

Future Observations, Techniques and Methodology in Astrochemistry

Annual Meeting of the Astrophysical Chemistry Group

Scientific Programme 24 June 2019

Astronomical Observations as Tools to Constrain the Chemical Routes of Interstellar Complex Organic Molecules

Cecilia Ceccarelli (Invited Speaker)

Grenoble Observatory, FR

Organic molecules have been detected in the Inter-Stellar Medium for decades, some of which have more than five atoms and are called iCOMs for interstellar Complex Organic Molecules. This class of interstellar molecules, especially those detected in solar-type planetary systems, are particularly interesting because they might have been the seeds from which larger pre-biotic molecules could have grown and started/facilitated the appearance of life on Earth.

Despite this far reaching interest, there is still a debate on the formation routes of iCOMs. In principle, they can either be synthesized on the grains surfaces, like many current models assume, or on the gas phase, as mounting evidence suggests.

In this presentation, I will review how astronomical observations can be used to put constraints on the formation routes of iCOMs and will present specific examples.

First Detection of the Pre-biotic Molecule Glycolonitrile (HOCH₂CN) in the Interstellar Medium

Shaoshan Zeng

Queen Mary University of London, UK

Theories of a pre-RNA world suggest that glycolonitrile (HOCH₂CN) is a key species in the process of ribonucleotide assembly, which is considered as a molecular precursor of nucleic acids. We report the first detection of this pre-biotic molecule in the interstellar medium (ISM) by using ALMA data obtained at frequencies between 86.5 GHz and 266.5 GHz toward the Solar-type protostar IRAS16293-2422 B. A total of 15 unblended transitions of HOCH₂CN were identified. Our analysis indicates the presence of a cold ($T_{\text{ex}}=24\pm 8$ K) and a warm ($T_{\text{ex}}=158\pm 38$ K) component meaning that this molecule is present in both the inner hot corino and the outer cold envelope of IRAS16293 B. The relative abundance with respect to H₂ is $(6.5\pm 0.6) \times 10^{-11}$ and $\geq (6\pm 2) \times 10^{-10}$ for the warm and cold components respectively.

Our chemical modelling seems to underproduce the observed abundance for both the warm and cold component under various values of the cosmic-ray ionisation rate (ζ). Key gas phase routes for the formation of this molecule might be missing in our chemical network.

A Detailed Chemical View of the Circumstellar Environment and Disk of the Forming O-Star AFGL4176

Katharine G. Johnston

University of Leeds, UK

In this talk, I will present results of a detailed analysis of the disk and circumstellar environment of the forming O-type star AFGL4176, with a particular focus on its chemistry. To do this, we have utilized a combination of observations from ALMA, ATCA and APEX. With ALMA, we detect seventeen 1.2 mm continuum sources within 21,000 AU of the main source AFGL4176 mm1, which is surrounded by a circumstellar disk. Within the ALMA bands, we detect over 250 lines from 25 molecules toward the source mm1, which we categorize into several morphological types. All molecules that contain nitrogen trace the disk. Lines that have a morphology that peaks on the blue-shifted side of the disk are predominantly oxygen-bearing. We suggest these molecules are tracing a disk accretion shock. The molecules $C^{34}S$, H_2CS and CH_3CCN trace a slow wide-angle wind or dense structures in the outflow cavity walls. With APEX, we detect a compact and optically thin continuum source ($<2000 \times 760$ AU) at 1.2 cm, associated with mm1, of which $>96\%$ is due to ionized gas. The $NH_3(1,1)$ and $(2,2)$ emission traces a large-scale ($r \sim 0.5$ pc) rotating toroid with mm1 in the blue-shifted part of this structure offset to the NW. Our results show that AFGL 4176 mm1 provides an example of a forming O-star with a large and chemically complex disk, embedded in a large-scale rotating toroid.

Gas-Ice-Dust Mapping in the JWST Era

Helen J. Fraser¹, J. Jorgensen, L. Kristensen, G. Perotti, W. Rocha, J.A. Noble, A. Suutarinen, T.R. Kendall & the ICEAGE JWST ERS team

¹Open University, UK

To fully understand the synergy between gas-phase and solid-state chemistry requires us to be able to accurately map all the components of our star / planet forming chemical cauldron, i.e. gas dust and ice. Building on expertise from the AKARI mission, we have previously shown that we can map H₂O CO and CO₂ ices on scales of around 1000 AU, and compare these to dust and gas column densities. Worryingly for the whole understanding of astrochemistry – this doesn't paint a picture of "more is more" where more dust implies more ice, or a generic picture of what ices we can find (or predict) to be in certain environments. In fact despite knowing for years that ices are our chemical clocks, reflecting prevailing physical and chemical conditions at their formation and evolving as a function of chemistry and physics thereafter, we actually observe a huge diversity in ice chemistries; one that cannot be predicted from gas-phase or dust column densities alone. Are ices the last "missing" link between astrochemical and astrophysical conditions in star forming regions? What can ice mapping reveal about COMS formation and distributions?

Using SVS4 as our latest "laboratory" I'll demonstrate how a combination of observational and laboratory astrochemistry can be used to better understand the unique chemical environments in complex star forming regions, and set the scene for the prospect of JWST ice-mapping to come.

Bad Vibrations: The Anharmonic Infrared Spectrum of PAHs at Beginning of the JWST Era

Alessandra Candian

University of Leiden

Dusty, ultraviolet-irradiated regions of the interstellar medium show strong emission bands in their infrared spectra, the so-called Aromatic Infrared Bands (AIBs), generally attributed to Polycyclic Aromatic Hydrocarbon (PAH) molecules. PAHs absorb UV photons and relax through a collision-less cascade of IR photons, producing the AIBs. Emission spectroscopy experiments in interstellar conditions are incredibly challenging [1], thus theoretical approaches are the way forward. In the past years ([2] and references therein) we have calculated the anharmonic infrared spectrum of a sample of small PAHs using second order vibrational perturbation theory (VPT2) applied to Density Functional Theory-level quartic force fields. Comparison with high-resolution, low-temperature, gas-phase absorption spectra validated our methods. Building up on these results, we developed [3] a fully theoretical IR cascade spectra of PAHs including: an anharmonic VPT2 treatment; the inclusion of Fermi resonances through polyads; and the calculation of anharmonic temperature band shifts and broadenings (including resonances) through a Wang-Landau approach. We also suggest a simplified scheme to calculate vibrational emission spectra that retains the essential characteristics of the full IR cascade treatment and can directly transform low temperature absorption spectra in IR cascade spectra. We show that past astronomical models were in error in assuming a 15 cm^{-1} correction was needed to account for anharmonic emission effects. This work will be crucial to interpret the AIB spectrum once the James Webb Space Telescope comes online.

References:

- [1] Cook D.J. et al, *Nature*, 1996, 380, 227
- [2] Candian A. and Mackie C.J., 2017, *Int. J. Quant. Chem.*, 117 (2), 146
- [3] Mackie C.J. et al, *J. Chem. Phys.*, 149 (13), 134302

Complex Organic Molecules Tracing the Comet-Forming Regions in Protoplanetary Disks

Catherine Walsh (Invited Speaker)

University of Leeds, UK

ALMA has shone light on the diversity in molecular composition and emission morphology of nearby planet-forming disks. These data highlight that gas and ice chemistry ongoing during the epoch of planet formation, not only determines the composition of planet-building material, but also emphasizes many different physical effects. The unprecedented sensitivity of ALMA has allowed the first detection of so-called 'complex organic molecules', or COMs, defined in astrochemistry as molecules with greater than five atoms. The detection and analysis of COM emission from planet-forming disks is vital for understanding the chemical archaeological record of our Solar System contained within comets. I will give an update of recent state-of-the-art results from observations and models of protoplanetary disk chemistry. I will discuss how chemistry affects the dust-ice-gas balance and influences the composition of forming comets, the building blocks of planets.

Measuring the Chemical Inventory of Exoplanet Atmospheres with High-Resolution Spectroscopy

Matteo Brogi

University of Warwick, UK

Two decades of discoveries have revealed an astonishing number of exoplanets, and allowed us to draw robust conclusions about their size distribution. In contrast, accurate determination of physical and chemical properties of exoplanets is still uncharted territory and relies on challenging spectroscopic observations of their atmospheres. As we typically discover evolved systems, it is even more challenging to relate these measurements to how and where planets formed. Numerous detections of water vapour with the Hubble Space Telescope have been recently backed up with ground-based high-resolution spectroscopy. This greatly expanded the number of detected molecular (CO, CH₄, TiO, HCN) and atomic species (H, He, Na, Ca). I will show how in the next few years the yield of the TESS mission and ongoing progress in the analysis of high resolution spectra will produce a large comparative sample of exoplanet atmospheres with measured abundances. Not only will this be vital to shed light on the current exoplanet population, but possibly it will reveal hints about their initial formation. Ultimately, this research will deliver the next step up in sensitivity leading to the detection of biomarkers with the next-generation Extremely Large Telescope.

Chemical Diagnostics of J-type Shocks: An Application to L1157

Tomas James¹, S. Viti, J. Holdship, I. Jimenez-Serra

¹University College London, UK

Shocks are often considered to be of 2 types: C-type and J-type (Draine 1980). Both types exist under different physical, or pre-shock, conditions, giving rise to different final, or post-shock, conditions and chemistry. Tracing the type of each shock, however, is challenging. The differences in post-shock chemistry between C and J shocks can, in theory, be used as a tracer of the type of shock existing within that region owing to the different physical structure within each shock-type.

We have developed a J-shock module for the astrochemical code UCLCHEM (Holdship et al. 2017) aimed at simulating a parameterised J-shock. By using this in conjunction with the existing parameterised C-shock module of UCLCHEM we aim to identify molecules that behave distinctly under different shock types and shock conditions. As an example we apply our models to a prototypical, chemically rich, outflow in L1157 (Umamoto et al. 1992; Bachiller et al. 2001). L1157 is of particular interest given that it not only represents a ubiquitous molecular outflow, but this outflow is thought to host both C-type and J-type shocks in the B1 and B2 knots (Vasta et al. 2012), making it the ideal laboratory in which to apply our models.

We will present results indicating that the dominant mechanism in the chemical evolution of a shock is not the shock-type. Instead, the pre-shock conditions of the shocked material have far more influence on the shock evolution. As such our application to L1157 shows that shock-type diagnostics remain elusive.

References:

- [1] Bachiller, R., Perez-Gutierrez, M., Kumar, M. S. N., & Tafalla, M. (2001). Chemically active outflow L1157. *Astronomy & Astrophysics*, 372(2), 899–912. <https://doi.org/10.1051/0004-6361>
- [2] Draine, B. T. (1980). Interstellar Shock Waves with Magnetic Precursors. *The Astrophysical Journal*, 241, 1021-1038.
- [3] Holdship, J., Viti, S., Jimenez-Serra, I., Makrymallis, A., & Priestley, F. (2017). UCLCHEM: A Gas-grain Chemical Code for Clouds, Cores, and C-Shocks. *The Astronomical Journal*. <https://doi.org/10.3847/1538-3881/aa773f>
- [4] Umamoto, T., Iwata, T., Fukui, Y., Mikami, H., Yamamoto, S., Kameya, O., & Hirano, N. (1992). The outflow in the L1157 dark cloud - Evidence for shock heating of the interacting gas. *The Astrophysical Journal*, 392(i), L83-L86.
- [5] Vasta, M., Codella, C., Lorenzani, A., Santangelo, G., Nisini, B., Giannini, T., Kristensen, L. (2012). Water emission from the chemically rich outflow L1157. *Astronomy & Astrophysics*, 537, A98. <https://doi.org/10.1051/0004-6361/201118201>

Can a Varying Dust-to-Gas Ratio Have an Effect on Chemistry? An Application to the Wardle Instability

Tomas James¹, J. M. C. Rawlings & S. A. E. G. Falle

¹University College London, UK

The Wardle Instability is an effect observed in unstable C-type shocks (Wardle 1990). In a two-fluid scheme consisting of a charged fluid and a neutral grain fluid, perturbations in the magnetic field produce over densities of ions where the field is concave to the direction of propagation and under densities of ions where the field is convex to the direction of propagation. As the dust-grains and ions are weakly coupled, this introduces an inhomogeneity in the number density of dust-grains along the field line, thus changing the dust-to-gas ratio on relatively small scales.

This study aims to analyse the effect these inhomogeneities have on the chemistry within this instability by utilising a one-dimensional ideal MHD simulation of the Wardle Instability (Falle et al. 2009) coupled to a time-dependent chemical code. We aim to assess not only whether the presence of such an instability has an appreciable effect on the physics (and/or chemistry) of the post-shock region, but also whether we can use such chemistry as a tracer of the shock and/or the instability itself.

Preliminary results indicate that the chemistry in a shock is far more temperature dependent than dust-to-gas ratio dependent. However, we aim to present more comprehensive results from a larger chemical network including more grain surface chemistry. We theorise that given the Wardle Instability induces dust-to-gas ratio variations, the greatest enhancement is likely to be observed in molecules which are strongly dependent on grain surface chemistry, such as CH₃OH.

References:

- [1] Wardle, M. (1990). The stability of magnetohydrodynamic shock waves in molecular clouds. *MNRAS*. 98–109. 246.
- [2] Falle, S A E G. Hartquist, T W. Van Loo, S. (2009). Numerical Simulations of the Wardle Instability.

Determination of Refractive Indices of Astrochemical Ices Using Ultraviolet/Visible Reflection Absorption Spectroscopy

James W. Stubbing¹, Tara L. Salter¹, Wendy A. Brown¹, Skandar Taj², Martin R.S. McCoustra²

¹University of Sussex, UK

²Heriot-Watt University, UK

Dust grains occur in many regions in space including the interstellar medium (ISM) and protoplanetary nebulae and provide a surface onto which adsorption and processing of molecules can occur. This in part accounts for the rich chemistry observed. Knowledge of the optical parameters of adsorbed species can be used to predict spectra of interstellar ices, allowing a direct comparison to observational data. In addition, these can be used to more accurately model regions of the ISM in terms of their photoabsorption behaviour.

Determining these parameters experimentally is challenging. Conditions pertinent to the ISM are required, along with a suitable dust grain analogue surface. Additionally, where this surface is optically opaque, a reflection absorption setup is necessary. To the best of our knowledge, no previous work has been undertaken which can satisfy all of these requirements.

We present results from a novel ultraviolet/visible (UV/vis) reflection absorption apparatus which has been installed onto the existing ultra-high vacuum chamber at the University of Sussex. Analysis of the reflectance UV/vis reflectance spectra allows the real part of the refractive index, n , and the thickness, d , of the ice to be measured. Advantages of our analysis method over previously used analyses are discussed. Additionally, an iterative fitting method has been developed to determine wavelength dependent, complex refractive indices which is presented. Data for benzene and methyl formate are shown, both of which have been detected in space and have been shown in this laboratory to undergo a thermally induced phase change.

Unravelling the Isomers of Reactive Ionic Intermediates Using FELIX

Sandra Brünken (Invited Speaker)

FELIX Laboratory, Radboud University Nijmegen, NL

Hydrocarbon and nitrile ions play an important role in the chemistry of planetary atmospheres and the interstellar medium. Laboratory spectroscopic studies of these essential reaction intermediates give valuable insights on their geometrical and electronic structure, and provide accurate transition frequencies needed for their identification in space. Conventional absorption spectroscopy has in the past been successfully applied for spectroscopic studies of molecular ions, but is often hampered by low number densities and spectral congestion due to the multitude of species produced at high excitation energies during their formation process. These limitations can be overcome by performing experiments on mass-selected ions in cryogenic ion trap instruments. Here I will present laboratory data on the gas phase spectra of several hydrocarbon and nitrile cations ranging in size from comparatively small systems (e.g., $C_3H_2^+$, CH_2CN^+) to PAH cations, made possible by recent developments of sensitive methods for action spectroscopy in cryogenic ion traps. A focus will be on broadband infrared experiments and methods to disentangle the isomeric composition of ionic samples, using the unique combination of a cryogenic ion trap instrument interfaced to the free electron lasers at the FELIX Laboratory.

Laboratory Investigation of Atomic Oxygen (O) Gas-Phase Chemistry with Organic Molecules in the ISM: Destruction Routes and O Addition.

Demian Marchione¹, P. Recio, A. Caracciolo, N. Balucani, and P. Casavecchia

¹Università degli Studi di Perugia, IT

Oxygen is the third most abundant element in the universe, and although in the interstellar medium most of it is depleted as H₂O, CO and CO₂, a significant fraction of residual atomic oxygen might play an important role in the formation and destruction of interstellar complex organic molecules (COMs). It is assumed that grain surface chemistry is solely responsible for the formation of COMs. However, this established view was challenged by recent laboratory results on the negligible photodesorption of intact methanol [1] and by the detection of methyl formate and dimethyl ether in cold objects, reevaluating the role of gas-phase chemistry in the synthesis of COMs [2]. For instance, a recent theoretical study proposed a new scheme of reactions for the formation of glycolaldehyde, acetic acid, and formic acid following the H abstraction of ethanol and subsequent oxidation of the possible products [3]. The conclusions of this work strengthened the idea that reactions of neutrals in the gas-phase chemistry can indeed be important and should not be overlooked to explain astronomical observations.

Within this context, we performed crossed molecular beams (CMB) reactive scattering experiments coupled with time-of-flight (TOF) mass spectrometry detection to investigate the reactivity of O atoms with organic molecules in single-collision conditions. A brief overview of the relevant published works is outlined and new data on the reactivity of an important COM, pyridine (C₅H₅N), with O radicals are presented. Preliminary analysis of the laboratory data reveals that the reaction C₅H₅N + O(³P) leads 1) to the addition of the O atom to the aromatic ring via H abstraction (C₅H₄NO + H), and 2) to ring contraction via CO elimination (C₄H₅N + CO). Implications in O-rich space environments are briefly discussed.

References:

- [1] Bertin, M.; Romanzin, C.; Doronin, M.; Philippe, L.; Jeseck, P.; Ligterink, N.; Lin-nartz, H.; Michaut, X.; Fillion, J.-H. UV photodesorption of methanol in pure and CO-rich ices: desorption rates of the intact molecule and of the photofragments. *Astrophys. J.* 2016, 817, L12.
- [2] Balucani, N.; Ceccarelli, C. and Taquet, V. Formation of complex organic molecules in cold objects: the role of gas-phase reactions *Mon. Not. R. Astron. Soc.* 2015, 449, L16.
- [3] Skouteris, S.; Balucani, N.; Ceccarelli, C.; Vazart, F.; Puzzarini, C.; Barone, V.; Codella, C. and Lefloch, B. The Genealogical Tree of Ethanol: Gas-phase Formation of Glycolaldehyde, Acetic Acid, and Formic Acid *Astrophys. J.* 2018, 854, 135.

A Systematic, Experimental Investigation into CO₂:NH₃ Interstellar Ice Analogues

Rachel James¹, Anita Dawes¹, Sergio Ioppolo², Nigel J. Mason³

¹Open University, UK

²Queen Mary University of London, UK

³University of Kent, UK

Despite the variety of molecules discovered in the interstellar medium, the exact formation mechanism for most of these molecules remains unknown. However, most of the larger molecules are presumed to form through solid-phase reactions in the ice which surrounds the interstellar dust grains. Laboratory investigations have shown that it is relatively easy to induce molecular synthesis within interstellar ice analogue mixtures via processing of the ice. Yet, there is still a general lack of understanding on how the molecules within the mixtures interact with each other and whether this has any significant bearing on the molecules being formed. In order to understand this interaction, we need to go back and perform systematic experiments on simple binary ice mixtures before building up to the larger, more realistic compositions. In this contribution, I will present the results of a systematic study on the binary ice mixture of CO₂ and NH₃. Using mid-IR spectroscopy, the effect of the initial mixing ratio of CO₂ and NH₃ ice mixtures was investigated at 20 K, as a result of thermal processing and as a result of electron irradiation. These results will show that not only does the initial mixing ratio appear to have an effect on the products being formed, but it also appears to affect the structure of the ice. Recent investigations suggests that the ice structure plays just as important part in reactivity of the ice. Therefore more systematic, experimental studies may help better inform us of the formation mechanisms of molecules in space.

Infrared Resonant Vibrational Restructuring of Amorphous Solid Water

Jennifer A. Noble¹, Herma Cuppen², Stephane Coussan¹, Britta Redlich³, Sergio Ioppolo⁴

¹Aix-Marseille University, FR

²IMM, Radboud University Nijmegen, NL

³FELIX Laboratory, Radboud University Nijmegen, NL

⁴Queen Mary University of London, UK

Water ices form in dense, cold molecular clouds in the form of amorphous solid water, before undergoing various types of processing (thermal, shocks, irradiation, bombardment) which may alter their original structure. Crystalline ices have been observed in protoplanetary disks, on satellites and planets, as well as here on Earth. All of these environments represent later stages in the star and planet formation process, and are subject to irradiation processes. How is the energy injected into the vibrational modes of ices dissipated, and what structural modification results?

Here, we present the first results from a joint experimental and theoretical study of the selective mid-IR and THz irradiation of amorphous and crystalline ices. Experiments were carried out in a UHV surface science experiment at the FELIX laser facility and interpreted by comparison with molecular dynamics simulations. We will describe the new UHV setup at FELIX available to the astrochemistry community.

Terahertz High Spectral Resolution Astrophysics - A Technical Overview

Brian Ellison (Invited Speaker)

Rutherford Appleton Laboratory, UK

The presentation will first provide a brief introduction to the requirement for performing astronomical spectral observations in the terahertz (THz) spectral range. This will be followed by a short overview of related instrumentation and processes of selection. Substantial emphasis will then be placed on high-resolution spectroscopy as performed via frequency down-conversion, i.e. heterodyne frequency translation. Within this portion of the presentation, the basic operation of a heterodyne system will be explained and a summary of the related technical evolution of the technique to the present day expounded. Finally, future heterodyne system developments will be suggested and their related potential impact on astronomical observations discussed.

Terahertz Desorption Emission Spectroscopy

Olivier Auriacombe¹, H. Fraser², B. Ellison¹, S. Ioppolo^{2,3}, S. Rea¹

¹Rutherford Appleton Laboratory, UK

²Open University, UK

³Queen Mary University of London, UK

Enhancing our understanding of the formation and evolution of the Universe is strongly dependent upon the observation of matter that forms the interstellar medium (ISM), using Radio-telescopes based on heterodyne detection (such as ALMA). Whilst molecules, such as H₂O and CH₃OH, can only form in the solid state, the formation of complex organic molecules (COMs) is not fully known. Are they forming in the solid phase and then desorbing to the gas phase? Are they formed in the gas-phase from chemical reactions of ions and smaller molecules which desorb from ice grains? How is the rotational state occupancy of these molecules affected by desorption processes?

A new experimental technique has been developed to tackle these questions, namely Terahertz Desorption Emission Spectroscopy (THz-DES). The basis of THz-DES is to recreate the chemical conditions found in interstellar environments by emulating the astronomical detection techniques. The emission spectroscopy is based on the integration of a total-power Schottky-barrier based radiometer operating between 320-350 GHz (overlapping with ALMA band 7), with a vacuum chamber where interstellar ice analogues can be grown in situ on a 77 K cold-finger. The ice is then thermally desorbed, enabling the identification of molecular spectra and desorption energies.

Thermal desorption was observed in pure, layered or mixed ices of nitrous oxide, water and methanol molecules. The THz-DES results were compared to existing values in the literature in the subject area of desorption energies, and known spectral features. The preliminary findings suggest that certain energy levels of desorbing species (A and E populations of methanol) were under-populated compared the population expected in local thermodynamic equilibrium conditions. This impact of surface constraints on the dynamics and internal energy of desorbing molecules, largely ignored in astronomy, shows interesting promise for the future of the THz-DES techniques and the understanding of the formation of COMs.

Nanoscale Structure of Amorphous Solid Water: What Determines the Porosity in ASW?

Sabrina Gärtner^{1,2}, Thomas F. Headen², Tristan G. A. Youngs², Catherine R. Hill¹, Natalia Pascual¹, Olivier Auriacombe^{1,3}, Sergio Ioppolo^{1,4}, Thomas Loerting⁵, Daniel T. Bowron² and Helen J. Fraser¹

¹Open University, UK

²ISIS Facility, STFC Rutherford Appleton Laboratory, UK

³RAL Space, STFC Rutherford Appleton Laboratory, UK

⁴Queen Mary University of London, UK

⁵University of Innsbruck, AT

Vapour deposited amorphous solid water (ASW) is supposed to be the most common solid material in space. Low-temperature depositions are porous, suggesting that in space it may incorporate trace gases, influencing grain chemistry, Burke & Brown (2010), and grain collisions Wang et al. (2005). However, the underlying structure of ASW is poorly understood. Laboratory experiments on interstellar ice analogues often yield seemingly contradictory results, as the porosity and ice phase are highly sensitive to the growth conditions employed. Moreover, the structures crystallise and lose porosity with temperature and potentially with time. This annealing process again depends on the ice's environmental conditions and thermal history. Building on earlier work by Hill et al. (2016), herein we attempt to quantify some structural aspects of ASW. We have grown vapour-deposited D₂O ices in a systematic and reproducible manner, and employed neutron scattering as a non-destructive probe of their structure from 18 to 180 K over intramolecular to nanometric length scales using the NIMROD instrument at STFC Rutherford Appleton Laboratory (beamtime allocations RB1610318 & RB1510246). An Arrhenius-type model is able to describe both the loss of surface area and the porosity over the temperature range studied. The activation energy for this process is (428 ± 104) K, which is in the range expected for van der Waals forces acting between ice structures of several nanometers in size, and over a distance of a few nanometers. Structural changes evidence enhanced mobility from 100 to 150 K and while derived structural descriptors such as the widths of pores and ice widths change by an order of magnitude, their effects on the kinetic parameters appear to cancel out. Both surface area and porosity may be described utilising a common set of kinetic parameters, but differing high-temperature equilibria. Despite the same mechanism driving both changes, this then indicates that surface area is not a measure for porosity.

Our findings imply that models for ASW must include macroscopic effects and long-range forces in order to reliably predict these structures in astrophysical environments. Furthermore, since changes in structure are well-described by an activation energy, these ices will always change over time, even at low temperatures, which demands critical reassessment of our picture of ice astrophysics.

References:

[1] Burke, D. J. & Brown W. A. 2010, PCCP, 12.23, 5947

[2] Hill, C.R., Mitterdorfer, C., Youngs, T.G.A., Bowron, D.T., Fraser, H.J. & Loerting, T. 2016, PRL, 116, 215501

[3] Wang H., Bell R. C., Iedema M. J., Martin J., Tsekouras, A.A. & Cowin, J.P. 2005, ApJ, 620, 1027

Production and Analysis of Cosmic Dust Analogues by Stardust Machine

Mario Accolla¹, Lidia Martínez¹, Pablo Merino¹, Gonzalo Santoro¹, Jesús M. Sobrado², José Cernicharo³, Christine Joblin⁴ and José A. Martín-Gago¹

¹Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), ES

²Centro de Astrobiología (CAB, INTA-CSIC), ES

³Instituto de Física Fundamental (IFF-CSIC), ES

⁴IRAP, Université de Toulouse, FR

Stardust machine is a new experimental setup designed to mimic in the laboratory both the complex conditions of cosmic dust formation and the processing in the environment of evolved stars. It comprises six interconnected ultra-high-vacuum (UHV) modules, offering a high level of control over fabrication, processing and analysis of cosmic dust analogues. In Stardust machine, the chemistry proceeds via atom aggregation under conditions in which most of the reactions that occur are neutral-neutral, closely resembling what happens in the circumstellar envelopes of Asymptotic Giant Branch (AGB) stars.

The first experiments with astrophysical interest performed by this setup consisted in the fabrication of carbon nanoparticles in the gas phase, starting from carbon atoms and molecular hydrogen. The dust grains so produced have been characterized by both in situ and ex situ analysis.

My talk will be focused on the description and on the potentialities of the experimental setup. Then, I will explain both the experimental procedure to produce carbon dust grains by Stardust machine and the characterization of these cosmic dust analogues.

Programme 24 June 2019

Time	Speaker	Affiliation	Title
10:00	COFFEE		
10:25	Introduction/Welcome		
	Chair: Izaskun Jimenez-Serra		
10:30-11:30	Cecilia Ceccarelli (I)	Grenoble Observatory	Astronomical Observations as Tools to Constrain the Chemical Routes of Interstellar Complex Organic Molecules
11:30-11:50	Shaoshan Zeng	Queen Mary University of London	First Detection of the Pre-biotic Molecule Glycolonitrile (HOCH ₂ CN) in the Interstellar Medium
11:50-12-10	Katharine G. Johnston	University of Leeds	A Detailed Chemical View of the Circumstellar Environment and Disk of the Forming O-Star AFGL4176
12:10-12:30	Helen J. Fraser	Open University	Gas-Ice-Dust Mapping in the JWST Era
12:30	LUNCH & POSTER SESSION		
	Chair: Anthony J.H.M. Meijer		
13:30-14:00	Alessandra Candian	Leiden Observatory	Bad Vibrations: the Anharmonic Infrared Spectrum of PAHs at the Beginning of the JWST Era
14:00-15:00	Catherine Walsh (I)	University of Leeds	Complex Organic Molecules Tracing the Comet-Forming Regions in Protoplanetary Disks
15:00	COFFEE		
	Chair: Wendy A. Brown		
15:30-16:00	Matteo Brogi	University of Warwick	Measuring the Chemical Inventory of Exoplanet Atmospheres with High-Resolution Spectroscopy
16:00-16:20	Tomas James	University College London	Chemical Diagnostics of J-type Shocks: An Application to L1157
16:20-16:40	Tomas James	University College London	Can a Varying Dust-to-Gas Ratio Have an Effect on Chemistry? An Application to the Wardle Instability
16:40-17:00	James W. Stubbing	University of Sussex	Determination of Refractive Indices of Astrochemical Ices Using Ultraviolet/Visible Reflection Absorption Spectroscopy
17:00-18:00	AMG & POSTER SESSION		

(I) = Invited Speaker

Programme 25 June 2019

Time	Speaker	Affiliation	Title
10:00	COFFEE		
10:25	Introduction/Welcome		
	Chair: Martin R.S. McCoustra		
10:30-11:30	Sandra Brünken (I)	FELIX Laboratory	Unravelling the Isomers of Reactive Ionic Intermediates Using FELIX
11:30-12:00	Demian Marchione	Perugia University	Laboratory Investigation of Atomic Oxygen (O) Gas-Phase Chemistry with Organic Molecules in the ISM: Destruction Routes and O Addition
12:00-12:30	Rachel James	Open University	A Systematic, Experimental Investigation into CO ₂ :NH ₃ Interstellar Ice Analogues
12:30	LUNCH & POSTER SESSION		
	Chair: Nigel J. Mason		
13:30-14:00	Jennifer A. Noble	Aix-Marseille University	Infrared Resonant Vibrational Restructuring of Amorphous Solid Water
14:00-15:00	Brian Ellison (I)	RAL Space	Terahertz High Spectral Resolution Astrophysics - A Technical Overview
15:00	COFFEE		
	Chair: Sergio Ioppolo		
15:30-16:00	Olivier Auriacombe	RAL Space	Terahertz Desorption Emission Spectroscopy
16:00-16:30	Sabrina Gärtner	ISIS Facility	Nanoscale Structure of Amorphous Solid Water: What Determines the Porosity in ASW?
16:30-17:00	Mario Accolla	ICMM-CSIC	Production and Analysis of Cosmic Dust Analogues by Stardust Machine
17:00	END OF MEETING		

(I) = Invited Speaker