellar envelope is well traced by C18O, DCO+ and N2D+, with the freeze-out of CO governing the chemistry at envelope scales. Molecular outflows are seen in classical shock tracers like SiO and SO, but ice-mantle products such as CH3OH and HNCO released with the shock are also observed. The molecular jet is prominent not only in

SiO and SO but also occasionally in H2CO. The cavity walls show tracers of UV-irradiation such as C2H c-C3H2 and CN. The hot inner envelope, apart from showing emission from complex organic molecules (COMs), also presents compact emission from small molecules like H2S, SO, OCS and H13CN, most likely related to ice sublimation and high-temperature chemistry. Sub-arcsecond millimeter-wave observations allow to identify those (simple) molecules that best trace each of the physical components of a protostellar system. COMs are found both in the hot inner envelope (high excitation lines) and in the outflows (lower-excitation lines) with comparable abundances. COMs can coexist with hydrocarbons in the same protostellar sources, but they trace different components. In the near future, mid-IR observations with JWST-MIRI will provide complementary information about the hottest gas and the ice mantle content, at unprecedented sensitivity and at resolutions comparable to ALMA for the same sources.

A&A, Forthcoming article
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Can Cytosine, Uracil, and Thymine Be Formed from HC3N and H2NCO+ in Interstellar Space?

Joong Chul Choe

Syntheses of cytosine, uracil, and thymine starting from interstellar molecules were examined theoretically. Potential energy surfaces for the formation of protonated cytosine (CyH+), uracil (UrH+), and thymine (ThH+) from cyanoacetylene (HC3N), protonated isocyanic acid (H2NCO+), and one of NH3, H2O, and CH3OH, respectively, were determined by quantum chemical calculation using the CBS-QB3 method. Barrierless pathways were found for all the three reactions. Investigation of the energetics and kinetics of further possible reactions of CyH+, UrH+, and ThH+ led to the conclusion that cytosine, uracil, and thymine could not be formed along the proposed pathways in the interstellar gas phase, whereas their formation might be possible on interstellar icy grain mantles.

Astrophys. J. 914:136 (2021)
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Full-text URL: https://iopscience.iop.org/article/10.3847/1538-4357/abfd34/pdf

Laboratory Investigations Coupled to VIR/Dawn Observations to Quantify the Large Concentrations of Organic Matter on Ceres

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Organic matter directly observed at the surface of an inner planetary body is quite infrequent due to the usual low abundance of such matter and the limitation of the infrared technique. Fortuitously, the Dawn mission has revealed, thanks to the Visible and InfraRed mapping spectrometer (VIR), large areas rich in organic matter at the surface of Ceres, near Ernutet crater. The origin of the organic matter and its abundance in association with minerals, as indicated by the low altitude VIR data, remains unclear, but multiple lines of evidence support an endogenous origin. Here, we report an experimental investigation to determine the abundance of the aliphatic carbon signature observed on Ceres. We produced relevant analogues containing ammoniated-phyllosilicates, carbonates, aliphatic carbons (coals), and magnetite or amorphous carbon as darkening agents, and measured their reflectance by infrared spectroscopy. Measurements of these organic-rich analogues were directly compared to the VIR spectra taken from different locations around Ernutet crater. We found that the absolute reflectance of our analogues is at least two orders of magnitude higher than Ceres, but the depths of absorption bands match nicely the ones of the organic-

rich Ceres spectra. The choices of the different components are discussed in comparison with VIR data. Relative abundances of the components are extrapolated from the spectra and mixture composition, considering that the differences in reflectance level is mainly due to optical effects. Absorption bands of Ceres' organic-rich spectra are best reproduced by around 20 wt.% of carbon (a third being aliphatic carbons), in association with around 20 wt.% of carbonates, 15 wt.% of ammoniated-phyllosilicate, 20 wt.% of Mg-phyllosilicates, and 25 wt.% of darkening agent. Results also highlight the pertinence to use laboratory analogues in addition to models for planetary surface characterization. Such large quantities of organic materials near Ernutet crater, in addition to the amorphous carbon suspected on a global scale, requires a concentration mechanism whose nature is still unknown but that could potentially be relevant to other large volatile-rich bodies.

Minerals 2021, 11(7), 719
DOI: 10.3390/min11070719
Full-text URL: https://www.mdpi.com/2075-163X/11/7/719

Fitting infrared ice spectra with genetic modelling algorithms. Presenting the ENIIGMA fitting tool

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A variety of laboratory ice spectra simulating different chemical environments, ice morphology as well as thermal and energetic processing are demanded to provide an accurate interpretation of the infrared spectra of protostars. To answer which combination of laboratory data best fit the observations, an automated statistically-based computational approach becomes necessary. To introduce a new approach, based on evolutionary algorithms, to search for molecules in ice mantles via spectral decomposition of infrared observational data with laboratory ice spectra. A publicly available and open-source fitting tool, called ENIIGMA dEcompositioN of Infrared Ice features using Genetic Modelling Algorithms), is introduced. The tool has dedicated Python functions to carry out continuum determination of the protostellar spectra, silicate extraction, spectral decomposition and statistical analysis to calculate confidence intervals and quantify degeneracy. As assessment of the code, fully blind and fully sighted tests were conducted with known ice samples and constructed mixtures. Additionally, a complete analysis of the Elias 29 spectrum was performed and compared with previous results in the literature. The ENIIGMA fitting tool can identify the correct ice samples and their fractions in all checks with known samples tested in this paper. In the cases where Gaussian noise was added to the experimental data, more robust genetic operators and more iterations became necessary. Concerning the Elias 29 spectrum, the broad spectral range between 2.5-20 microns was successfully decomposed after continuum determination and silicate extraction. This analysis allowed the identification of different molecules in the ice mantle, including a tentative detection of CH3CH2OH. The ENIIGMA is a toolbox for spectroscopy analysis of infrared spectra that is well-timed with the launch of the James Webb Space Telescope. Additionally, it allows for exploring different chemical environments and irradiation field in order to correctly interpret the astronomical observations.

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Spectroscopic measurements of CH3OH in layered and mixed interstellar ice analogues

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Context. The molecular composition of interstellar ice mantles is defined by gas-grain processes in molecular clouds, with the main components being H2O, CO, and CO2. CH3OH ice is detected towards the denser regions, where large amounts of CO freeze out and get hydrogenated. Heating from nearby protostars can further change the ice structure and composition. Despite the several observations of icy features towards molecular clouds and along the line of site of protostars, it is not yet clear if interstellar

ices are mixed or if they have a layered structure. Aims. We aim to examine the effect of mixed and layered ice growth in ice mantle analogues, with focus on the position and shape of methanol infrared bands, so future observations could shed light on the structure of interstellar ices in different environments. Methods. Mixed and layered ice samples were deposited on a cold substrate kept at T = 10 K using a closed-cycle cryostat placed in a vacuum chamber. The spectroscopic features were analysed by FTIR spectroscopy. Different proportions of the most abundant four molecules in ice mantles, namely H2O, CO, CO2, and CH3OH, were investigated, with special attention on the analysis of the CH3OH bands. Results. We measure changes in the position and shape of the CH and CO stretching bands of CH3OH depending on the mixed or layered nature of the ice sample. Spectroscopic features of methanol are also found to change due to heating. Conclusions. A layered ice structure best reproduces the CH3OH band position recently observed towards a pre-stellar core and in star-forming regions. Based on our experimental results, we conclude that observations of CH3OH ices can provide information about the structure of interstellar ices, and we expect JWST to put stringent constraints on the layered or mixed nature of ices in different interstellar environments.

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X-ray induced desorption and photochemistry in CO ice

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We report an investigation of X-ray induced desorption of neutrals, cations and anions from CO ice. The desorption of neutral CO, by far the most abundant, is quantified and discussed within the context of its application to astrochemistry. The desorption of many different cations, including large cations up to the mass limit of the spectrometer, are observed. In contrast, the only desorbing anions detected are O− and C−. The desorption mechanisms of all these species are discussed with the aid of their photodesorption spectrum. The evolution of the X-ray absorption spectrum shows significant chemical modifications of the ice upon irradiation, which along with the desorption of large cations gives a new insight into X-ray induced photochemistry in CO ice.

Phys. Chem. Chem. Phys., 2021,23, 15965-15979
DOI: 10.1039/D1CP02670D
Full-text URL: https://arxiv.org/abs/2107.10503

ORion Alma New GEneration Survey (ORANGES) I. Dust continuum and free-free emission of OMC-2/3 filament protostars

M. Bouvier, A. López-Sepulcre, C. Ceccarelli, N. Sakai, S. Yamamoto, Y-L. Yang

The spectral energy distribution (SED) in the millimetre (mm) to centimetre (cm) range is a useful tool for characterising the dust in protostellar envelopes as well as free-free emission from the protostar and outflow. While many studies have been carried out towards low- and high-mass protostars, little exists so far about solar-type protostars in high-mass star-forming regions, which are likely to be representatives of the conditions where the Solar System was born. We focus here on the OMC-2/3 solar-type protostars, which are bounded by nearby HII regions and which are, therefore, potentially affected by the high-UV illumination. We aim to understand whether the small-scale structure (≤1000 au) and the evolutionary status of these solar-type protostars are affected by the nearby HII regions, as is the case for the large-scale (≤1e4 au) gas chemical composition. We used ALMA in the 1.3 mm band (246.2 GHz) to image the continuum of 16 OMC-2/3 solar-type protostars, with an angular resolution of 0.25″ (100 au). We completed our data with archival data from the

VANDAM survey of Orion Protostars at 333 and 32.9 GHz, respectively, to construct the dust SED, extract several dust parameters and to assess whether free-free emission is contaminating their dust SED in the cm range. From the mm to cm range dust SED, we found low dust emissivity spectral indexes (Beta<1) for the majority of our source sample and free-free emission towards only 5 of the 16 sample sources. We were also able to confirm or correct the evolutionary status of the source sample. Finally, we did not find any dependence of the source dust parameters on their location in the OMC-2/3 filament. Our results show that the small-scale dust properties of the OMC-2/3 protostars are not affected by the high- UV illumination from the nearby HII regions.

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DOI: 10.1051/0004-6361/202141157
Full-text URL: https://arxiv.org/abs/2107.10743

Electron Irradiation and Thermal Chemistry Studies of Interstellar and Planetary Ice Analogues at the ICA Astrochemistry Facility

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The modelling of molecular excitation and dissociation processes relevant to astrochemistry requires the validation of theories by comparison with data generated from laboratory experimentation. The newly commissioned Ice Chamber for Astrophysics-Astrochemistry (ICA) allows for the study of astrophysical ice analogues and their evolution when subjected to energetic processing, thus simulating the processes and alterations interstellar icy grain mantles and icy outer Solar System bodies undergo. ICA is an ultra-high vacuum compatible chamber containing a series of IR-transparent substrates upon which the ice analogues may be deposited at temperatures of down to 20 K. Processing of the ices may be performed in one of three ways: (i) ion impacts with projectiles delivered by a 2 MV Tandetron-type accelerator, (ii) electron irradiation from a gun fitted directly to the chamber, and (iii) thermal processing across a temperature range of 20–300 K. The physico-chemical evolution of the ices is studied in situ using FTIR absorbance spectroscopy and quadrupole mass spectrometry. In this paper, we present an overview of the ICA facility with a focus on characterising the electron beams used for electron impact studies, as well as reporting the preliminary results obtained during electron irradiation and thermal processing of selected ices.

Eur. Phys. J. D (2021), 75: 182
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Full-text URL:
https://epjd.epj.org/articles/epjd/abs/2021/06/10053_2021_Article_192/10053_2021_Article_192.html

Chemulator: Fast, accurate thermochemistry for dynamical models through emulation

J. Holdship, S. Viti, T. J. Haworth, J. D. Ilee

Chemical modelling serves two purposes in dynamical models: accounting for the effect of microphysics on the dynamics and providing observable signatures.Ideally, the former must be done as part of the hydrodynamic simulation but this comes with a prohibitive computational cost which leads to many simplifications being used in practice. We aim to produce a statistical emulator that replicates a full chemical model capable of solving the temperature and abundances of a gas through time. This emulator should suffer only a minor loss of accuracy over including a full chemical solver in a dynamical model bu twould have a fraction of the computational cost. To do this, the gas-grain chemical code UCLCHEM was updated to include heating and cooling processes and a large dataset of model outputs from possible starting conditions was

produced. A neural network was then trained to map directly from inputs to outputs. Chemulator replicates the outputs of UCLCHEM with an overall mean squared error (MSE) of 0.0002 for a single time step of 1000 yr and is shown to be stable over 1000 iterations with an MSE of 0.003 the log scaled temperature after one time step and 0.006 after 1000 time steps. Chemulator was found to be approximately 50,000 times faster than the time dependent model it emulates but can introduce a significant error to some models.

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Full-text URL: https://arxiv.org/abs/2106.14789

Announcements

LaboAstroMolec 1st Announcement Thematic School LABORATORY ASTROPHYSICS : tracking the evolution of cosmic matter towards molecular complexity, Les HOUCHES, France, March 2022, Sunday 13- Friday 18

We are pleased to announce the organization of a thematic school on « Laboratory Astrophysics : tracking the evolution of cosmic matter towards molecular complexity » that will take place at “Les Houches School of Physics”, located in the Chamonix valley of the French Alps in March 13-18 2022. This winter school is a PCMI-supported initiative and is addressed to a very broad audience, extending well beyond its own frontiers. It includes the fields of astrochemistry and planetary sciences (observational, experimental, modelling).
This school focuses on advanced experimental and theoretical approaches used to produce, analyze and investigate the properties and the evolution of extraterrestrial analogs in the laboratory, dedicated to improve our understanding of the origin and evolution of complex molecular matter observed in space, from dense molecular clouds up to the formation of new stars, planetary bodies and comets. The program will present a wide range of complementary and advanced methods allowing the production, analysis and investigation of properties and evolution of extraterrestrial analogs, that were developed in recent years in close connection to the most relevant astronomical observations. Emphasis will be put on the degree of chemical and/or structural complexity which can be achieved in the gas and solid phases and at their interface under space conditions. The methods used to characterize the physics of silicates and carbonaceous dust, and to investigate the formation/destruction processes of ices will be detailed. Techniques used to analyze matter from cometary and asteroid origins will also be presented. During the school, interactive sessions with invited teachers will be organized and all participants are encouraged to present their own work during poster sessions.

More information is available at https://lab-astrophysic.sciencesconf.org

The organizing committee : Jean-Hugues Fillion, Ludovic Biennier, Grégoire Danger and Aude Simon