AstroChemical Newsletter #97

December 2023

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

Synthesis of urea on the surface of interstellar water ice clusters. A quantum chemical study

J. Perrero and A. Rimola

Urea is a prebiotic molecule that has been detected in few sources of the interstellar medium (ISM) and in Murchison meteorite. Being stable against ultraviolet radiation and high-energy electron bombardment, urea is expected to be present in interstellar ices. Theoretical and experimental studies suggest that isocyanic acid (HNCO) and formamide (NH2CHO) are possible precursors of urea. However, uncertainties still exist regarding its formation routes. Previous computational works characterised urea formation in the gas phase or in presence of few water molecules by reaction of formamide with nitrogen-bearing species. In this work, we investigated the reaction of HNCO + NH3 on an 18 water molecules ice cluster model mimicking interstellar ice mantles by means of quantum chemical computations. We characterised different mechanisms involving both closed-shell and open-shell species at B3LYP-D3(BJ)/ma-def2-TZVP level of theory, in which the radical-radical H2NCO + NH2 coupling has been found to be the most favourable one due to being almost barrierless. In this path, the presence of the icy surfaces is crucial for acting as reactant concentrators/suppliers, as well as third bodies able to dissipate the energy liberated during the urea formation.

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Full-text URL: https://www.sciencedirect.com/science/article/pii/S001910352300427X

SUNRISE: The rich molecular inventory of high-redshift dusty galaxies revealed by broadband spectral line surveys

Chentao Yang (□□□), Alain Omont, Sergio Martín, Thomas G. Bisbas, Pierre Cox, Alexandre Beelen, Eduardo González-Alfonso, Raphaël Gavazzi, Susanne Aalto, Paola Andreani, Cecilia Ceccarelli, Yu Gao (□□), Mark Gorski, Michel Guélin, Hai Fu (□□), R. J. Ivison, Kirsten K. Knudsen, Matthew Lehnert, Hugo Messias, Sebastien Muller, Roberto Neri, Dominik Riechers, Paul van der Werf, and Zhi-Yu Zhang (□□□).

Understanding the nature of high-redshift dusty galaxies requires a comprehensive view of their interstellar medium (ISM) and molecular complexity. However, the molecular ISM at high redshifts is commonly studied using only a few species beyond 12C16O, limiting our understanding. In this paper, we present the results of deep 3 mm spectral line surveys using the NOrthern Extended Millimeter Array (NOEMA) targeting two strongly lensed dusty galaxies observed when the Universe was less than 1.8Gyr old: APM08279+5255, a quasar at redshift z=3.911, and NCv1.143 (H-ATLAS J125632.7+233625), a z = 3.565 starburst galaxy. The spectral line surveys cover rest-frame frequencies from about 330 to 550 GHz for both galaxies. We report the detection of 38 and 25 emission lines in APM 08279+5255 and NCv1.143, respectively. These lines originate from 17 species, namely CO, 13CO, C18O, CN, CCH, HCN, HCO+, HNC, CS, C34S, H2O, H3O+, NO, N2H+, CH, c-C3H2, and the vibrationally excited HCN and neutral carbon. The spectra reveal the chemical richness and the complexity of the physical properties of the ISM. By comparing the spectra of the two sources and combining the analysis of the molecular gas excitation, we find that the physical properties and the chemical imprints of the ISM are different: the molecular gas is more excited in APM 08279+5255, which exhibits higher molecular gas temperatures and densities compared to NCv1.143; the molecular abundances in APM 08279+5255 are akin to the values of local active galactic nuclei (AGN), showing boosted relative abundances of the dense gas tracers that might be related to high-temperature chemistry and/or the X-ray-dominated regions, while NCv1.143 more closely resembles local starburst galaxies. The most significant differences between the two sources are found in H2O: the 448 GHz ortho-H2O(423 –330) line is significantly brighter in APM 08279+5255, which is likely linked to the intense far-infrared radiation from the dust powered by AGN. Our astrochemical model suggests that, at such high column densities, far-ultraviolet radiation is less important in regulating the ISM, while cosmic rays (and/or X-rays and shocks) are the key players in shaping the molecular abundances and the initial conditions of star formation. Both our observed CO isotopologs line ratios and the derived extreme ISM conditions (high gas temperatures, densities, and cosmic-ray ionization rates) suggest the presence of a top-heavy stellar initial mass function. From the∼330–550GHz continuum, we also find evidence of nonthermal millimeter flux excess in APM 08279+5255 that might be related to the central supermassive black hole. Such deep spectral line surveys open a new window into the physics and chemistry of the ISM and the radiation field of galaxies in the early Universe.

A&A in press
DOI: 10.1051/0004-6361/202347610
Full-text URL: https://arxiv.org/abs/2308.07368

A systematic mid-infrared spectroscopic study of thermally processed SO2 ices

DV Mifsud, P Herczku, KK Rahul, R Ramachandran, P Sundararajan, STS Kovács, B Sulik, Z Juhász, R Rácz, S Biri, Z Kanuchová, RW McCullough, B Sivaraman, S Ioppolo and NJ Mason

The use of mid-infrared spectroscopy to characterise the chemistry of icy interstellar and Solar System environments will be exploited in the near future to better understand the chemical processes and molecular inventories in various astronomical environments. This is, in part, due to observational work made possible by the recently launched James Webb Space Telescope as well as forthcoming missions to the outer Solar System that will observe in the mid-infrared spectroscopic region (e.g., the Jupiter Icy Moons Explorer and the Europa Clipper missions). However, such spectroscopic characterisations are crucially reliant upon the generation of laboratory data for comparative purposes. In this paper, we present an extensive mid-infrared characterisation of SO2 ice condensed at several cryogenic temperatures between 20 and 100 K and thermally annealed to sublimation in an ultrahigh-vacuum system. Our results are anticipated to be useful in confirming the detection (and possibly thermal history) of SO2 on various Solar System bodies, such as Ceres and the icy Galilean moons of Jupiter, as well as in interstellar icy grain mantles.

2023, Physical Chemistry Chemical Physics, 25, 26278-26288
DOI: 10.1039/d3cp03196a
Full-text URL: https://pubs.rsc.org/en/content/articlehtml/2023/cp/d3cp03196a

The evolution of sulphur-bearing molecules in high-mass star-forming cores

Fontani, F. ; Roueff, E. ; Colzi, L. ; Caselli, P.

To understand the chemistry of sulphur (S) in the interstellar medium, models need to be tested by observations of S-bearing molecules in different physical conditions. We analyse observations obtained with the IRAM 30m telescope towards 15 well-known cores classified in the three main evolutionary stages of the high-mass star-formation process: high-mass starless cores,high-mass protostellar objects, and ultracompact HII regions. We detected rotational lines of SO, SO+, NS, C34S, 13CS, SO2, CCS, H2S, HCS+, OCS, H2CS, and CCCS. From a local thermodynamic equilibrium approach, we have derived column densities of each species and excitation temperatures. Based on a statistical analysis on the line widths and the excitation temperatures, we find that: NS, C34S, 13CS, CCS, and HCS+ trace cold, quiescent, and likely extended material; OCS, and SO2 trace warmer, more turbulent, and likely denser and more compact material; SO and perhaps SO+ trace both quiescent and turbulent material depending on the target. The abundances of SO, SO2, and H2S show the strongest positive correlations with the kinetic temperature, believed to be an evolutionary indicator. Moreover, the sum of all molecular abundances show an enhancement of gaseous S from the less evolved to the more evolved stages. These trends could be due to the increasing amount of S sputtered from dust grains owing to the increasing protostellar activity with evolution. The average abundances in each evolutionary group increase especially in the oxygen-bearing molecules, perhaps due to the increasing abundance of atomic oxygen with evolution owing to photodissociation of water in gas phase. Our observational work represents a test-bed for theoretical studies aimed at modelling the chemistry of sulphur during the evolution of high-mass star-forming cores

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Full-text URL: https://arxiv.org/abs/2310.10356

ALMA Reveals Hidden Morphologies in the Molecular Envelope of VY Canis Majoris

A. P. Singh , A. M. S. Richards , R. M. Humphreys , L. Decin, and L. M. Ziurys

The J = 2 → 1 transition of CO near 230 GHz and the J = 3 → 2 line of HCN at 265 GHz have been imaged in the envelope of the red hypergiant star, VY Canis Majoris (VY CMa), using the Atacama Large Millimeter Array (ALMA) with angular resolutions 0farcs2–1farcs5; single-dish data were added to provide sensitivity up to 30". These images reveal a far more complex envelope, with previously unseen outflows extending 4"–9" from the star. These new structures include an arc-like outflow with an angular separation of ∼9" northeast from the stellar position ("NE Arc"), twin fingerlike features approximately 4" to the north/northeast ("NE Extension"), and a roughly spherical region observed ∼7" E of the star ("E Bubble"). The NE Arc appears to be decelerating from base (VLSR ∼ 7 km s−1) to tip (VLSR ∼ 18 km s−1), while the NE Extension is blueshifted with VLSR ∼ −7 km s−1. Among the new features, HCN is only detected in the NE Arc. In addition, known structures Arc 1, Arc 2, and NW Arc, as well as other features closer to the star, are closely replicated in CO, suggesting that the gas and dust are well mixed. The CO spectra are consistent with the kinematic picture of VY CMa derived from HST data. Arc 2, however, has added complexity. Preliminary results from CO suggest 12C/13C ∼ 22–38 across the envelope. The additional presence of at least three major episodic mass ejection events significantly broadens the current perspective of the envelope structure and mass-loss history of VY CMa.

2023 September 1, Astrophysical Journal Letters, 954:L1 (7pp)
DOI: 10.3847/2041-8213/ace7cb
Full-text URL: https://iopscience.iop.org/article/10.3847/2041-8213/ace7cb/meta

High throughput anharmonic vibrational and rotational spectral computations

B. R. Westbrook, R. C. Fortenberry

Theoretical spectroscopy is a powerful tool in the chemist’s toolbox, providing insight into experimental investigations here on Earth and into the observations of telescopes like the recently-operational JWST. This work presents recent developments in our group focused on extending the application of highly-accurate, theoretical spectroscopic techniques to large molecules. By leveraging composite and hybrid methods based on coupled cluster theory, molecules of study can increase in size from three to five atoms to upwards of ten atoms. In turn, using such results as a training set lays the foundation for methods capable of treating dozens, or potentially hundreds, of atoms in the future.

2023, Ann. Rep. Comput. Chem., in press
DOI: 10.1016/bs.arcc.2023.10.005
Full-text URL: https://www.sciencedirect.com/science/article/abs/pii/S1574140023000105

Taming semi-empirical methods for PAHs and vibrational spectra

B. R. Westbrook, R. C. Fortenberry

Semi-empirical methods offer a cost-effective means of computing explicit, anharmonic vibrational frequencies for large molecules, such as polycyclic aromatic hydrocarbons (PAHs), but their default parameters produce insufficiently accurate results for comparison to experiment, especially in the hydride stretching region where the NIRSpec instrument on JWST is most effective. This work delivers several reparameterized variants of the PM6 semi-empirical method trained to reproduce the experimental vibrational frequencies of 5 small hydrocarbon molecules. When benchmarked on the experimental frequencies of benzene and naphthalene, these reparameterized methods match the empirical values to within 38.7 cm-1 on average. Combining these values with the default PM6 frequencies below 3000 cm-1 brings the average deviation below 22 cm-1 for naphthalene, comparing favorably with the existing state of the art in B3LYP/4-31G, for a two order of magnitude decrease in the computational cost. As such, the present work offers a promising means of extending the computation of explicit, anharmonic vibrational frequencies to PAHs larger than those that can be examined anharmonically via B3LYP. Such large and accurate data sets are necessary to disentangle the unidentified spectral features observed around myriad astronomical bodies and the influx of observational data from JWST.

2023, J. Molec. Spectrosc., 398, 111846
DOI: 10.1016/j.jms.2023.111846
Full-text URL: https://www.sciencedirect.com/science/article/abs/pii/S002228522300111X

Photoelectron spectroscopic study of 2-naphthylnitrene and its thermal rearrangement to cyanoindenes

Mayank Saraswat, Adrian Portela-Gonzalez, Enrique Mendez-Vega, Ginny Karir, Wolfram Sander and Patrick Hemberger

2-Cyanoindene has recently been identified in the interstellar medium, however current models cannot fully account for its formation pathways. Herein, we identify and characterize 2-naphthylnitrene, which is prone to rearrange to 2- and 3-cyanoindene, in the gas phase using photoion mass-selective threshold photoelectron spectroscopy (ms-TPES). The adiabatic ionization energies (AIE) of triplet nitrene (3A″) to the radical cation in its lowest-energy doublet X̃+(2A′) and quartet ã+(4A′) electronic states were determined to be 7.72 ± 0.02 and 8.64 ± 0.02 eV, respectively, leading to a doublet–quartet energy splitting (ΔED–Q) of 0.92 eV (88.8 kJ mol−1). A ring-contraction mechanism yields 3-cyanoindene, which is selectively formed under mild pyrolysis conditions (800 K), while the lowest-energy isomer, 2-cyanoindene, is also observed under harsh pyrolysis conditions at 1100 K. The isomer-selective assignment was rationalized by Franck–Condon spectral modeling and by measuring the AIEs at 8.64 ± 0.02 and 8.70 ± 0.02 eV for 2- and 3-cyanoindene, respectively, in good agreement with quantum chemical calculations.

Phys. Chem. Chem. Phys., 2023, 25, 31146
DOI: 10.1039/D3CP04064J
Full-text URL: https://pubs.rsc.org/en/content/articlepdf/2023/cp/d3cp04064j

Collisional excitation of PO+ by para-H2: potential energy surface, scattering calculations, and astrophysical applications

F. Tonolo, L. Bizzocchi, V. M. Rivilla, F. Lique, M. Melosso and C. Puzzarini

We report the derivation of rate coefficients for the rotational (de-)excitation of PO+ induced by collisions with H2. The calculations were performed on a 4D potential energy surface, obtained on top of highly accurate ab initio energy points. Preliminary tests pointed out the low influence of the coupling between j = 0 and the higher rotational levels of H2 on the cross- sections values, thus allowing to neglect the rotational structure of H2. On this basis, state-to-state collisional rate coefficients were derived for temperatures ranging from 5 to 200 K. Radiative transfer calculations have been used to model the recent observation of PO+ in the G+0.693–0.027 molecular cloud, in order to evaluate the possible impact of non-LTE models on the determination of its physical conditions. The derived column density was found to be approximately ∼ 3.7e11 cm−2 , which is 60% (a factor of ∼ 1.7) smaller than the previously LTE-derived value. Extensive simulations show that PO+ low-j rotational lines exhibit maser behaviour at densities between 1e4 and 1e6 cm−3, thus highlighting the importance of a proper treatment of the molecular collisions to accurately model PO+ emissions in the interstellar medium.

MNRAS 527, 2279–2287 (2024)
DOI: 10.1093/mnras/stad3140
Full-text URL: https://arxiv.org/abs/2310.08052

Rotational spectroscopic characterisation of the [D2,C,S] system: an update from the laboratory and theory

N. Inostroza-Pino, V. Lattanzi, C. Z. Palmer, R. C. Fortenberry, D. Mardones, P. Caselli, O. E. Godwin, T. J. Lee

The synergy between high-resolution rotational spectroscopy and quantum-chemical calculations is essential for exploring future detection of molecules, especially when spectroscopy parameters are not available yet. By using highly correlated ab initio quartic force fields (QFFs) from explicitly correlated coupled cluster theory, a complete set of rotational constants and centrifugal distortion constants for D2CS and cis/trans-DCSD isomers have been produced. Comparing our new ab initio results for D2CS with new rotational spectroscopy laboratory data for the same species, the accuracy of the computed B and C rotational constants is within 0.1% while the A constant is only slightly higher. Additionally, quantum chemical vibrational frequencies are also provided, and these spectral reference data and new experimental rotational lines will provide additional references for potential observation of these deuterated sulfur species with either ground-based radio telescopes or space- based infrared observatories.

Molecular Physics e2280762 (2023)
DOI: 10.1080/00268976.2023.2280762
Full-text URL: https://arxiv.org/abs/2311.09063

Infrared Spectral Signatures of Nucleobases in Interstellar Ices I: Purines

CA Rosa, A Bergantini, P Herczku, DV Mifsud, G Lakatos, STS Kovács, B Sulik, Z Juhász, S Ioppolo, HM Quitián-Lara, NJ Mason, and C Lage

The purine nucleobases adenine and guanine are complex organic molecules that are essential for life. Despite their ubiquitous presence on Earth, purines have yet to be detected in observations of astronomical environments. This work therefore proposes to study the infrared spectra of purines linked to terrestrial biochemical processes under conditions analogous to those found in the interstellar medium. The infrared spectra of adenine and guanine, both in neat form and embedded within an ice made of H2O:NH3:CH4:CO:CH3OH (10:1:1:1:1), were analysed with the aim of determining which bands attributable to adenine and/or guanine can be observed in the infrared spectrum of an astrophysical ice analogue rich in other volatile species known to be abundant in dense molecular clouds. The spectrum of adenine and guanine mixed together was also analysed. This study has identified three purine nucleobase infrared absorption bands that do not overlap with bands attributable to the volatiles that are ubiquitous in the dense interstellar medium. Therefore, these three bands, which are located at 1255, 940, and 878 cm−1, are proposed as an infrared spectral signature for adenine, guanine, or a mixture of these molecules in astrophysical ices. All three bands have integrated molar absorptivity values (ψ) greater than 4 km mol−1, meaning that they should be readily observable in astronomical targets. Therefore, if these three bands were to be observed together in the same target, then it is possible to propose the presence of a purine molecule (i.e., adenine or guanine) there.

2023, Life, 13, 2208.
DOI: 10.3390/life13112208
Full-text URL: https://www.mdpi.com/2075-1729/13/11/2208

The UMIST Database for Astrochemistry 2022

T J Millar, C Walsh, M Van de Sande and A J Markwick

Detailed astrochemical models are a key component to interpret the observations of interstellar and circumstellar molecules since they allow important physical properties of the gas and its evolutionary history to be deduced. We update one of the most widely used astrochemical databases to reflect advances in experimental and theoretical estimates of rate coefficients and to respond to the large increase in the number of molecules detected in space since our last release in 2013. We present the sixth release of the UMIST Database for Astrochemistry (UDfA), a major expansion of the gas-phase chemistry that describes the synthesis of interstellar and circumstellar molecules. Since our last release, we have undertaken a major review of the literature which has increased the number of reactions by over 40% to a total of 8767 and increased the number of species by over 55% to 737. We have made a particular attempt to include many of the new species detected in space over the past decade, including those from the QUIJOTE and GOTHAM surveys, as well as providing references to the original data sources. We use the database to investigate the gas-phase chemistries appropriate to both O-rich and C-rich conditions in TMC-1 and to the circumstellar envelope of the C-rich AGB star IRC+10216 and identify successes and failures of gas-phase only models. This update is a significant improvement to the UDfA database. For both the dark cloud and C-rich circumstellar envelope models, calculations match around 60% of the abundances of observed species to within an order of magnitude. There are a number of detected species, however, that are not included in the model either because their gas-phase chemistry is unknown or because they are likely formed via surface reactions on icy grains. Future laboratory and theoretical work is needed to include such species in reaction networks.

Astronomy & Astrophysics, in press
DOI: 10.1051/0004-6361/202346908
Full-text URL: https://arxiv.org/abs/2311.03936

A Comparative Study of the Cold Collisions of H2O and D2O with Ne

R. M. García-Vázquez, O. Denis-Alpizar, and T. Stoecklin

The present work is dedicated to the first theoretical study of the rotationally inelastic collisions of Ne with H_2O and its isotopologue D_2O in an attempt to analyze the effect on the dynamics of H substitution by deuterium. To this aim two new potential energy surfaces are developed. Their quality is tested by computing the bound states of the complexes and comparing them with those most recently reported by other teams. System-specific collisional propensity rules are inferred for these two systems by analyzing the computed state-to-state cross sections at low and higher collision energy. The application of the Alexander parity index propensity rule is also discussed, and the present results are compared with those obtained for the collisions with other noble gases.

J. Phys. Chem. A 127: 4838−4847 (2023)
DOI: 10.1021/acs.jpca.3c02086
Full-text URL: https://pubs.acs.org/doi/full/10.1021/acs.jpca.3c02086

Quantum study of the radiative association of Cl^- + H_2 and Cl^- + D_2

M. Lara-Moreno and Thierry Stoecklin

We compute the radiative association (RA) of Cl^- with H_2 and D_2. We use potential energy and dipole moment surfaces recently tested by a combined theoretical and experimental study of the pre- dissociation spectrum of these complexes. The RA rates are calculated using a quantum approach based on the driven equations formalism and compared with those obtained for similar systems. An indirect comparison with experiment is also discussed using the three body rates measured recently for this system.

Eur. Phys. J. Spec. Top. (2023) 232:1961–1966
DOI: 10.1140/epjs/s11734-023-00944-z
Full-text URL: https://epjst.epj.org/articles/epjst/abs/2023/12/11734_2023_Article_944/11734_2023_Article_944.html

Bending relaxation of H_2O by collision with para- and ortho-H_2

Ricardo-Manuel Garcia-vasquez, Alexandre Faure, Thierry stoecklin

We extend our recent theoretical work on the bending relaxation of H_2O in collisions with H_2 by including the three water modes of vibration coupled with rotation, as well as the rotation of H_2. Our full quantum close-coupling method is combined with a high-accuracy nine-dimensional potential energy surface. The collisions of para-H_2O and ortho-H_2O with the two spin modifications of H_2 are considered and compared for several initial states of H_2O. The convergence of the results as a function of the size of the rotational basis set of the two colliders is discussed. In particular, near-resonant energy transfer between H_2O and H_2 is found to control the vibrational relaxation process, with a dominant contribution of transitions with $\Delta j_2=+2, +4$ in H_2. Finally, the calculated value of the H_2O bending relaxation rate coefficient at 295K is found to be in excellent agreement with its experimental estimate.

Phys. Chem. Phys (2023) published on line
DOI: 10.1002/cphc.202300698
Full-text URL: https://chemistry-europe.onlinelibrary.wiley.com/doi/epdf/10.1002/cphc.202300698

Radiative electron attachment to rotating C_3N through dipole-bound states

Joshua Forer , Viatcheslav Kokoouline , and Thierry Stoecklin

The role of a large dipole moment in rotating neutral molecules interacting with low-energy electrons is studied using an accurate ab initio approach accounting for electronic and rotational degrees of freedom. It is found that theory can reproduce weakly bound (dipole-bound) states observed in a recent photodetachment experiment with C_3N^- [Phys. Rev. Lett. 127, 043001 (2021)]. Using a similar level of theory, the cross section for radiative electron attachment to the C_3N molecule, forming the dipole-bound states, was determined. The obtained cross section is too small to explain the formation of C_3N^- in the interstellar medium, suggesting that it is likely formed by a different process.

Physical Review A 107, 043117 (2023)
DOI: 10.1103/PhysRevA.107.043117
Full-text URL: https://journals.aps.org/pra/abstract/10.1103/PhysRevA.107.043117

An explicitly correlated six-dimensional potential energy surface for the SiCSi + H_2 complex

Lisán David Cabrera-González, Dayán Páez-Hernández, Thierry Stoecklin and Otoniel Denis-Alpizar

The first six-dimensional potential energy surface (PES) for the SiCSi + H_2 complex is presented in this work. This surface is developed from a large number of ab initio energies computed at the explicitly correlated coupled-cluster level of theory together with the augmented correlation-consistent polarized valence triple zeta basis set (CCSD(T)-F12/aug-cc-pVTZ). These energies are fitted to an analytical function through a procedure that combines spline, least-squares, and kernel-based methods. Two minimums of similar depths were found at the equilibrium geometry of the SiCSi molecule. The dependence of the PES on the bending angle is analyzed. Furthermore, a reduced four-dimensional PES averaged over the H_2 orientation is presented. Finally, the six-dimensional PES is used for computing the second virial coefficient of the SiCSi + H_2 pair using classical and semi-classical methods.

Phys. Chem. Chem. Phys., 2023, 25, 4542
DOI: 10.1039/d2cp03872b
Full-text URL: https://pubs.rsc.org/en/content/articlelanding/2023/CP/D2CP03872B

Announcements

Call for Abstracts EGU GA PS3.2 Emergence, chemistry, and evolution of organic matter in the Solar System

Call for Abstracts EGU GA PS3.2 Emergence, chemistry, and evolution of organic matter in the Solar System

Conveners: Nora Hänni, Niels Ligterink, Kelly Miller, Fabian Klenner, Cécile Engrand

EGU General Assembly - Vienna, Austria & Online | 14–19 April 2024

Organic matter of variable degrees of chemical complexity is found throughout our Solar System – ranging from simple molecules like methane in Titan’s lakes to macromolecular matter in meteorites. While small bodies like comets and Kuiper Belt Objects (KBOs) are thought to have preserved a pristine material record, the organic chemistry in planets and their satellites can be strong indicators of environmental processes. The widespread nature of organic species leaves us wondering: How did these organics form? Was this chemical complexity inherited, did it emerge in the Solar System, or a combination of both? What do these molecules tell us about the physical conditions and formational history of planetary bodies and other objects in the Solar System? Is there a link between this organic matter and the emergence of life?
This session is dedicated to the study of organic molecules and their chemical reactions taking place within the Solar System as well as the nearby environments from which these compounds could be inherited. Scientists with backgrounds in laboratory experimentation, chemical modelling, space exploration, instrumentation, theoretical chemistry, and observations are brought together to share knowledge and progress our understanding of the evolution of organic chemistry in interplanetary / interstellar dust particles, meteorites, comets, asteroids, KBOs, icy moons, terrestrial planets, and planetary atmospheres. We also ask how future space exploration missions can push the boundaries of our current knowledge.

Submit your abstract for session PS3.2 here: https://meetingorganizer.copernicus.org/EGU24/session/48094

Rules and regulations for abstract submission are found here: https://www.egu24.eu/programme/how_to_submit.html

Registration opens for the 2024 edition of the RED School - An astrobiology introductory course

The RED School will take place in Le Teich (France) from March 17 to 23, 2024. Its aim is to offer interdisciplinary training in astrobiology to students and young scientists with a Master's degree in astronomy, planetology, geology, chemistry, biology, or the history and philosophy of science.

Thanks to the support of the school's partners, we will be able to cover almost all registration costs. Participants will only have to pay for their own transport.

Registration for the 2024 event is now open: https://red-astrobiology.fr/

COSPAR 2024, Scientific Event F3.4: "Interstellar Organic Molecules in the Age of JWST and ALMA."

Organizers Rob Garrod and Eric Herbst invite submissions for contributed talks and posters at their COSPAR 2024 Scientific Event F3.4: "Interstellar Organic Molecules in the Age of JWST and ALMA." COSPAR (Committee on Space Research) is a large international organization that sponsors scientific assemblies about space research every other year. COSPAR 2024 will be held in Busan, Korea from 13–21 July 2024, and will be a fully in-person meeting.

The event description and speakers are given below. Abstracts may be submitted on the assembly web page: https://www.cospar-assembly.org by going to "Abstract Submission" and "Log-in". The deadline for abstracts is Feb. 9, 2024.

A selection of refereed papers from the event will be published in Advances in Space Research or Life Sciences in Space Research, and authors are encouraged to submit manuscripts after the Assembly for consideration. Details about the scientific program, transportation, financial aid, and logistics can be found at the above website, and at the local website www.cospar2024.org. A number of interesting scientific sessions will take place during the conference, including others with astrochemistry-related topics. Questions about our session F3.4 can be addressed to Rob Garrod (rgarrod@virginia.edu).

Event Description:
Following its launch in December 2021, the James Webb Space Telescope has already shown itself to be a transformative instrument for astrochemistry, providing unparalleled interstellar infrared spectra, and being used to identify several new solid-phase interstellar molecules. Over the coming years, JWST is expected to provide a wealth of new information about the spatial distribution of ices and gas-phase molecular species, with unprecedented infrared spectral resolution and sensitivity. In combination with data from the now well-established ALMA telescope, our picture of interstellar organic chemistry - and the link between gas-phase and dust grain-surface chemistry - will be richer and clearer than ever. In this scientific event, we will bring together observers, experimentalists, computational modelers and theorists to present the

latest results in molecular astrochemical research pertinent to new JWST and ALMA results, interstellar molecular complexity, and the origins of life. We will provide a platform for young researchers, especially those from developing countries, to present their work to an international audience.

Scientific Organizing Committee:
Rob Garrod, Main Scientific Organizer (University of Virginia, USA)
Eric Herbst, Deputy Scientific Organizer (University of Virginia, USA)
Ryan Fortenberry (University of Mississippi, USA)
Miwha Jin (NASA Goddard Space Flight Center, USA)
Jeong-Eun Lee (Seoul National University, Korea)
Alexey Potapov (Friedrich Schiller University Jena & Max Planck Institute for Astronomy, Germany)
Victor Rivilla (Centro de Astrobiologia (CSIC, INTA), Spain)
Yao-Lun Yang (RIKEN, Japan)

Speakers:
Stefanie Milam (NASA Goddard)
Albert Rimola (Universitat Autònoma de Barcelona, Spain)
Naoki Watanabe (Institute of Low Temperature Science, Hokkaido University, Japan)
Yao-Lun Yang (Star and Planet Formation Laboratory, RIKEN, Japan)
Melisse Bonfand (University of Virginia, USA)
Kenji Furuya (National Astronomical Observatory, Japan)
Daniel Harsono (Institute of Astronomy, National TsingHua University, Taiwan)
Natalia Inostroza-Pino (Universidad Autónoma de Chile, Chile)
Jaeyeong Kim (Korea Astronomy and Space Science Institute, Korea)
German Molpeceres (University of Tokyo, Japan)
Pooneh Nazari (University of Leiden, Netherlands)
Yuki Okoda (Star and Planet Formation Laboratory, RIKEN, Japan)
Takashi Onaka (University of Tokyo, Japan)
Takashi Shimonishi (Niigata University, Japan)
Kotomi Taniguchi (National Astronomical Observatory, Japan)

PhD position: Untangling Ice, Dust and Gas Astrochemistry with JWST Ice- Ma= pping (closing date Jan 25th 2024)

We expect to recruit to this PhD project, funded by DISCnet (www.discnet.co.uk), an STFC Centre for Doctoral Training, for a PhD position starting in October 2024.

For more information email helen.fraser@open.ac.uk (Dr Helen Jane Fraser)

JWST is revolutionising Astrochemistry of star-forming regions. When JWST data are coupled with gas-phase observations on the same spatial scales, (e.g. ALMA NOEMA JCMT IRAM) or archival observations of dust and astrophysics in the same regions (e.g. Gaia Eucld Herschel Spitzer) we have the potential to disentangle the astrochemistry of these environments, and understand the chemical influences on star and planet formation. There are three key outcomes to this PhD
* Generate new JWST ice maps of star-forming regions
* Interpret the astrochemistry of these regions by combining ice mapping and archival (or new) gas-phase and dust observations of the same regions
* To develop the unique computing techniques required to process of high volumes of complex data concurrently, first to generate ice maps, and second to interpret them; focusing especially on where there are lots of possible explanations of an observation, and establishing which is most feasible: this is the kind of big data challenge that lends itself to modern computing analysis in the machine learning / AI sphere.

Full details of the project can be found at: https://www5.open.ac.uk/science/physical-science/sites/www.open.ac.uk.science.physical-science/files/files/SPS_Studentships/FRASER%202024%20Project%20Proposal%20DISCnet.pdf
How to apply
If you would like to apply then please read the guidance on applying for a PhD studentship here and e-mail the following to STEM-SPS-PHD@open.ac.uk by the application deadline 25th January 2024:
* a completed Application form UK https://www.open.ac.uk/students/research/system/files/documents/application-form-uk.docx if you are classed as a home studenthttps://www.ukri.org/what-we-offer/developing-people-and-skills/esrc/funding-for-postgraduate-training-and-development/eligibility-for-studentship-funding/, or Application form non-UK https://www.open.ac.uk/students/research/system/files/documents/application-form-international.docx if you are an international student.
* an up to date CV.
* a list of individual courses taken and grades obtained.
* a personal statement identifying your interest in the project and suitability for it.
* copy of your passport.
* a copy of your settled status document (if you are an EU citizen requesting a PhD place as a home student).
You do not need to submit a research proposal.

Interviews will take place remotely on 7-9th February 2024.

Funding and Eligibility
These studentships are funded for 4 years, 3½ years research study and a 6-month placement, attract a stipend of £18,622 per year (2023/24 rate) directly payable to the student, and cover the home-student University fees: in some cases international fees may also be covered. To be eligible for funding, applicants must meet the UKRI academic requirements. We normally require that the candidates have at least a 2:1 at UK equivalent BSc or MSc level in physics or astronomy, but some flexibility is offered where applicants have significant research experience as evidenced by publications or other research assistant experience.

We are committed to widening participation and awarding PhD studentships toa diverse community of applicants. We particularly welcome applications from under-represented groups. Equal Opportunity is University policy.