DIG (Dust, Ice and Gas) Astrochemistry

17-18th November, 2022
(virtual)

ABSTRACT BOOK

http://iases.org.in/dig-astrochem.html

Scientific topic

Using modern technologies and facilities, scientists unveiled the fingerprints of the chemicals in the interstellar medium down to stellar and planetary environments. High-sensitive and high-resolution telescopes like ALMA are providing amazing results by mapping the gas phase molecules down to the planetary scale. Further, JWST will complement chemical inventory by looking deep into the protoplanetary disk, planetary atmospheres, PDR, etc., and will investigate the ice compositions with a much deeper insight. Astrochemistry has now evolved as an emerging branch of many astrophysical fields, where molecules are used as a diagnostic tool to understand the physical and chemical properties of various astronomical objects. This webinar aims to bring together experimentalists, observers, and modelers to allow the astrochemical community to assemble and confer on recent accomplishments and upcoming challenges.

SOC

Prof. Nigel Mason (University of Kent, UK)
Prof. Anil Bhardwaj (PRL, India)
Prof. Elangannan Arunan (Indian Institute of Science, India)
Prof. B. N. Rajasekhar (BARC, India)
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Dr. Ankan Das (IASES, India)
Dr. Bhalamurugan Sivaraman (PRL, India)

Solicited Speakers

Prof. Eric Herbst (University of Virginia, US)
Dr. Robin Garrod (University of Virginia, US)
Dr. Victor Manuel Rivilla (Center for Astrobiology, Spain)
Prof. Cristina Puzzarini (University of Bologna, Italy)
Dr. Christine Joblin, (Université Toulouse III / CNRS, France)
Prof. Liv Hornekaer (Aarhus university, Denmark)
Prof. Sergio Pilling (UNIVAP, Brazil)
Dr. Kei Tanaka (University of Colorado Boulder, US)
Dr. Sergio Ioppolo (Aarhus university, Denmark)
Dr. Kotomi Taniguchi (NAOJ, Japan)

Dr. Kenji Furuya (NAOJ, Japan)
Dr. Niels F.W. Ligterink (University of Bern, Switzerland)
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Dr. Prasanta Gorai (Chalmers University of Technology, Sweden)
Dr. Divita Gupta (University of Cologne, Germany)
Dr. Giacomo Mulas (INAF-OAC Cagliari, Italy)
Dr. Mathias Rapacioli (LCPQ, Toulouse, France)
Dr. Tien-Hao Hsieh (Center for Astrochemical Studies, MPE, Germany)

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Andrés Megías (CAB, CSIC-INTA, Spain)
Dr. Heidy M. Quitián-Lara (University of Kent)
Álvaro López-Gallifa (CAB, CSIC-INTA, Spain)
Dr. David Dubois (NASA Ames Research Center, USA)
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Synthetic Approaches to Complex Organi Molecules in the Cold Interstellar Medium

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The detection of large organic molecules in interstellar space is an exciting development in astrochemistry. At present, approximately 270 molecules have been observed in interstellar clouds of gas and dust where new stars and planets have formed and are forming. In this talk, we emphasize the production of so-called complex organic molecules, abbreviated by the terms COMs or iCOMs, where the lower case i stands for "interstellar." These partially saturated gas-phase species are characterized by six atoms or more with at least one carbon atom. Although COMs have been detected in warm regions of clouds for some time, their more recent detection in cold regions has proved to be more difficult to understand. Both gas-phase reactions and reactions on and in dust particles are thought to be involved in their synthesis. Although gas-phase reactions were the first to be suggested, the role of granular reactions has been strengthened by experiments showing that COMs as complicated as glycine can be produced on cold dust grains under conditions somewhat related to dust surfaces in cold interstellar clouds. In addition, new mechanisms of reactions on cold dust such as non-diffusive motions and cosmic ray bombardment have been suggested. Nevertheless, the role of gas-phase reactions has not been ruled out. Both mechanisms will be discussed.

New models of hot and cold chemistry in star-forming regions

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Reactions on dust-grain surfaces are responsible for the production of many important interstellar molecules, including gas-phase H2, grain-surface ice species such as water, ammonia and methanol, and arguably some of the most complex molecules detected in star-forming regions. However, our view of the temperature dependence of this chemistry has recently been changing. A major driver in this shift is the gas-phase detection of complex organic molecules (COMs) such as methyl formate in cold pre-stellar cores. These detections have pushed back the astronomical clock on COM production, to a time much earlier than the warm proto-stellar stage in which they are usually detected (albeit in much greater abundance). Experimental evidence also suggests that COMs may be formed on very cold surfaces (~10 K), through mechanisms that do not require thermal diffusion of the reactants. Past models that rely solely on diffusive reaction mechanisms now appear inadequate.

I will discuss new modeling treatments that adopt a more comprehensive framework for grain-surface and ice-mantle chemistry, allowing reactants to meet in a variety of ways that do not rely solely on diffusion. This allows COMs to form as the ice mantles grow, while processing of the ices by external and cosmic-ray-induced UV fields can also lead to COM production. The period when the water-dominated ices desorb from the grains also allows trapped radicals to meet and react on the warm ice surfaces, prior to desorption. Gas-phase chemistry can further enhance COM production in some cases. In combination, these processes allow COMs to form over a range of temperatures, through a variety of mechanisms. I will discuss the implications of this new picture of COM chemistry on the origins and abundances of both familiar and more unusual COMs in star-forming regions.

Molecular precursors of the RNA-world in the interstellar medium: the astrochemical mine found in G+0.693-0.027

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We still do not understand how simple molecules combined together to form large molecules essential for living organisms. Recent prebiotic experiments, based on the RNA-world hypothesis for the origin of Life, have suggested that the three basic macromolecular systems (nucleic acids, proteins and lipids) could have formed from relatively simple precursors. The detection of some of these molecules in space, thanks to the unprecedented capabilities of current astronomical facilities, has opened a new window for astrobiology from the astrochemical point of view. In this talk I will present the most recent results of an ultradeep unbiased spectral survey towards the molecular cloud G+0.693-0.027 with the Yebes 40m, IRAM 30m and APEX telescopes. We have recently discovered 13 new interstellar species, including key precursors of RNA nucleotides such as hydroxylamine (NH2OH); of sugars, such as the glycolaldehyde isomer 1,2-ethenediol ((CHOH)2); of proteins, such as ethyl isocyanate (C2H5NCO), and propargylimine (HCCCHNH); of lipids, such as ethanolamine (NH2CH2CH2OH) and propanol (CH3CH2CH2OH); and new species with phosphorus, such as the ion PO+. This amazing chemical complexity, which might be only the tip of the iceberg, means that interstellar chemistry offers an extremely rich feedstock for triggering prebiotic chemistry.

Rotational spectroscopy and chemical reactivity in Astrochemistry: experiment and theory

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Understanding the chemical evolution of the universe is one of the main aims of Astrochemistry, with the starting point being the knowledge whether a molecule is present in the astronomical environment under consideration and, if so, its abundance. In this context, rotational spectroscopy plays the central role. The astronomical observation of the spectroscopic features of a given molecule is the definitive, unequivocal proof of its presence in the astronomical environment under consideration, with the overwhelming majority of gas-phase chemical species being discovered via their rotational signatures. Among the goals of astrochemistry, the detection of prebiotic COMs in astrophysical environments is fundamental in view of possibly understanding the origin of life. While the evidence for molecular complexity in the universe is undisputed, there is still much to be understood about what prebiotic molecules are present and how they are formed in the typically cold and (largely) collision free environment of the interstellar medium. By means of selected examples, it will be shown that: (i) the interplay of experiment and theory in the field of rotational spectroscopy is a powerful tool in astrochemistry; (ii) state-of-the-art computational approaches allow for deriving formation pathways able to explain the molecular abundances derived from astronomical observations.

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Modeling the aromatic infrared bands in the JWST era

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Aromatic infrared bands (AIBs) are used in astronomy to trace the ultraviolet (UV) radiation field in star-forming regions, from the small scale of protoplanetary disks to the large scale of galaxies. Their observation is at the heart of the Early Release Science programme, PDRs4all, of the James Webb Space Telescope. AIBs result from the cooling of large carbonaceous molecules following the absorption of UV photons. They contain information on the chemical complexity of their carriers and their evolution with physical conditions. Polycyclic aromatic hydrocarbons (PAHs) and related species are good candidates to explain AIBs, but other species such as fullerenes also contribute (so far, C60 and C60+ have been firmly identified). A detailed analysis of AIB spectra requires taking into account molecular diversity as well as excitation conditions. To disentangle these two effects, a detailed comparison of observed spectra with synthetic spectra is necessary. In this context, the LAIBrary project brings together a team of experimentalists, theorists and modelers to calculate the photophysical evolution of a given PAH molecule in a given UV field and extract the associated infrared (IR) spectrum. Such a calculation requires all the necessary molecular ingredients, including empirical anharmonic parameters that describe the evolution of IR band widths and positions with temperature. The objectives and current achievements of the LAIBrary project will be presented.

Imaging Interstellar Dust Grain Model Surfaces with Atomic Resolution

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Interstellar space is home to surprisingly complex chemistry. In spite of the low temperatures and pressures more than 250 different molecules have so far been detected. Catalytic reactions on dust grain surfaces are expected to play a dominant role in interstellar chemistry. Such heterogenous catalytic reactions are highly dependent on the specifics of the catalytic surface. The elemental composition, defects, nano-structure, porosity, ice coatings and thick icy layers all impact heavily on reactivity. Scanning tunneling microscopy (STM) allow us to image surface structures and adsorbate molecules at the atomic level. Such measurements allow us to detect reaction products with single molecule detection sensitivity and to study the structure of low temperature icy clusters forming on surfaces of interstellar relevance. Here I present results on water ice cluster formation at temperatures down to 12 K and on imaging of reaction products from PAH hydrogenation reactions.

Chemical evolution of CO2 ices under processing by ionizing radiation employing the PROCODA code

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Astrophysical ices are being exposed to ionizing radiation in space environments, which trigger new reactions and desorption processes. In the lab, such processing by radiation has revealed the appearance of several new species and complements the study of the chemical evolution of icy astrophysical scenarios. Here, we present our new computational methodology developed to clarify the chemical evolution of ices investigated experimentally under photolysis/radiolysis processes until reach chemical equilibrium (CE). Briefly, the code (named PROCODA) solves a system of coupled differential equations and describes the evolution of the molecular abundances with the irradiation time for ices under processing by radiation (Pilling et. al. 2022, ApJ, in press). Two experimental icy samples containing pure CO2 and irradiated by two ionizing agents (cosmic ray (CR) analogue and ultraviolet (UV) photons) were considered prototype systems. We considered 11 different chemical species within the ice (4 observed: CO2, CO, O3, and CO3; 7 non-observed or unknown: O, O2, C, C2, C2O, C2O2, and C2O3), 100 reaction routes (e.g. direct dissociation reactions, bimolecular and termolecular reactions) and radiation-induced desorption processes. The best-fit models provide the reaction rates, several desorption parameters, as well as, the characterization of the chemical equilibrium phase. At CE the percentage of non-observed species in the UV model was almost triple the one calculated in the CR model (which also includes a lot of O and C atoms). The determined values can be employed in future astrochemical models to map chemical evolution embedded species in astrophysical under the presence of an ionizing radiation field.

Massive Protostellar Disks as a Hot Laboratory

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Recent high-resolution observations reveal detailed structures and chemistry in protoplanetary disks around low-mass stars, yet mostly limited to outside of their snowlines with low temperatures of <200K. On the other hand, massive protostellar disks are typically as hot as ~100-1000 K, due to the intense stellar radiation and high accretion heating. Therefore, we propose to utilize massive protostellar disks as a hot laboratory for investigating the physics and chemistry of solid materials at such high temperatures. In hot disks at >100K, silicate grains are exposed as water ice sublimates. We successfully constrain the threshold fragmentation velocity of silicate grains to ~6-10 m/s by comparing our disk model calculations with polarization observations (Yamamuro, Tanaka, and Okzumi, to be submitted). Also, at > several hundred Kelvin, even refractory materials begin to evaporate. Our ALMA high-resolution observations have shown that rare molecular lines, e.g., salts (NaCl, KCl) and silicon compounds (SiO, SiS), are good tracers for massive protostellar disks (Tanaka, Zhang et al. 2020, etc.). Those hot-disk researches will provide new insights into the formation of rocky planets, as well as CAIs and chondrules in primitive meteorites.

Laboratory Ice Astrochemistry at Large Scale Facilities

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Complex organic species are expected to be formed in a variety of interstellar environments at the surface of ice grains by means of a combination of energetic and nonenergetic processing, e.g., photons, electrons, ions, and atoms. However, to date, many fundamental questions on the physicochemical origin of the observed molecular complexity in space and its link to life on Earth remain unanswered. The recent scientific achievements of the James

Webb Space Telescope (JWST) are marking the onset of a new era for space science, astrophysics, astrochemistry, and astrobiology. The unprecedented combination of JWST and the ground-based Atacama Large Millimeter/submillimeter Array (ALMA) will respectively map and characterize the ice and the gas content of the interstellar medium toward a variety of space environments and physicochemical conditions, revolutionizing our understanding of the star formation process. In my talk, I will discuss new emerging laboratory techniques at larger scale facilities in Europe that will allow for a correct interpretation of observational ice data to help address some of the “Grand Challenges” in astrochemistry of the next decade.

Carbon-Chain Chemistry around Massive Young Stellar Objects

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Carbon-chain molecules had been considered to be abundant in young starless cores. Warm Carbon-Chain Chemistry (WCCC) was discovered around low-mass protostars in the late 2000s. However, our knowledge about carbon-chain chemistry in high-mass star-forming regions is poor. Are carbon-chain molecules formed around massive young stellar objects (MYSOs)? If so, does WCCC explain their abundances? We have investigated carbon-chain chemistry around MYSOs by observations and chemical simulations. We found that the observed HC5N abundances around MYSOs cannot be explained by WCCC, but can be reproduced after the temperature reaches its sublimation temperature above 100 K. I will give a talk about results of ALMA data and chemical simulations, and future plans regarding carbon-chain chemistry around protostars.

Chemistry and transport of volatiles in protoplanetary disks

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Recent observations have revealed that volatile elemental abundances in some protoplanetary disks are different from those in the local ISM. For example, the abundance of volatile carbon in some disks is found to be lower than that in the local ISM by a factor of 10-100. These findings indicate that the transport of volatiles via the turbulent mixing and the vertical settling/radial drift of icy dust grains occurs efficiently in the disks. In this talk, I will discuss how the combination of gas-ice chemistry and the transport processes shape the chemical compositions of protoplanetary disks in light of our recent modeling studies.

Cooking with the stars: creating a hot corino soup

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Hot corinos are protostars that are surrounded by warm gas that is rich in molecules. To create this molecular soup, we need to know how its ingredients are created and how they are heated up. In this talk I will present recent studies we have conducted on this topic. We employ cryogenic laboratory studies to simulate interstellar ice chemistry. In electron irradiation experiments, a wealth of molecules are formed, but the degree of complexity varies significantly depending on the starting ice mixture that is used. To understand how these products transfer from the ice to the gas, we have used data analysis and machine learing tools to determine binding energies of these molecules. With this computationally low-cost method we can determine the binding energy of a large number of complex molecules. Bringing ice experiments and knowledge of desorption parameters together, helps us to understand how the chemical complexity in hot corinos arrises.

Complex Chemistry in Star Formation: The Synergy of ALMA and JWST

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The Discovery of complex organic molecules (COMs) in solar-type protostars highlights the extensive chemical evolution at the onset of planet formation. These molecules, which are potential precursors to pre-biotic molecules, are also found in comets that contain the most pristine matter in the solar system. In recent years, the increasing detection of COMs by interferometric sub-mm/mm observations, such as ALMA and VLA, suggest a common presence of COMs in the early stage of star formation. However, the formation pathways of COMs and whether most protostars undergo similar chemical evolution remain open questions with incomplete observational constraints. It is thought that COMs form in the ice mantles on dust grains followed by thermal sublimation near protostars. While ALMA provides sub-100 au resolution, a resolution necessary to resolve sites of planet formation, to characterize gaseous COMs in nearby embedded protostars, measurements of chemical composition in ices had been limited by low-resolution and limited sensitivity spectroscopy until JWST, which can probe ices at a spatial scale comparable to that by ALMA with unprecedented sensitivity. In this talk, I will highlight the frontier of complex chemistry from observations of COMs in both gas- and ice-phase. Particularly, I will discuss the prospect of connecting the COM formation and evolution from prestellar cores to planet-forming disks in the era of JWST.

Nitrogen isotopic ratios across the Milky Way

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One of the most important tools to investigate the chemical history of our Galaxy and our own Solar System is to measure the isotopic ratios of chemical elements. The isotopic ratios are governed by two main processes: 1. chemical evolution of the whole Galaxy due to stellar nucleosynthesis; and 2. local fractionation effects. The latter is the process that distributes the less abundant stable isotopes of an element in different molecules. For the case of nitrogen (N), the 14N/15N isotopic ratio found for the proto-Solar nebula, 440, is significantly higher than that measured in pristine Solar System materials, like comets (around 140). This suggests a local chemical enrichment of 15N during the Solar System formation. However, the causes of the 15N-enrichment are still uncertain.

In this talk I will briefly review the state-of-the-art of the astronomical observations and theoretical chemical models devoted to the study of nitrogen isotopic ratios. I will show the overall behavior of the 14N/15N ratio across the Galaxy. In particular, based on a large survey of star-forming regions, we have confirmed that the 14N/15N ratio increases with galactocentric distances up to 11 kpc, and found for the first time that it decreases after 11 kpc. This overall trend can be explained by nucleosynthesis Galactic chemical evolution models. Furthermore, I will present the first interferometric maps of N-fractionation of N2H+ towards a star-forming region. Our results highlight the importance of local effects, and in particular of isotope-selective photodissociation of N2, in determining the 15N-enrichments in star-forming regions. I will also review recent works studying the importance of this chemical effect.

Grain surface ice astrochemistry of MgNC

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Density functional theory cluster calculations were used to characterize the chemistry that may occur when magnesium isocyanide, MgNC is deposited on amorphous water ice. The spectrum of ice-bound MgNC was simulated on a range of cluster sizes. Subsequent reactions with H, acetylene, and HCN were studied in clusters with 17 and 24 water molecules. MgNC is an intriguing reactant: it is a reasonably reactive radical with a mix of covalent and ionic bonding. Pathways were identified to form HMgNC (a known astromolecule) and various divalent open shell and radical compounds containing Mg. Two catalytic pathways were found to form the vinyl and methaniminyl radicals.

Astrochemical Modeling of Massive Protostellar Core Envelopes

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A large number of molecular species have been identified in hot molecular cores, i.e., the gas that is directly involved in massive star formation. Chemical evolution is expected to be closely coupled to physical evolution. In particular, it is crucial to include the evolution of densities and temperatures along infalling streamlines in the chemical modeling to predict the spatial distribution of abundances in protostellar core envelopes. In this talk, I will present the results of astrochemical models of massive protostellar core envelopes based on the framework of the Turbulent Core Accretion model (McKee & Tan 2003; Zhang et al. 2014). I will discuss the evolution of abundances of various interstellar species in the ice and gas phases within a 60 solar mass core that eventually forms stars with different masses. The location of ice lines in the infalling envelope is one particular focus.

High-resolution spectroscopy of astrophysically-relevant hydrocarbon ions

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Molecular ions are long known to be key intermediates in the evolution of molecular complexity in the interstellar medium. However, they have historically proved challenging to study in terrestrial laboratory experiments due to their reactivity and transient nature. The 22-pole ion trap instruments, like the ones available at Cologne [1,2], have been revolutionary in this field as mass-selected, cryogenically cooled ions provide very clear spectroscopic information. Ionic species are investigated using ion trap instruments which feature mass selection via quadrupole mass analyzers, long storage times in cryogenic 22-pole ion traps, and cooling of the ions via He buffer gas to temperatures as low as 4 K. Due to the low number of stored ions (typically less than 105), so-called action spectroscopic techniques have to be applied, in which the ion count is used as the spectroscopic signal. These high resolution rovibrational and pure rotational spectra are also crucial to provide information for unambiguous identification of ions in space using the recently launched James Webb Space Telescope and/or other ground-based radio observatories, like ALMA, NRAO, etc. I will talk about a new action spectroscopy technique, “leak-out spectroscopy” [3], recently developed in Cologne which has been employed to measure the spectra of the various cations of astrochemical relevance. In particular, I will focus on c-C3H3+, which is the smallest aromatic hydrocarbon ion, and its isotopologues. Hydrocarbon ions in the interstellar medium, especially in the diffuse clouds and photodissociation regions, can act as an excellent tracer of the interplay between polyaromatic hydrocarbon formation and photo-destruction[4].

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Computing the ingredients to simulate the photophysics of PAHs in space

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Polycyclic Aromatic Hydrocarbons (PAHs), and their close derivatives, are believed to be a key component of the interstellar medium (ISM). They should collectively use between 10 and 20% of the available interstellar carbon, provide a large contribution to the interstellar extinction in the UV, dominate gas heating in photodissociation regions (PDRs), contribute as catalysts to the formation of H2. Their most prominent observational signatures are an ubiquitous set of infrared bands, the aromatic infrared bands (AIBs), corresponding to the vibrational frequencies of C-H and C-C bonds in all aromatic species. PAHs in the ISM are supposed to absorb UV photons via electronic transitions, convert the electronic excitation to vibrational excitation via a series of ultrafast non-radiative transitions, then relax via a cascade of vibrational transitions. Modelling this emission properly for an individual PAH hence requires a number of "ingredients", from the electronic photoabsorption cross-section to a quantitative estimate of anharmonicity. An overview will be given on which, and how, these ingredients can be obtained through (feasible) theoretical calculations.

Large carbonaceous molecules and molecular clusters : Insights from theoretical modelling

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Astronomical observations and matter evolution models suggest a strong diversity carbon based materials in the interstellar medium including amorphous carbonaceous grains, PAHs, PAH clusters and PAH on/in ices. Quantum chemistry is a powerfull tool to investigate their properties but original developpements are often required to address astrophysically relevant systems. In particular, it is challenging to describe the large number of atoms/electrons and processes like the charge delocalization in molecular clusters. We will show that Density Functional based Tight Binding, an approximated quantum chemistry scheme, allows to adress such large systems and is a powerfull tool to compute their structural, energetic and spectral properties. Its coupling with dynamical simulations allows to adress fragmentation dynamics and to identify the main dissociation processes. Recent results will be presented showing the main differences between energetic, structural and spectral properties for neutral and cationic PAH clusters. PAH clusters evaporation following a collision or photon absorption is investigated and good agreement is obtained with experimental works. We will also report recent developments allowing to simulate beyond the Born-Oppenheimer approximation the evolution of an electronically excited system (collision or photon absorption).

Temperature and kinematic structure of the burst-phase protostar SVS13A using DCN and COMs

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We present new NOEMA observation with high-spectral resolution and sensitivity toward the Class O/I binary system SVS13A. Protostars are believed to stay in a quiescent accretion phase for most of the time and accretion bursts occasionally occur while delivering material onto the central protostar. Recently, large-scale accretion flows have been found to funnel chemically fresh material onto the disk scale; this material accumulates on the disk, triggering accretion bursts. During a burst phase, the source luminosity can increase by 1-2 order of magnitude and surrounding dust grain icy mantles can sublimate, changing the chemical composition in the gas phase. However, how such mechanism affects the chemical and physical evolution is not well understood. SVS13A is a low-mass proto-binary system; given the high bolometric luminosity, 45 Lsun, SVS13A is considered to be undergoing an accretion burst. We observe CH3CN and DCN line emission toward SVS13A. With the high-spectral-resolution data, we find that the complicated line profiles cannot be explained by a simple component or Keplerian motion. By adopting a two-component model, we suggest that the temperature and/or density of the emitting gas traced via CH3CN can change dramatically within the circumbinary disk. In addition, combining our DCN observation with previous ALMA high-resolution observation, we find that the binary system (or Per-emb-44B) is fed by an infalling streamer from an outer region (~700 au). This streamer contributes to an accretion of material onto the system with a rate of at least 1.2x10^-6 M yr^-1. Furthermore, with the high-spectral resolution data for O-bearing COMs, we find that the COM emission can be decomposed several velocity components with a big variety in temperature (100--500 K) and source size (0.03--0.24 arcsec). Given this complex structure, we suggest that the central region is inhomogeneous and unlikely be heated by only the protostellar radiation. Accretion shocks or shocked gas in the disk likely exists to induce the complex COM emission. We conclude that the COM emission in SVS13A originates from gas in a complex structure in the binary system. The large-scale infalling streamer is affecting the binary formation in an early evolutionary stage.

Spectroscopy of Interstellar Aromatics

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Single or fused Benzene rings constitute aromatics that are highly stable due to the presence of delocalized electrons. These molecules are ubiquitous in terrestrial environments and are formed by the burning of hydrocarbons (viz. vehicle exhausts, smokes, etc.). We focus on aromatics, specifically Polycycylic Aromatic Hydrocarbon (PAH) molecules that are expected to be present in interstellar space and are inherently involved with the chemistry of the local environment. The presence of PAH molecules is known by the observation of strong emission features at 3.3, 6.2, 7.7, 8.6 and 11.2 μm in the Milky Way and in external galaxies1. Confirmation of the presence of fullerene cation in the interstellar medium (ISM)2 strongly supports the presence of PAHs. In the harsh interstellar conditions, PAHs experience physical and chemical processing that brings changes in the molecule. Ionization, dehydrogenation, etc. produce significant spectral signatures that are being diagnosed spectroscopically. We have been studying variants of PAHs, viz., deuterated3, dehydrogenated4 and also with addition of aliphatic side groups5. Density functional theory (DFT) has been used to calculate the theoretical vibrational spectra of PAHs. The spectra obtained matches well with available experimental spectra and provides important clues to the form of PAHs present in the ISM. We also present rotational spectra of nitrogen containing PAHs that may help in detection of these PAHs6.

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Comparative study of the chemical composition of G31.41 with different phases of the star formation

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There is growing evidence that our Sun, like most stars, was born in a rich and dense stellar cluster that also contained massive stars. Therefore, the study of the chemical reservoir of galactic massive star-forming regions is crucial to understand the basic chemical ingredients that were available prior the formation of our Solar System, and the subsequent emergence of life. With this purpose, the ALMA project GUAPOS (G31.41+0.31 Unbiased ALMA sPectral Observational Survey) studies the full molecular inventory of the massive star-forming region G31.41+0.31, one of the most chemically rich sources in the Galaxy. In this talk, I will present the results of the comparative study of the abundances of more than 60 different molecules (including complex organic molecules with prebiotic relevance) identified in G31.41+0.31 with those previously derived in other well-studied sources: the low-mass Solar-like protostar IRAS 16293–2422 B, and the comets 67P/Churyumov-Gerasimenko and 46P/Wirtanen. We have used three complementary statistical tests (Spearman, Kendall and Theil-Sen) to study the correlations between the chemical content of these different objects. This comparison gives us important hints about how the chemical complexity of the interstellar medium can be inherited during the process of star and planet formation.

Modeling Titan's Upper Atmospheric Gas Chemistry at Low Temperature

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The Cassini spacecraft measured the molecular mass of ions for the first time in the atmosphere of Saturn’s largest moon, Titan. These observations uncovered the complexity of Titan’s upper atmospheric chemistry, which results in the production of radicals, ions and aerosols. Photochemical models have helped explain the gas phase chemistry involved in the production of organic aerosols. Alongside those models, laboratory experiments have helped fill gaps in the reaction networks through detailed studies of the effects of precursors and energy source(s) on the chemical pathways leading to aerosol production.

Here, we present a new study using an existing 1D model, which simulates the plasma chemistry in the Titan Haze Simulation (THS) experiment developed on the COSmIC Simulation Chamber (COSmIC) at NASA Ames Research Center. THS uses a pulsed plasma discharge in the stream of a supersonic jet expansion to simulate the different steps in Titan’s atmospheric chemistry at low (~150 K) Titan-like temperature. Using newly published reaction rates, we have updated the model and report new computational results and their comparison to experimental mass spectra obtained with THS in three gas mixing ratio conditions (N2-CH4, N2-CH4-C2H4 and N2-CH4-HCN) relevant to Titan's ionosphere.

Chemical complexity in starless and pre-stellar cores

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Observations carried out toward starless and pre-stellar cores have revealed that complex organic molecules are prevalent in these objects, but it is unclear what chemical processes are involved in their formation. In 2016, Jiménez-Serra et al. observed the L1544 pre-stellar core and found that complex organic molecules are preferentially produced at an intermediate-density shell at radial distances of several thousands astronomical units with respect to the core center [1]. Later, in 2021, Jiménez-Serra et al. performed similar observations toward the L1498 starless core, believed to be at an earlier stage of evolution than L1544 [2]. In this talk, I will present a related study toward another starless core, L1517B, which seems even younger than L1498 and L1544. L1517B has been observed in the 3 mm atmospheric window using the 30-meter telescope of IRAM at Pico Veleta (Spain), with the aim of determining its level of chemical complexity and to compare it with that of L1544 and L1498. We observed a lower level of chemical complexity than in L1498 and L1544, and we suggest that the differences between these three cores are due to their evolutionary stage, where the nitrogen-bearing organics are formed first followed by the oxygen-bearing organics once the catastrophic depletion of CO sets in.

[1] Jiménez-Serra et al., 2016, ApJL 830 L6. https://doi.org/10.3847/2041-8205/830/1/L6
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X-Ray Photoinduced Fragmentation of Prebiotic Molecules in Interstellar Clouds: Ethanolamine

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Ethanolamine (C2H7NO), recently identified in object G+0.693–0.027 [1] within SgB2, is a biologically important molecule that is part of the hydrophilic head of the second most abundant group of phospholipids present in cell membranes. The identification of this molecular species in a region close to the galactic centre opens up a whole series of questions about the mechanisms of formation and stability of complex organic molecules in astrophysical environments. For this reason, we study the fragmentation mechanisms and estimate the half-life of ethanolamine in the G+0.693 object, using experimental x-ray data taken at the National Synchrotron Light Laboratory (LNLS) facility, Campinas, Brazil. The data allow us to identify the dominant fragmentation profiles and to propose potential precursors present even in other objects, which may be important for the synthesis of prebiotic species in molecular clouds and possibly as part of the chemical content in forming planetary regions.,

[1]Rivilla Víctor M., et al., PNAS, 118, 22, 2021.

Towards a better understanding of sulphur radiation chemistry in astrochemical ices

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The chemistry of sulphur represents one of the least understood facets of astrochemistry, both in terms of chemistry occurring within interstellar regions as well as within the icy Solar System. In dense interstellar regions, sulphur is depleted by two to three orders of magnitude compared to its expected cosmic abundance. Various modelling efforts have outlined different reservoirs that may possibly host this 'missing' sulphur, though scientific consensus has yet to be achieved. In the Solar System, the presence of SO_2 ice on the surfaces of the Galilean moons of Jupiter has long been attributed to the implantation of magnetospheric sulphur ions into the surfaces of these moons, which contain several oxygen-bearing molecules (e.g., H_2O, CO_2, O_2). However, experimental work has provided little in the way of evidence for a reasonable formation mechanism of SO_2 via sulphur ion surface implantation, and systematic studies are lacking. In this talk, I will provide a detailed overview of these problems, as well as recent experimental work that has been performed in our group in an attempt to gain a clearer understanding of the underlying processes relevant to sulphur ice astrochemistry, with particular reference to these as yet unanswered problems.

H-Atom-Abstraction and H-Atom-Addition Reactions of Fulminic Acid (HCNO) and Formaldoxime (H2CNOH) in Solid para-H2

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Until the end of 2021 more than 260 molecules were identified in the interstellar medium (ISM). The most abundant of them in the ISM is H_2. One of the central questions of astrochemistry is how H_2 is formed in dense molecular clouds. According to recent theoretical studies, it is possible that H_2 is generated in catalytic cycles [1]. In the catalytic cycles two H atoms recombine to an H_2 molecule with the help of a catalyst. The aim of our research work was to investigate the catalytic cycle of fulminic acid (HCNO) and formaldoxime (H_2CNOH). The molecules were trapped in para-H_2 matrix at 3.1 K. Then, H atoms were generated in the matrix. In para-H_2, the H atoms can diffuse efficiently, which enabled the examination of the reactions of the trapped molecules with H atoms. The chemical changes were followed by IR spectroscopy. According to our experimental results, fulminic acid and formaldoxime can react with H atoms in para-H_2 matrix at 3.1 K. This observation indicates that the same reactions might also occur in the dense molecular clouds and these reactions can catalyze the H_2 formation. While fulminic acid is present in a large amount in the ISM, formaldoxime has not been detected yet. The experimental results have shown that the quantity of fulminic acid and formaldoxime is connected to each other through a quasi-equilibrium reaction. This quasi-equilibrium is shifted towards the fulminic acid, which may explain the non-detection of formaldoxime in the ISM.

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Metallic buckyballs as promising carriers of mysterious unidentified infrared emission bands

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Unidentified infrared emission (UIE) bands with wavelengths between 3–20 μm are observed in a variety of astrophysical environments, but over 40 years of research efforts still leave the source of these emission bands largely unknown. In this talk, I will present our innovative approach that combines gas-phase synthesis of fullerene-metal complexes and their in-situ characterization by mass spectrometry, infrared action spectroscopy, and theoretical modeling to understand the carriers of UIE bands. We obtained for the first time the high-quality laboratory infrared (6–25 μm) spectra of gas-phase fullerene-metal complexes, and conducted a detailed comparison with observational Spitzer spectra. We propose that fullerene-metal complexes are promising carriers of astronomical infrared bands, opening a new chapter for studying cosmic fullerene species and carbon chemistry in the Universe.

Contribution of small hydrocarbons from dust photo-dissociation

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I will present the results of study of evolution of hydrogenated amorphous carbon (HAC) grains under harsh UV radiation in photo-dissociation regions (PDRs) near young massive stars. The aim of the study is to evaluate the impact of the HAC grains and PAHs on formation of observed small hydrocarbons: C_2H, C_2H_2, C_3H+, C_3H, C_3H_2, C_4H, in PDRs. We developed a microscopic model of the HAC grains based on available experimental results. The model includes processes of photo- and thermodesorption, accretion of hydrogen and carbon atoms and subsequent formation of carbonaceous mantle on dust surface. H_2, CH_4, C_2H_2, C_2H_4, C_2H_6, C_3H_4, C_3H_6, C_3H_8 are considered as the main fragments of the HAC photo-destruction. We simulated evolution of the HAC grains under the physical conditions of two PDRs, the Orion Bar and the Horsehead nebula. We estimated the production rates of the HAC' fragments in gas phase chemical reactions and compared them with the production rates of fragments due to the HAC destruction. The latter rates may dominate under some conditions, namely, at AV=0.1 in both PDRs. We coupled our model with the gas-grain chemical model MONACO and calculated abundances of observed small hydrocarbons. We conclude that the contribution of the HAC destruction fragments to chemistry is not enough to match the observed abundances, although it increases the abundances by several orders of magnitude in the Orion Bar at AV=0.1. Additionally, we found that the process of carbonaceous mantle formation on dust surface can be an inhibitor for the formation of observed small hydrocarbons in PDRs.

Theoretical and observational study of PAHs up to ten hexagon rings

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The present study reports the comparison of theoretical infrared and optical absorption spectra with the observational data of 01 to 10 hexagons in their neutral and ionic states. The hexagons' structural arrangements make isomers viz. cata, peri-condensed and branched structures. The five-member benzene ring has 22 isomers viz 02 branched, 10 peri, and 10 cata-condensed structures. The closed, linear structural arrangement from peri and cata condensed shows the lowest energy isomer for five-membered hexagons. These structural arrangements followed for the remaining hexagons. All these structures are optimized at the B3LYP/TZVP level of theory to confirm the lowest energy structure. Significant changes have been observed in their vibrational and electronic absorption spectra of ions compared to neutral. The geometrical parameters such as dipole moment, symmetry, and energies for these isomers are reported. $C_{22}H_{12}$ in its peri-condensed form has a significant dipole moment with low symmetry at C1 in neutral and its ionic form. The average theoretical spectra of cata and peri-condensed PAH molecules show the features at 3.25 µm, 7.65 µm, 8.69 µm, and 11.25 µm respectively. These features are observed in the reflection nebula NGC 2023 and planetary nebula NGC 7027. To compare with the bump feature at 217.5nm in the interstellar extinction curve, we also studied the electronic absorption spectra of the up to ten hexagons in their neutral and their ionic states using time-dependent density functional theory (TDDFT) at the same level of theory. The electronic transition, oscillator strength, and HOMO-LUMO gap were also reported. The present study also is to understand the emission features of the 217 nm (2200 Å) astronomical UV bump. We have compared this theoretical study with the available observational data.

Neutral atomic hydrogen as an efficient catalyst for interstellar gas-phase formation of adenine and guanine

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Using quantum chemical calculations, we simulate multiple possible gas-phase synthesis pathways towards adenine and guanine in interstellar condition. Neutral atomic hydrogen (HI) is found active in promoting a series of fundamental proton transfer processes of organic synthesis, including bond formation, cyclization, dehydrogenation, and H migration. The reactive potential barriers are significantly reduced by the alternative pathways created by HI, leading to a remarkable increase in the reaction rate. The reactive activation temperature is accordingly reduced by HI from 757.8 to 131.5-147.0 K, pointing to a thermally feasibility of the proposed pathways in star-forming regions, towards which parts of the reactants are astronomically detected. Our results suggest that a catalytic effect of HI in the formation of interstellar complex organic molecules.

Metal-Ion Mediation in Interstellar Chemistry

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The chemistry of metal-ions is well understood in terrestrial chemistry. However in the Interstellar medium (ISM), a lot of interesting and open questions pertaining to the role of metal-ions in assisting molecular evolution are yet to be adequately addressed. In this presentation, we shall highlight how metal-ions may be of relevance in three particular gas-phase interstellar reactions : (a) glycoaldehyde formation from formaldehyde, (b) the generation of formamide, and (c) epoxide synthesis. This presentation features an account of our computational research work which actively advocates the possible role played by organometallic species in the formation of interstellar complex organic molecules. Some key open questions in this nascent area of organometallic astrochemistry shall also be discussed.

Density Structure of Centrally Condensed Prestellar Cores from Multiscale Observations

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Starless cores represent the initial stage of evolution toward (proto) star formation. Only a subset of starless cores - known as prestellar cores, however, can be embryos to (proto)stars. Therefore, estimating the density profile of prestellar cores provides the best opportunity to gauge the initial conditions of star formation. Prestellar cores are expected to be highly dense (~ 10^6 cm^−3 or higher) and centrally concentrated. However, a limited number of dense prestellar cores have been reported to date. Based on a recent observation, we have detected five highly dense prestellar cores, and in this work, we perform rigorous modeling to estimate the density profiles of three of them presenting nearly spherical geometry. We use single-dish SCUBA-2 observation (beam ~ 5600 au) to high resolution (~ 480 au) ALMA observations to constrain models of the observed dust continuum emission and density profile. A simple physical model with a compact region of flat density in the center of each cores and an r^-2 profile outside is able to reproduce consistently the observed emission from large to small scales. The result suggests that a single power law should be able to describe the density profile of the spherical prestellar cores. Additionally, we use the size of the compact central region as a proxy for the dynamical stage of the cores. We find that all the modeled cores are likely gravitationally unstable and on the verge of collapse. Importantly, we estimated that the size of one compact region can be as small as ~ 500 au. Possibly, they represent the most evolved prestellar core known to date.

Ultraviolet photon-induced trapping of photoproducts in amorphous solid water

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In the interior of cold and dense molecular clouds, along with H_2O other molecular species, including CH_4, CO_2, CO, CH_3OH, and NH_3, exist on icy dust grains. These ice mantles undergo photoprocessing by secondary ultraviolet (UV) photons. Such a photon-irradiation initiates different physicochemical processes affecting the molecular abundances detected in the gas and solid phase. However, this work aims to understand the UV photon-induced synthesis and trapping of CO_2 and CO in porous water ice. Upon VUV irradiation of CO-H_2O ice at 10 K in an experiment conducted in ultrahigh vacuum, reflection absorption infrared spectroscopy and temperature-programmed desorption (TPD) mass spectrometry analyses have shown that CO and CO_2 are trapped in clathrate hydrate (CH) cages. CHs are inclusion compounds in which different guest molecules are encased in H-bonded water cages. CHs are ubiquitous on earth under high-pressure conditions but are also known to exist in the interstellar medium (ISM).

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