AstroChemical Newsletter #90

May 2023

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Abstracts

The effect of thermal non-equilibrium on kinetic nucleation

Sven Kiefer, David Gobrecht, Leen Decin, Christiane Helling

Nucleation is considered to be the first step in dust and cloud formation in the atmospheres of asymptotic giant branch (AGB) stars, exoplanets, and brown dwarfs. In these environments dust and cloud particles grow to macroscopic sizes when gas phase species condense onto cloud condensation nuclei (CCNs). Understanding the formation processes of CCNs and dust in AGB stars is important because the species that formed in their outflows enrich the interstellar medium. Although widely used, the validity of chemical and thermal equilibrium conditions is debatable in some of these highly dynamical astrophysical environments. We aim to derive a kinetic nucleation model that includes the effects of thermal non-equilibrium by adopting different temperatures for nucleating species, and to quantify the impact of thermal non-equilibrium on kinetic nucleation. Forward and backward rate coefficients are derived as part of a collisional kinetic nucleation theory ansatz. The endothermic backward rates are derived from the law of mass action in thermal non-equilibrium. We consider elastic collisions as thermal equilibrium drivers. For homogeneous TiO2 nucleation and a gas temperature of 1250 K, we find that differences in the kinetic cluster temperatures as small as 20 K increase the formation of larger TiO2 clusters by over an order of magnitude. An increase in cluster temperature of around 20 K at gas temperatures of 1000 K can reduce the formation of a larger TiO2 cluster by over an order of magnitude. Our results confirm and quantify the prediction of previous thermal non-equilibrium studies. Small thermal non-equilibria can cause a significant change in the synthesis of larger clusters. Therefore, it is important to use kinetic nucleation models that include thermal non-equilibrium to describe the formation of clusters in environments where even small thermal non-equilibria can be present.

Accepted to A&A
DOI: 10.1051/0004-6361/202244685
Full-text URL: https://arxiv.org/abs/2302.08358

The chemistry of H2NC in the interstellar medium and the role of the C + NH3 reaction

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We carried out an observational search for the recently discovered molecule H2NC, and its more stable isomer H2CN, toward eight cold dense clouds (L1544, L134N, TMC-2, Lupus-1A, L1489, TMC-1 NH3, L1498, and L1641N) and two diffuse clouds (B0415+379 and B0355+508) in an attempt to constrain its abundance in different types of interstellar regions and shed light on its formation mechanism. We detected H2NC in most of the cold dense clouds targeted, 7 out of 8, while H2CN was only detected in 5 out of 8 clouds. The column densities derived for both H2NC and H2CN are in the range 1e11-1e12 cm-2 and the abundance ratio H2NC/H2CN varies between 0.51 and >2.7. The metastable isomer H2NC is therefore widespread in cold dense clouds where it is present with an abundance similar to that of H2CN. We did not detect either H2NC or H2CN in any of the two diffuse clouds targeted, which does not allow to shed light on how the chemistry of H2NC and H2CN varies between dense and diffuse clouds. We found that the column density of H2NC is correlated with that of NH3, which strongly suggests that these two molecules are chemically linked, most likely ammonia being a precursor of H2NC through the C + NH3 reaction. We performed electronic structure and statistical calculations which show that both H2CN and H2NC can be formed in the C + NH3 reaction through two different channels involving two different transition states which lie very close in energy. The predicted product branching ratio H2NC/H2CN is very method dependent but values between 0.5 and 0.8 are the most likely ones. Therefore, both the astronomical observations and the theoretical calculations support that the reaction C + NH3 is the main source of H2NC in interstellar clouds.

Accepted for publication in A&A.
DOI: 10.1051/0004-6361/202346279
Full-text URL: https://arxiv.org/abs/2303.12011

Detection of ethanol, acetone, and propanal in TMC-1: New O-bearing complex organics in cold sources

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We present the detection of ethanol (C2H5OH), acetone (CH3COCH3), and propanal (C2H5CHO) toward the cyanopolyyne peak of TMC-1. These three O-bearing complex organic molecules are known to be present in warm interstellar clouds, but had never been observed in a starless core. The addition of these three new pieces to the puzzle of complex organic molecules in cold interstellar clouds stresses the rich chemical diversity of cold dense cores in stages prior to the onset of star formation. The detections of ethanol, acetone, and propanal were made in the framework of QUIJOTE, a deep line survey of TMC-1 in the Q band that is being carried out with the Yebes 40m telescope. We derive column densities of (1.1 +/- 0.3)e12 cm-2 for C2H5OH, (1.4 +/- 0.6)e11 cm-2 for CH3COCH3, and (1.9 +/- 0.7)e11 cm-2 for C2H5CHO. The formation of these three O-bearing complex organic molecules is investigated with the aid of a detailed chemical model which includes gas and ice chemistry. The calculated abundances at a time around 2e5 yr are in reasonable agreement with the values derived from the observations. The formation mechanisms of these molecules in our chemical model are as follows. Ethanol is formed on grains by addition of atomic carbon on methanol followed by hydrogenation and non-thermal desorption. Acetone and propanal are produced by the gas-phase reaction between atomic oxygen and two different isomers of the C3H7 radical, where the latter follows from the hydrogenation of C3 on grains followed by non-thermal desorption. A gas-phase route involving the formation of (CH3)2COH+ through several ion-neutral reactions followed by its dissociative recombination with electrons do also contribute to the formation of acetone.

Accepted for publication in A&A
DOI: 10.1051/0004-6361/202346076
Full-text URL: https://arxiv.org/abs/2303.16121

FAUST VIII. The protostellar disk of VLA 1623-2417 W and its streamers imaged by ALMA

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More than 50% of solar-mass stars form in multiple systems. It is therefore crucial to investigate how multiplicity affects the star and planet formation processes at the protostellar stage. We report continuum and C18O (2-1) observations of the VLA 1623-2417 protostellar system at 50 au angular resolution as part of the ALMA Large Program FAUST. The 1.3 mm continuum probes the disks of VLA 1623A, B, and W, and the circumbinary disk of the A1+A2 binary. The C18O emission reveals, for the first time, the gas in the disk-envelope of VLA 1623W. We estimate the dynamical mass of VLA 1623W, Mdyn=0.45±0.08 M⊙, and the mass of its disk, Mdisk∼6e−3 M⊙. C18O also reveals streamers that extend up to 1000 au, spatially and kinematically connecting the envelope and outflow cavities of the A1+A2+B system with the disk of VLA 1623W. The presence of the streamers, as well as the spatial (∼1300 au) and velocity (∼2.2 km/s) offset of VLA 1623W suggest that either sources W and A+B formed in different cores, interacting between them, or that source W has been ejected from the VLA 1623 multiple system during its formation. In the latter case, the streamers may funnel material from the envelope and cavities of VLA 1623AB onto VLA 1623W, thus concurring to set its final mass and chemical content.

Accepted to MNRAS
DOI: 10.1093/mnras/stad964
Full-text URL: https://arxiv.org/abs/2303.16257

Digging into the Interior of Hot Cores with ALMA (DIHCA). III: The Chemical Link between NH2CHO, HNCO, and H2CO

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We have analyzed the NH2CHO, HNCO, H2CO, and CH3CN (13CH3CN) molecular lines at an angular resolution of ∼0.3″ obtained by the Atacama Large Millimeter/submillimeter Array (ALMA) Band 6 toward 30 high-mass star-forming regions. The NH2CHO emission has been detected in 23 regions, while the other species have been detected toward 29 regions. A total of 44 hot molecular cores (HMCs) have been identified using the moment 0 maps of the CH3CN line. The fractional abundances of the four species have been derived at each HMC. In order to investigate pure chemical relationships, we have conducted a partial correlation test to exclude the effect of temperature. Strong positive correlations between NH2CHO and HNCO (ρ=0.89) and between NH2CHO and H2CO (0.84) have been found. These strong correlations indicate their direct chemical links; dual-cyclic hydrogen addition and abstraction reactions between HNCO and NH2CHO and gas-phase formation of NH2CHO from H2CO. Chemical models including these reactions can reproduce the observed abundances in our target sources.

Accepted for The Astrophysical Journal
Full-text URL: https://arxiv.org/abs/2304.00267

Understanding the temperatures of H3+ and H2 in diffuse interstellar sightlines

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The triatomic hydrogen ion H3+ is one of the most important species for the gas phase chemistry of the interstellar medium. Observations of H3+ are used to constrain important physical and chemical parameters of interstellar environments. However, the temperatures inferred from the two lowest rotational states of H3+ in diffuse lines of sight - typically the only ones observable - appear consistently lower than the temperatures derived from H2 observations in the same sightlines. All previous attempts at modelling the temperatures of H3+ in the diffuse interstellar medium failed to reproduce the observational results. Here we present new studies, comparing an independent master equation for H3+ level populations to results from the Meudon PDR code for photon dominated regions. We show that the populations of the lowest rotational states of H3+ are strongly affected by the formation reaction and that H3+ ions experience incomplete thermalisation before their destruction by free electrons. Furthermore, we find that for quantitative analysis more than two levels of H3+ have to be considered and that it is crucial to include radiative transitions as well as collisions with H_2. Our models of typical diffuse interstellar sightlines show very good agreement with observational data, and thus they may finally resolve the perceived temperature difference attributed to these two fundamental species.

Accepted in "Molecular Physics"
DOI: [10.1080/00268976.2023.2182612](https://doi.org/10.1080/00268976.2023.2182612)
Full-text URL: https://arxiv.org/abs/2303.16070

Fine-structure transitions of Si and S induced by collisions with atomic hydrogen

Pei-Gen Yan, James F. Babb

Using a quantum-mechanical close-coupling method, we calculate cross-sections for fine-structure excitation and relaxation of Si and S atoms in collisions with atomic hydrogen. Rate coefficients are calculated over a range of temperatures for astrophysical applications. We determine the temperature-dependent critical densities for the relaxation of Si and S in collisions with H and compare these to the critical densities for collisions with electrons. The present calculations should be useful in modelling environments exhibiting the [S I] 25 μm and [S I] 57 μm far-infrared emission lines or where cooling of S and Si by collisions with H is of interest.

Accepted for publication in MNRAS
DOI: [10.1093/mnras/stad1050](https://doi.org/10.1093/mnras/stad1050)
Full-text URL: https://arxiv.org/abs/2304.02727

Cosmo-tomography toward PKS1830-211: Variability of the quasar and of its foreground molecular absorption monitored with ALMA

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Time variability of astronomical sources provides crude information on their typical size and on the implied physical mechanisms. PKS1830-211 is a remarkable radio-bright lensed quasar with a foreground molecular absorber at z=0.89. Small-scale morphological changes in the core-jet structure of the quasar -which is magnified by the lensing- result in a varying illumination of the absorber screen, which in turn causes variations in the absorption profile. We aim to study the time variations of the system [...] in order to obtain constraints on both the quasar activity and small-scale structures in the ISM of the absorber. We used ALMA to monitor the submm continuum emission, together with the absorption spectra of the H_2O and CH molecules, with 17 visits spread over six months in 2016. [...] From the continuum data, we followed the evolution of the flux density, flux-density ratio, spectral index, and differential polarization between the two lensed images of the quasar; all quantities show significant variations related to the intrinsic activity of the quasar. We propose a simple parametric model of a core plus a ballistic plasmon to account for the continuum evolution, from which we constrain a time delay of 25+/-3 days between lensed images. The spectral lines reveal significant variations in the foreground absorption. A principal component analysis highlights apparent wavy time variations, possibly linked to the helical jet precession period of the quasar. From the deep averaged spectra towards the SW image, we detect the absorption of 13CH and estimate an abundance ratio of 12CH/13CH~150. We also measure the oxygen isotopic ratios, 16O/18O=65.3+/-0.7 and 18O/17O=11.5+/-0.5. Finally, we find a remarkable continuous shallow trough in the water absorption spanning a velocity interval of nearly 500 km/s. This broad absorption could be the signature of an extra-planar molecular component. [Abridged]

Accepted for publication in A&A
DOI: [10.1051/0004-6361/202245768](https://doi.org/10.1051/0004-6361/202245768)
Full-text URL: https://arxiv.org/abs/2304.09002

Gas-phase electronic action absorption spectra of protonated oxygen-functionalized polycyclic aromatic hydrocarbons (OPAHs)

Anne P. Rasmussen, Gabi Wenzel, Liv Hornekær, Lars H. Andersen

Context. Extended red emission (ERE) denotes a broad unassigned feature extending from 540 to 800 nm observed in many regions of the interstellar medium (ISM), and is thought to originate from photoluminescence of cosmic dust. However, definitive assignment of specific carriers remains to be achieved. Aims. Our aim is to investigate the photoabsorption spectra of astrophysically relevant protonated oxygen-functionalized polycyclic aromatic hydrocarbons (OPAHs) to probe their ability to absorb photons in the near-ultraviolet (UV) and visible (vis) spectral region and to search for any low-lying electronic states that may account for the ERE. Methods. Gas-phase electronic action absorption spectra of the protonated OPAHs were recorded in the spectral range of 200−700 nm using the ELISA ion-storage ring. Additional time-dependent density functional theory (TD-DFT) calculations were performed to compute excited state transitions that complement the experimental spectra. Results. A set of five protonated (O)PAHs was considered, namely pentacene and the four oxygen-functionalized PAHs, pentacenequinone,pentacenetetrone, anthraquinone, and phenathrenequinone. All pentacene-related species show a main absorption band between 400 and 500 nm, while the smaller OPAHs, anthraquinone and phenanthrenequinone, generally absorb further to the blue compared to the pentacenes. Interestingly, pentacenequinone and phenanthrenequinone exhibit wide absorption plateaus towards the red side of their main absorption band(s), which places them among the potential candidates to contribute to ERE. Additional photodissociation mass spectra reveal the formation of smaller functionalized PAHs and small oxygen-bearing species. Conclusions. Our results demonstrate the ability of OPAHs to absorb in the UV/vis spectral region. Among the four studied OPAHs, two revealed very broad absorption characteristics at wavelengths up to 700 nm, which makes them suitable candidates to contribute to a part of the ERE spectrum. Moreover, these two OPAHs, pentacenequinone and phenanthrenequinone, could dissociate efficiently into oxygen-bearing molecules and smaller functionalized PAHs in photon-dominated regions (PDRs) of the ISM.

Accepted for publication in Astronomy & Astrophysics
DOI: 10.1051/0004-6361/202346003
Full-text URL: https://www.aanda.org/component/article?access=doi&doi=10.1051/0004-6361/202346003

Sensitivity study of chemistry in AGB outflows using chemical kinetics

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Asymptotic Giant Branch (AGB) stars shed a significant amount of their mass in the form of a stellar wind, creating a vast circumstellar envelope (CSE). Owing to the ideal combination of relatively high densities and cool temperatures, CSEs serve as rich astrochemical laboratories. While the chemical structure of AGB outflows has been modelled and analysed in detail for specific physical setups, there is a lack of understanding regarding the impact of changes in the physical environment on chemical abundances. A systematic sensitivity study is necessary to comprehend the nuances in the physical parameter space, given the complexity of the chemistry. This is crucial for estimating uncertainties associated with simulations and observations. In this work, we present the first sensitivity study of the impact of varying outflow densities and temperature profiles on the chemistry. With the use of a chemical kinetics model, we report on the uncertainty in abundances, given a specific uncertainty on the physical parameters. Additionally, we analyse the molecular envelope extent of parent species and compare our findings to observational studies. Mapping the impact of differences in physical parameters throughout the CSE on the chemistry is a strong aid to observational studies.

2023, accepted by MNRAS
Full-text URL: https://arxiv.org/abs/2304.05924

Announcements

Funded 3-year Ph.D, starting October 1st, 2023: "From Interstellar Clouds to Planetary Systems: Investigating the Formation and Evolution of Molecules in Space"

Context: The detection of nearly 200 different molecular species in space over the last 50 years demonstrates that the interstellar medium (ISM) is home to a rich chemistry. In the last decade our laboratory has contributed greatly to the understanding of how molecular complexity develops in space, by synthesizing new molecules under interstellar cloud conditions, by publishing a couple of papers about the sticking properties of hydrogen on dust grains, by exploring the thermal and non-thermal mechanisms of the return of molecules to the gas phase, and by impacting the scientific scene with papers concerning the diffusion at low temperatures of key atoms (H, O, and N) on surfaces of astrophysical interest.

Thesis work: Given the variety of laboratory techniques used at LERMA-CY, that is 1) Surface science mechanisms in astrophysics, 2) Mass spectrometry, temperature-controlled desorption (TPD) and temperature-controlled during exposure desorption (TP-DED), 3) Fourier Transform Infrared (FTIR) spectroscopy, and the various ongoing research topics (see https://cylerma.cyu.fr/), an example of thesis work could be to expand the experimental study of the mobility of species to selected molecules and radicals (CO, NO, OH, ...) adsorbed on ice mantles. In fact, one of the important parameters that sparks chemistry in very cold cosmic environments is the diffusion capability of adsorbed species, which can lead to the formation of more complex organic molecules, especially if atoms are locked-up in heavy and almost immobile radicals (HCO, NH2). Depending on the background and specific skills of the successful candidate, however, the thesis work may equally unfold on the infrared spectroscopy of pure, mixed, and processed interstellar ices. In fact, a robust and a fairly reliable identification of the chemical species in the ISM can only be based on the comparison of laboratory experiments and telescopic observations. As a further alternative, the project could address the reactivity of selected species leading to complex organic molecules in the interstellar medium, protoplanetary disks, and comets.

Skills: Master degree in chemistry, physics, astrophysics, or similar fields; prior experience with laboratory experiments and/or astrochemical modelling would be an asset, but is not required. Coding skills are a plus (e.g., Python), as well as a good written and oral level of English.

Procedure: Informal inquires are welcome (francois.dulieu@cyu.fr, emanuele.congiu@cyu.fr). Applicants should submit a detailed CV, letter of motivation, letter of intent, and arrange for at least one recommendation letter, to be sent by June 1st 2023.
Each application will receive full consideration and applicants will be interviewed.
The successful Ph.D. student will be hosted at the LERMA-CY Lab (5, mail Gay-Lussac, 95000 Neuville sur Oise – CERGY-PONTOISE).