

AstroChemical Newsletter #103

June 2024

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

Correlations among complex organic molecules around protostars: Effects of physical structure

P. Nazari , B. Tabone, G. P. Rosotti, E. F. van Dishoeck

Column density ratios of complex organic molecules are generally constant across protostellar systems with some low-level scatter. However, the scatter in formamide (NH₂CHO) to methanol (CH₃OH) column density ratio is one of the highest. This larger scatter is sometimes interpreted as evidence of gas-phase formation of NH₂CHO. In this work we propose an alternative interpretation in which this scatter is produced by differences in the snowline locations related to differences in binding energies of these species and the small-scale structure of the envelope and the disk system. We also include CH₃CN in our work as a control molecule which has a similar binding energy to CH₃OH. We use radiative transfer models to calculate the emission from these species in protostellar systems with and without disks. The abundances of these species are parameterized in our models. Then we fit the calculated emission lines to find the column densities as done in real observations. We find a correction factor of ~ 10 to be multiplied by gas-phase $N_{\text{NH}_2\text{CHO}}/N_{\text{CH}_3\text{OH}}$ to give the true abundance ratio of these two species in the ices. We find that models with different physical parameters produce a scatter in $N_{\text{NH}_2\text{CHO}}/N_{\text{CH}_3\text{OH}}$, comparable with that of observations. The scatter in $N_{\text{NH}_2\text{CHO}}/N_{\text{CH}_3\text{OH}}$ is larger than that of $N_{\text{CH}_3\text{CN}}/N_{\text{CH}_3\text{OH}}$ in models consistent with the observations. We show that the scatter in $N_{\text{NH}_2\text{CHO}}/N_{\text{CH}_3\text{OH}}$ will be lower if we correct for the difference in sublimation temperatures of these two species in observations of ~ 40 protostellar systems with ALMA. The scatter in $N_{\text{NH}_2\text{CHO}}/N_{\text{CH}_3\text{OH}}$ can be partially explained by the difference in their binding energies. We conclude that gas-phase chemistry routes for NH₂CHO are not necessary to explain the larger scatter of $N_{\text{NH}_2\text{CHO}}/N_{\text{CH}_3\text{OH}}$ compared with other ratios.

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Laboratory and astronomical discovery of cyanthioketene, NCCHCS, in the cold starless core TMC-1

C. Cabezas, M. Agúndez, Y. Endo, B. Tercero, Y.-P. Lee, N. Marcelino, P. de Vicente, and J. Cernicharo

We present the detection of cyanthioketene, NCCHCS, in the laboratory and toward TMC-1. This transient species was produced through a discharge of a gas mixture of CH₂CHCN and CS₂ using argon as carrier gas, and its rotational spectrum between 9

and 40 GHz was characterized using a Balle-Flygare narrowband-type Fourier-transform microwave spectrometer. A total of 21 rotational transitions were detected in the laboratory, all of them exhibiting hyperfine structure induced by the spin of the N nucleus. The spectrum for NCCHCS was predicted in the domain of our line surveys using the derived rotational and distortion constants. The detection in the cold starless core TMC-1 was based on the QUIJOTE line survey performed with the Yebes 40m radio telescope. Twenty-three lines were detected with $K_a=0, 1, \text{ and } 2$ and $J_u=9$ up to 14. The derived column density is $(1.2 \pm 0.1) \times 10^{11} \text{ cm}^{-2}$ for a rotational temperature of $8.5 \pm 1 \text{ K}$. The abundance ratio of thioketene and its cyano derivative, H₂CCS/NCCHCS, is 6.5 ± 1.3 . Although ketene is more abundant than thioketene by about 15 times, its cyano derivative NCCHCO surprisingly is not detected with a 3 σ upper level to the column density of $3.0 \times 10^{10} \text{ cm}^{-2}$, which results in an abundance ratio H₂CCO/NCCHCO > 430. Hence, the chemistry of CN derivatives seems to be more favored for S-bearing than for O-bearing molecules. We carried out chemical modeling calculations and found that the gas-phase neutral-neutral reactions $\text{CCN} + \text{H}_2\text{CS}$ and $\text{CN} + \text{H}_2\text{CCS}$ could be a source of NCCHCS in TMC-1.

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CN stretches around 4.4 microns dominate the IR absorption spectra of cyano-polycyclic aromatic hydrocarbons

V. J. Esposito, R. C. Fortenberry, C. Boersma, A. Maragkoudakis, L. J. Allamandola

Anharmonic quantum chemical computations reveal a strong, narrow (width = 0.075 microns) band in the 4.3 - 4.5 micron region of the absorption spectra of the cyano-substituted polycyclic aromatic hydrocarbons (CN-PAHs) cyanonaphthalene, cyanoanthracene, cyanophenanthrene, and cyanopyrene. This narrow window with intense IR lines implies that CN-PAHs of various shapes and sizes offer little variation in both wavelength and intensity in this region. Subsequently, this band can be used as a tracer for CN-PAHs. The distinct features making up the band are assigned to mixed vibrational states consisting of the CN stretch fundamental and various combination bands, including in-plane CH bends, CC skeletal bends, and CC skeletal breathing motions. The extraordinarily large intrinsic intensity of the fundamental CN stretch is redistributed to nearby states via anharmonic coupling, which is readily captured when using second order vibrational perturbation theory with resonance polyad matrices. This redistribution of intensity leads to a complex spectrum. The intense bands in this wavelength region may contribute to the baseline continuum and undulating macroscopic structure seen in recent JWST NIRSpec observations.

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MACE: a Machine learning Approach to Chemistry Emulation

S. Maes, F. De Ceuster, M. Van de Sande, L. Decin

The chemistry of an astrophysical environment is closely coupled to its dynamics, the latter often found to be complex. Hence, to properly model these environments a 3D context is necessary. However, solving chemical kinetics within a 3D hydro simulation is

computationally infeasible for an even a modest parameter study. In order to develop a feasible 3D hydro-chemical simulation, the classical chemical approach needs to be replaced by a faster alternative. We present MACE, a Machine learning Approach to Chemistry Emulation, as a proof-of-concept work on emulating chemistry in a dynamical environment. Using the context of AGB outflows, we have developed an architecture that combines the use of an autoencoder (to reduce the dimensionality of the chemical network) and a set of latent ordinary differential equations (that are solved to perform the temporal evolution of the reduced features). Training this architecture with an integrated scheme makes it possible to successfully reproduce a full chemical pathway in a dynamical environment. MACE outperforms its classical analogue on average by a factor 26. Furthermore, its efficient implementation in PyTorch results in a sub-linear scaling with respect to the number of hydrodynamical simulation particles.

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First detection of CF⁺ in the Large Magellanic Cloud

Yan Gong, Karl M. Menten, Arshia M. Jacob, Christian Henkel, C.-H. Rosie Chen

CF⁺ has been established as a valuable diagnostic tool for investigating photo-dissociation regions (PDRs) and fluorine abundances in the Milky Way. However, its role in extragalactic environments remains largely uncharted. Our objective is to explore the significance of CF⁺ in the Large Magellanic Cloud (LMC) and assess its utility as a valuable probe for examining C⁺ and fluorine abundances in external galaxies. We performed pointed CF⁺ observations toward an active star-forming region, N113 in the LMC, using the Atacama Pathfinder EXperiment 12m submillimeter telescope. We report the first discovery of CF⁺ in the LMC through the successful detection of the CF⁺ (2→1) and (3→2) lines. The excitation models indicate that CF⁺ emission originates from dense PDRs characterized by an H₂ number density of (0.5–7.9)e4 cm⁻³ in N113. Our observations provide the first constraint on the fluorine abundance in molecular clouds in the LMC, disclosing a value of $\lesssim 1.7e-9$. This value is about an order of magnitude lower than those previously measured toward red giants in the LMC, indicative of fluorine deficiency in the molecular gas. The estimated column density ratio between C⁺ and CF⁺ appears to be lower than the anticipated equilibrium ratio derived from the fluorine abundance in red giants. Both phenomena can be explained by the deficiency of CF⁺ caused by the freeze-out of its primary chemical precursor, HF, onto dust grains. The deficiency of CF⁺ within molecular clouds suggests that the measurements presented in this work serve exclusively as conservative estimates, establishing lower bounds for both the fluorine abundance and C⁺ column densities in external galaxies.

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The rotation-tunneling spectrum of 3-hydroxypropenal and confirmation of its detection toward IRAS 16293-2422 B

H. S. P. Müller, A. Coutens, J. K. Jørgensen, L. Margulès, R. A. Motiyenko, and J.-C. Guillemin

3-Hydroxypropenal (HOCHCHCHO) is the lower energy tautomer of malonaldehyde which displays a complex rotation-tunneling spectrum. It was detected tentatively toward the solar-type protostar IRAS 16293-2422B with ALMA in the framework of the

Protostellar Interferometric Line Survey (PILS). Several transitions, however, had large residuals, preventing not only their detection, but also the excitation temperature of the species from being determined unambiguously. We want to extend the existing rotational line list of 3-hydroxypropenal to shed more light on the recent observational results and to facilitate additional radio astronomical searches for this molecule. We analyzed the rotation-tunneling spectrum of 3-hydroxypropenal in the frequency regions between 150 and 330 GHz and between 400 and 660 GHz. Transitions were searched for in the PILS observations of IRAS 16293-2422. Local thermodynamic equilibrium (LTE) models were carried out and compared to the observations to constrain the excitation temperature. Additional transitions were searched for in other ALMA archival data of the same source to confirm the presence of 3-hydroxypropenal. More than 11500 transitions were assigned in the course of our investigation with quantum numbers $2 \leq J \leq 100$, $K_a \leq 59$, and $K_c \leq 97$, resulting in a greatly improved set of spectroscopic parameters. The comparison between the LTE models and the observations yields an excitation temperature of 125 K with a column density $N = 1e15 \text{ cm}^{-2}$ for this species. We identified seven additional lines of 3-hydroxypropenal that show a good agreement with the model in the ALMA archive data. The calculated rotation-tunneling spectrum of 3-hydroxypropenal has sufficient accuracy for radio astronomical searches. The detection of 3-hydroxypropenal toward IRAS 16293-2422B is now secure.

Astron. Astrophys., in press.

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An ALCHEMI inspection of sulphur-bearing species towards the central molecular zone of NGC 253

M. Bouvier, S. Viti, E. Behrens, J. Butterworth, K.-Y. Huang, J. G. Mangum, N. Harada, S. Martín, V. M. Rivilla, S. Müller, K. Sakamoto, Y. Yoshimura, K. Tanaka, K. Nakanishi, R. Herrero-Illana, L. Colzi, M. D. Gorski, C. Henkel, P. K. Humire, D. S. Meier, P. P. van der Werf, and Y. T. Yan

Sulphur-bearing species are detected in various environments within Galactic star-forming regions and are particularly abundant in the gas phase of outflows and shocks, and photo-dissociation regions. In this work, we aim to investigate the nature of the emission from the most common sulphur-bearing species observable at millimetre wavelengths towards the nuclear starburst of the galaxy NGC 253. We intend to understand which type of regions are probed by sulphur-bearing species and which process(es) dominate(s) the release of sulphur into the gas phase. We used the high-angular resolution (1.6" or 27 pc) observations from the ALCHEMI ALMA Large Program to image several sulphur-bearing species towards the central molecular zone (CMZ) of NGC 253. We performed local thermodynamic equilibrium (LTE) and non-LTE large velocity gradient (LVG) analyses to derive the physical conditions of the gas in which S-bearing species are emitted, and their abundance ratios across the CMZ. Finally, we compared our results with previous ALCHEMI studies and a few selected Galactic environments. We found that not all sulphur-bearing species trace the same type of gas: strong evidence indicates that H₂S and part of the emission of OCS, H₂CS, and SO, are tracing shocks whilst part of SO and CS emission rather trace the dense molecular gas. For some species, such as CCS and SO₂, we could not firmly conclude on their origin of emission. The present analysis indicates that the emission from most sulphur-bearing species throughout the CMZ is likely dominated by shocks associated with ongoing star formation. In the inner part of the CMZ where the presence of super star clusters was previously indicated, we could not distinguish between shocks or

thermal evaporation as the main process releasing the S-bearing species.

Accepted in A&A

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Shock and Cosmic-Ray Chemistry Associated with the Supernova Remnant W28

Tian-Yu Tu, Yang Chen, Ping Zhou, Samar Safi-Harb, Qian-Cheng Liu

Supernova remnants (SNRs) exert a strong influence on the physics and chemistry of the nearby molecular clouds through shock waves and the cosmic rays (CRs) they accelerate. To investigate the SNR-cloud interaction in the prototype interacting SNR W28 (G6.4-0.1), we present new observations of the HCO⁺, HCN, and HNC J = 1-0 lines, supplemented by archival data of CO isotopes, N₂H⁺ and H¹³CO⁺. We compare the spatial distribution and spectral line profiles of different molecular species. Using the local thermodynamic equilibrium assumption, we obtain an abundance ratio of N(HCO⁺)/N(CO) ~ 1e-4 in the northeastern shocked cloud, which is higher by an order of magnitude than the values in unshocked clouds. This can be accounted for by the chemistry jointly induced by shock and CRs, with the physical parameters previously obtained from observations: preshock density n_H ~ 2e5 cm⁻³, CR ionization rate ζ = 2.5e-15 s⁻¹, and shock velocity V_s = 15-20 km s⁻¹. Toward a point outside the northeastern boundary of W28 with a known high CR ionization rate, we estimate the abundance ratio N(HCO⁺)/N(N₂H⁺) ≈ 0.6-3.3, which can be reproduced by a chemical simulation if a high density n_H ~ 2e5 cm⁻³ is adopted.

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Chemical inventory of the envelope of the Class I protostar L1551 IRS 5

P. Marchand, A. Coutens, J. Scigliuto, F. Cruz-Sáenz de Miera, A. Andreu, J.-C. Loison, Á. Kóspál, P. Ábrahám

Episodic accretion in protostars leads to luminosity outbursts that end up heating their surroundings. This rise in temperature pushes the snow lines back, enabling the desorption of chemical species from dust grain surfaces, which may significantly alter the chemical history of the accreting envelope. However, a limited number of extensive chemical surveys of eruptive young stars have been performed thus far. In the present study, we carry out a large spectral survey of the binary Class I protostar L1551 IRS 5, known to be a FUor-like object, in the 3mm and 2mm bands with the IRAM-30m telescope. As a result, we detected more than 400 molecular lines. The source displays a great chemical richness with the detection of 75 species, including isotopologues. Among these species, there are 13 hydrocarbons, 25 N-bearing species, 30 O-bearing species, 15 S-bearing species, 12 deuterated molecules, and a total of 10 complex organic molecules (l-C₄H₂, CH₃CCH, CH₂DCCH, CH₃CHO, CH₃CN, CH₃OCH₃, CH₃OCHO, CH₃OH, CH₂DOH, and HC₅N). With the help of local thermodynamic equilibrium (LTE) and non-LTE models, we determined the column densities of most molecules as well as excitation and kinetic temperatures. While most of those molecules trace the cold envelope (< 20 K), the OCS and CH₃OH emission arise from the warm (> 100 K) innermost (< 2") regions. We compared the chemical inventory of L1551 IRS 5 and its column density ratios, including isotopic ratios, with other protostellar sources.

A broad chemical diversity is seen among Class I objects. More observations with both single-dish telescopes and interferometers are needed to characterize the diversity in a larger sample of protostars, while more astrochemical models would help explain this diversity, in addition to the impact of luminosity outbursts on the chemistry of protostellar envelopes.

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Chemistry across dust and gas gaps in protoplanetary disks: modelling the co-spatial molecular rings in the HD 100546 disk

M. Leemker, A. S. Booth, E. F. van Dishoeck, L. Wölfer, and B. Dent

High-resolution observations show that typically both the dust and the gas in nearby extended protoplanetary disks are structured, possibly related to radial and azimuthal variations in the disk density and/or chemistry. The aim of this work is to identify the expected location and intensity of rings seen in molecular line emission of HCN, CN, C₂H, NO, [CI], and HCO⁺ in gapped disks while exploring a range of physical conditions across the gap. In particular, we model HD 100546 disk where molecular rings are co-spatial with the dust rings at ~20 and ~200 au, in contrast to most other gapped disks. The fiducial model of a gapped disk with a 15 au gas cavity, a 20 au dust cavity, and a shallow (a factor of ≤ 10) gas and deep dust gap at 40-175 au provides a good fit to the continuum, CO isotopologues, HCN, and HCO⁺ in the HD 100546 disk. However, the predictions for [CI], CN, C₂H and NO do not match the intensity nor the morphology of the observations. An exploration of the parameter space shows that in general the molecular emission rings are only co-spatial with the dust rings if the gas gap between the dust rings is depleted by at least four orders of magnitude in gas or if the C/O ratio of the gas is varying as a function of radius. For shallower gaps the decrease in the UV field roughly balances the effect of a higher gas density for UV tracers such as CN, C₂H, and NO. Therefore, these radicals are not good tracers of the gas gap depth. The C/O ratio primarily effects the intensity of the lines without changing the morphology much. The co-spatial rings observed in the HD 100546 disk could be indicative of a radially varying C/O ratio in the HD 100546 disk with a C/O above 1 in a narrow region across the dust rings, together with a shallow gas gap that is depleted by a factor of ~10 in gas, and a reduced background UV field.

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HCN as a probe of the inner disk in a candidate proto-brown dwarf

B. Riaz, W.-F. Thi, M. Machida

The detection of Keplerian rotation is rare among Class 0 protostellar systems. We have investigated the high-density tracer HCN as a probe of the inner disk in a Class 0 proto-brown dwarf candidate. Our ALMA high angular resolution observations show the peak in the HCN (3-2) line emission arises from a compact component near the proto-brown dwarf with a small bar-like structure and a deconvolved size of ~50 au. Radiative transfer modelling indicates that this HCN feature is tracing the innermost, dense regions in the proto-brown dwarf where a small Keplerian disk is expected to be

present. The limited velocity resolution of the observations, however, makes it difficult to confirm the rotational kinematics of this feature. A brightening in the HCN emission towards the core center suggests that HCN can survive in the gas phase in the inner, dense regions of the proto-brown dwarf. In contrast, modelling of the HCO⁺ (3-2) line emission indicates that it originates from the outer pseudo-disk/envelope region and is centrally depleted. HCN line emission can reveal the small-scale structures and can be an efficient observational tool to study the inner disk properties in such faint compact objects where spatially resolving the disk is nearly impossible.

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Formation of AlO, AlOH, and Al(OH)₃ in the Interstellar Medium and Circumstellar Envelopes of AGB Stars

R. Firth, K. Bell, R. Fortenberry

AlO, AlOH, and Al(OH)₃ can be formed in the gas-phase starting from nothing more than simple aluminum hydrides (AlH and AlH₂) and water molecules. All three products are probable precursors to aluminum oxide clusters that may initiate the nucleation of dust grains in the interstellar medium. Chemically accurate CCSD(T)-F12b/cc-pVTZ-F12 computations provide exothermic energetic values for these pathways. For example, the fully submerged formation of AlO is exothermic by 51.3 kcal mol⁻¹, and this should also lead to favorable kinetics. To aid in the detection of the recurring intermediate cis/trans-HAlOH with instrumentation located on the James Webb Space Telescope (JWST), rotational and vibrational spectroscopic data are reported utilizing a highly-accurate quartic force field methodology. The ν₂ stretching frequency at 1807.9 cm⁻¹ exhibits an anharmonic intensity of 185 km mol⁻¹ and the antisymmetric bend (ν₄) at 534.2 cm⁻¹ exhibits an anharmonic intensity of 213 km mol⁻¹ for the cis and trans isomers, respectively. These are roughly three times the antisymmetric stretch intensity of water. The cis isomer has a smaller dipole moment of 0.83 D while the trans isomer contains a moderate dipole moment of 1.49 D. These properties indicate that both of these isomers are observable through vibrational and rotational spectroscopic techniques.

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Radial and vertical constraints on the icy origin of H₂CO in the HD 163296 Protoplanetary Disk

Claudio Hernández-Vera, Viviana V. Guzmán, Elizabeth Artur de la Villarmois, Karin I. Öberg, L. Ilseore Cleeves, Michiel R. Hogerheijde, Chunhua Qi, John Carpenter, Edith C. Fayolle

H₂CO is a small organic molecule widely detected in protoplanetary disks. As a precursor to grain-surface formation of CH₃OH, H₂CO is considered an important precursor of O-bearing organic molecules that are locked in ices. Still, since gas-phase reactions can also form H₂CO, there remains an open question on the channels by which organics form in disks, and how much the grain versus the gas pathways impact the overall organic reservoir. We present spectrally and spatially resolved Atacama Large Millimeter/submillimeter Array observations of several ortho- and para-H₂CO transitions toward the bright protoplanetary disk around the Herbig Ae star HD

163296. We derive column density, excitation temperature, and ortho-to-para ratio (OPR) radial profiles for H₂CO, as well as disk-averaged values of $N_T \sim 4e12 \text{ cm}^{-2}$, $T_{\text{ex}} \sim 20 \text{ K}$, and $\text{OPR} \sim 2.7$, respectively. We empirically determine the vertical structure of the emission, finding vertical heights of $z/r \sim 0.1$. From the profiles, we find a relatively constant $\text{OPR} \sim 2.7$ with radius, but still consistent with 3.0 among the uncertainties, a secondary increase of N_T in the outer disk, and low T_{ex} values that decrease with disk radius. Our resulting radial, vertical, and OPR constraints suggest an increased UV penetration beyond the dust millimeter edge, consistent with an icy origin but also with cold gas-phase chemistry. This Herbig disk contrasts previous results for the T Tauri disk, TW Hya, which had a larger contribution from cold gas-phase chemistry. More observations of other sources are needed to disentangle the dominant formation pathway of H₂CO in protoplanetary disks.

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Full-text URL: <https://arxiv.org/abs/2404.06133>

Announcements

Fractionation of isotopes in space II: from the Solar System to galaxies

We are pleased to announce the second edition of the conference Fractionation of isotopes in space II: from the Solar System to galaxies that will be held on November 4-7 2024 in Florence, Italy.

In the last two decades the number of studies focused on isotopic ratios has grown thanks to the unprecedented capabilities of current astronomical facilities. This growth is mainly due to the improved sensitivity of the instrumentation of different facilities such as the single-dish IRAM 30m, GBT 100m, and Yebes 40m telescopes, and the interferometers IRAM NOEMA and ALMA. Near IR observations obtained with the VLT and JWST have also recently allowed the first detection of ¹³CO and ¹⁵NH₃ in the atmosphere of a young exoplanet and a brown dwarf, opening new clues on local fractionation effects in exoplanetary objects. Moreover, new laboratory works and updated theoretical astrochemical and stellar Galactic chemical evolution models have been developed. The second edition of this conference aims to bring a multidisciplinary community together, covering topics that range from astronomical observations in different Galactic environments, to the Solar System, exoplanetary systems, and (extra)galactic molecular clouds, as well as laboratory works and theoretical astrochemical and stellar Galactic chemical evolution models. Moreover, ALMA Band 2 (67-116 GHz frequency window) and the Square Kilometer Array (SKA) are now under construction and the meeting will open discussion about the possible future projects related to the conference topic to be carried out with these new facilities. The meeting will also discuss future projects related to the topic and what are the best facilities, including under construction or future, that are best suited for them.

Here is the conference website: <https://sites.google.com/view/fractionation2>

Registration and Abstract submission is now open:

https://docs.google.com/forms/d/e/1FAIpQLScNqgfk-_eVRXOQ2RBV_HAKAZMj7dO9aQj5YorYszpdrLLwgA/viewform?usp=sf_link

The abstract submission deadline is June, 30th 2024. We aim to notify acceptance of

contributed talks and posters by the end of July 2024.

Confirmed invited speakers: Paola Caselli (Max Planck Institute for Extraterrestrial Physics, Germany), Mattia Melosso (Università di Bologna, Italy), Kotomi Taniguchi (National Astronomical Observatory of Japan, Japan), Donatella Romano (INAF - OAS Bologna, Italy), Serena Viti (Leiden University, Netherlands), Laurent Remusat (IMPMC, Museum National d'Histoire Naturelle, France), Yapeng Zhang (California Institute of Technology, California, USA)

The SOC includes: Laura Colzi (co-chair), Maite Beltrán (co-chair), Francesco Fontani (co-chair), Elena Redaelli, Evelyne Roueff, Pierre Hily-Blant, Nicolas Biver, Silvia Spezzano, and Christian Henkel

The LOC includes: Laura Colzi, Maite Beltrán, Francesco Fontani, Patrizia Braschi, Chi Yan Law, and Jofre Allande González

PhD Position in Molecular Astrophysics

We have an opening for a 3-year PhD position at the Institute for Fundamental Physics, CSIC, Madrid, Spain. The project, entitled "Unconventional Processes in the Synthesis of Interstellar PAHs: Theory and Modeling," seeks to understand the most favorable pathways for the formation of simple aromatic compounds, like benzene, benzyne, or cyclopentadiene, under the stringent conditions of the interstellar medium. For this, you will use automatic reaction discovery routines (supported by quantum chemical calculations) in tandem with astrochemical kinetic models to investigate the role of two types of reactions, ion-molecule reactions and radiative associations, in the synthesis of these molecules.

Requirements:

MSc in Chemistry or Physics.

Prior experience with quantum chemical calculations and theoretical reaction kinetics.

Good programming skills in Fortran and/or Python.

Good oral and written communication skills in English.

Knowledge of astrochemistry and physical and chemical processes in space (advantageous).

If you are interested, please send a short CV and a certificate of grades to german.molpeceres@iff.csic.es and marcelino.agundez@csic.es.

The position is open until a suitable candidate is found.

Kick-off Meeting for the COST Action - PLANETS - The birth of solar systems

The COST Action PLANETS - The birth of solar systems - will hold its kick-off meeting on 9 - 11 July 2024 in Torun in Poland. Further information on the Action members and objectives can be found at the link below.

A COST Action is an interdisciplinary research network that enables researchers to interact and investigate a specific topic, in our case, planet formation (<https://www.cost.eu/cost-actions/what-are-cost-actions/>). The mission of this Action is to "Build an interdisciplinary network, with expertise in experimental studies, observations, and models, to advance our understanding of planet formation, by determining the computational and data needs of the community, and how to best exploit current and future observations." COST Actions provide funding over four years

to fund meetings, training schools, attendance at conferences (to report research results under the remit of the Action), short-term scientific missions (to visit international collaborators or build new collaborations) and dissemination (e.g., publications) and public engagement material (<https://www.cost.eu/what-do-we-fund/>).

The Action kick-off meeting will take place at the Hotel Copernicus in Torun, Poland, and will consist of a combination of scientific talks under the remit of the five scientific working groups of the Action,

- Planet formation: laboratory perspectives
- Advancing planet formation models
- Planet formation theory confronts observations
- Emerging habitable environments
- Towards the first database on planet-forming discs

as well as dedicated discussion sessions to draft ideas and plans on how to meet the aims and objectives and ultimately, the deliverables, of the Action (which can be found in the MoU: https://e-services.cost.eu/files/domain_files/CA/Action_CA22133/mou/CA22133-e.pdf).

We currently have capacity for additional in-person and online attendees at the kick-off meeting, and we cordially invite members of the community working in planet formation and/or exoplanets to join the Action, and also to register and take part in the meeting. We also have capacity for poster presentations for in-person attendees to the meeting; note that there is no conference fee. Instructions on how to book the hotel and sample travel itineraries to Torun will be sent to all new in-person registrations.

Next steps are:

- Step 1: Set up an eCOST account - <https://e-services.cost.eu/user/login>
- Step 2: Join the Action - <https://e-services.cost.eu/action/CA22133/working-groups/apply>
- Step 3: Register for the meeting - <https://forms.office.com/e/vNHytM3jbM>