AstroChemical Newsletter #32

June 2018

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

Interferometric Imaging of Titan's HC3N, H13CCCN, and HCCC15N

M. A. Cordiner, C. A. Nixon, S. B. Charnley, N. A. Teanby, E. M. Molter, Z. Kisiel, and V. Vuitton

We present the first maps of cyanoacetylene isotopologues in Titan's atmosphere, including H13CCCN and HCCC15N, detected in the 0.9 mm band using the Atacama Large Millimeter/submillimeter array (ALMA) around the time of Titan's (southern winter) solstice in 2017 May. The first high-resolution map of HC3N in its v7 = 1 vibrationally excited state is also presented, revealing a unique snapshot of the global HC3N distribution, free from the strong optical depth effects that adversely impact the ground-state (v = 0) map. The HC3N emission is found to be strongly enhanced over Titan's south pole (by a factor of 5.7 compared to the north pole), consistent with rapid photochemical loss of HC3N from the summer hemisphere combined with production and transport to the winter pole since the 2015 April ALMA observations. The H13CCCN/HCCC15N flux ratio is derived at the southern HC3N peak, and implies an HC3N/HCCC15N ratio of 67 ± 14. This represents a significant enrichment in 15N compared with Titan's main molecular nitrogen reservoir, which has a 14N/15N ratio of 167, and confirms the importance of photochemistry in determining the nitrogen isotopic ratio in Titan's organic inventory.

ApJL, 859, L15
DOI: 10.3847/2041-8213/aac38d
Full-text URL: http://iopscience.iop.org/article/10.3847/2041-8213/aac38d/pdf

Structure and Spectroscopic Properties of Imine Acetaldehyde: A Possible Interstellar Molecule

P. Redondo, A. Largo, C. Barrientos

A previous theoretical study shows that imine acetaldehyde can be obtained from the reaction between protonated vinyl alcohol and azanone. Therefore, imine acetaldehyde could be considered as a good molecule candidate to be found in space and could evolve to more complex organic molecules of prebiotic interest. In the present work, we carried out a computational study of the different conformers of imine acetaldehyde. For characterize its conformers we apply a composite approach which considers the extrapolation to the complete basis set (CBS) limit and core-valence (CV) electron correlation corrections at the at the CC level including single and double excitations and a perturbative treatment of triple excitations (CCSD(T)). This approach provides bond distances with an accuracy of 0.001-0.002 Å and angles accurate to 0.05-0.1º. Vibrational harmonic and anharmonic frequencies and IR intensities are also reported at the CCSD level. The most stable structure corresponds to an antiperiplanar disposition of the oxygen atom and of NH group with the hydrogen atom of the NH group addressed outside the skeleton. Interconversion processes between the four conformers characterized are studied. The lowest isomerization barrier is estimated to be around 1.2 kcal/mol, making these processes unlikely under low temperature conditions, such as those reigning in the interstellar medium. The reported, at "spectroscopic" accuracy, stabilities, molecular structures, as well as spectroscopic parameters for the four imine acetaldehyde conformers that could help in their laboratory or astronomical detection.

Monthly Notices of the Royal Astronomical Society
DOI: 10.1093/mnras/sty1175
Full-text URL: https://academic.oup.com/mnras/advance-article-abstract/doi/10.1093/mnras/sty1175/4992776

The efficiency of photodissociation for molecules in interstellar ices

Juris Kalvans

Processing by interstellar photons affects the composition of the icy mantles on interstellar grains. The rate of photodissociation in solids differs from that of molecules in the gas phase. The aim of this work was to determine an average, general ratio between photodissociation coefficients for molecules in ice and gas. A 1D astrochemical model was utilized to simulate the chemical composition for a line of sight through a collapsing interstellar cloud core, whose interstellar extinction changes with time. At different extinctions, the calculated column densities of icy carbon oxides and ammonia (relative to water ice) were compared to observations. The latter were taken from literature data of background stars sampling ices in molecular clouds. The best-fit value for the solid/gas photodissociation coefficient ratio was found to be ≈0.3. In other words, gas-phase photodissociation rate coefficients have to be reduced by a factor of 0.3 before applying them to icy species. A crucial part of the model is a proper inclusion of cosmic-ray induced desorption. Observations sampling gas with total extinctions in excess of ≈22 mag were found to be uncorrelated to modelling results, possibly because of grains being covered with non-polar molecules.

Accepted in MNRAS
DOI: 10.1093/mnras/sty1172
Full-text URL: https://arxiv.org/abs/1805.03618

PCCP Themed Collection: Theory, experiment, and simulations in laboratory astrochemistry - now online and currently free to access

Editors: Laurent Wiesenfeld, Allan Shi-Chung Cheung, Jos Oomens

Guest-edited by Laurent Wiesenfeld (Université Grenoble Alpes), Allan Shi-Chung Cheung (The University of Hong Kong) and Jos Oomens (Radboud University), this themed issue of PCCP overviews the recent developments showing physical insights in the areas of theory, experiment, and simulation as applied to molecular astrophysics environments.

PCCP
Full-text URL: http://blogs.rsc.org/cp/2018/05/21/pccp-themed-collection-theory-experiment-and-simulations-in-laboratory-astrochemistry/

Cold Chemistry : Molecular Scattering and Reactivity Near Absolute Zero

Editors: Olivier Dulieu and Andreas Osterwalder,

Recent years have seen tremendous progress in research on cold and controlled molecular collisions, both in theory and in experiment. The advent of techniques to prepare cold and ultracold molecules and ions, to store them in optical lattices or in charged quasicristalline structures, and to use them in crossed or merged beam experiments have opened many new possibilities to study the most fundamental aspects of molecular interactions. At the same time, theoretical work has made progress in tackling these problems and accurately describing quantum effects in complex systems, and in proposing viable options to control chemical reactions at ultralow energies. Through tutorials on both the theoretical and experimental aspects of research in cold and ultracold molecular collisions, this book provides advanced undergraduate students, graduate students and researchers with the foundations needed to understand this exciting field.

The Royal Society of Chemistry (2018) ISBN 978-1-78262-597-1
DOI: 10.1039/9781782626800
Full-text URL: http://pubs.rsc.org/en/content/ebook/978-1-78262-597-1

On Cosmic Ray-Driven Grain Chemistry in Cold Core Models

Christopher N. Shingledecker, Jessica D. Tennis, Romane Le Gal, Eric Herbst

In this paper, we present preliminary results illustrating the effect of cosmic rays on solid-phase chemistry in models of both TMC-1 and several sources with physical conditions identical to TMC-1 except for hypothetically enhanced ionization rates. Using a recent theory for the addition of cosmic ray-induced reactions to astrochemical models, we calculated the radiochemical yields, called G values, for the primary dust grain ice-mantle constituents. We show that the inclusion of this non-thermal chemistry can lead to the formation of complex organic molecules from simpler ice-mantle constituents, even under cold core conditions. In addition to enriching ice-mantles, we find that these new radiation-chemical processes can lead to increased gas-phase abundances as well, particularly for HOCO, NO2, HC2O, methyl formate (HCOOCH3), and ethanol (CH3CH2OH). These model results imply that HOCO - and perhaps NO2 - might be observable in TMC-1. Future detections of either of these two species in cold interstellar environments could provide strong support for the importance of cosmic ray-driven radiation chemistry. The increased gas-phase abundance of methyl formate can be compared with abundances achieved through other formation mechanisms such as pure gas-phase chemistry and three-body surface reactions.

ApJ, accepted
Full-text URL: https://arxiv.org/abs/1805.05764

Ion collision-induced chemistry in pure and mixed loosely bound clusters of coronene and C60 molecules

Alicja Domaracka, Rudy Delaunay, Arkadiusz Mika, Michael Gatchell, Henning Zettergren, Henrik Cederquist, Patrick Rousseau and Bernd A Huber

Ionization, fragmentation and molecular growth have been studied in collisions of 22.5 keV He2+- or 3 keV Ar+-projectiles with pure loosely bound clusters of coronene (C24H12) molecules or with loosely bound mixed C60 -C24H12 clusters by means of mass spectrometry. The heavier and slower Ar+ projectiles induce prompt knockout-fragmentation – C- and/or H-losses – from individual molecules and highly efficient secondary molecular growth reactions before the clusters disintegrate on picosecond timescales. The lighter and faster He2+ projectiles have a higher charge and the main reactions are then ionization by ions that are not penetrating the clusters. This leads mostly to cluster fragmentation without molecular growth. However, also here penetrating collisions may lead to molecular growth but to a much smaller extent than with 3 keV Ar+. Here we present fragmentation and molecular-growth mass distributions with 1 mass unit resolution, which reveals that the same numbers of C- and H-atoms often participates in the formation and breaking of covalent bonds inside the clusters. We find that masses close to those with integer numbers of intact coronene molecules, or with integer numbers of both intact coronene and C60 molecules are formed where often one or several H-atoms are missing or have been added on. We also find that super-hydrogenated coronene is formed inside the clusters.

Phys. Chem. Chem. Phys., 2018, Accepted Manuscript
DOI: 10.1039/C8CP01179F
Full-text URL:
http://pubs.rsc.org/en/Content/ArticleLanding/2018/CP/C8CP01179F#!divAbstract

The maser emitting structure and time variability of the SiS lines J=14-13 and 15-14 in IRC+10216

J. P. Fonfría, M. Fernandez-Lopez, J. R. Pardo, M. Agundez, C. Sanchez Contreras, L. Velilla Prieto, J. Cernicharo, M. Santander-Garcia, G. Quintana-Lacaci, A. Castro-Carrizo, S. Curiel

We present new high angular resolution interferometer observations of the v=0 J=14-13 and 15-14 SiS lines towards IRC+10216, carried out with CARMA and ALMA. The maps, with angular resolutions of ~0.25"and 0.55", reveal (1) an extended, roughly uniform, and weak emission with a size of ~0.5", (2) a component elongated approximately along the East-West direction peaking at ~0.13" and 0.17" at both sides of the central star, and (3) two blue- and red-shifted compact components peaking around 0.07" to the NW of the star. We have modeled the emission with a 3D radiation transfer code finding that the observations cannot be explained only by thermal emission. Several maser clumps and one arc-shaped maser feature arranged from 5 to 20R* from the central star, in addition to a thin shell-like maser structure at ~13R* are required to explain the observations. This maser emitting set of structures accounts for 75% of the total emission while the other 25% is produced by thermally excited molecules. About 60% of the maser emission comes from the extended emission and the rest from the set of clumps and the arc. The analysis of a time monitoring of these and other SiS and 29SiS lines carried out with the IRAM 30m telescope from 2015 to present suggests that the intensity of some spectral components of the maser emission strongly depends on the stellar pulsation while other components show a mild variability. This monitoring evidences a significant phase lag of ~0.2 between the maser and NIR light-curves.

Accepted for publication in ApJ
Full-text URL: https://arxiv.org/abs/1805.05218

Complex organic molecules in the Galactic Centre: the N-bearing family

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Requena-Torres, J. Armijos-Abendaño, D. Riquelme, R. Aladro

We present an unbiased spectral line survey toward the Galactic Centre (GC) quiescent giant molecular cloud (QGMC), G+0.693 using the GBT and IRAM 30 telescopes. Our study highlights an extremely rich organic inventory of abundant amounts of nitrogen (N)-bearing species in a source without signatures of star formation. We report the detection of 17 N-bearing species in this source, of which 8 are complex organic molecules (COMs). A comparison of the derived abundances relative to H2 is made across various galactic and extragalactic environments. We conclude that the unique chemistry in this source is likely to be dominated by low-velocity shocks with X-rays/cosmic rays also playing an important role in the chemistry. Like previous findings obtained for O-bearing molecules, our results for N-bearing species suggest a more efficient hydrogenation of these species on dust grains in G+0.693 than in hot cores in the Galactic disk, as a consequence of the low dust temperatures coupled with energetic processing by X-ray/cosmic ray radiation in the GC.

Monthly Notices of the Royal Astronomical Society, Advance Access
DOI: [10.1093/mnras/sty1174](https://doi.org/10.1093/mnras/sty1174)
Full-text URL: https://arxiv.org/abs/1804.11321

Tracing the cold and warm physico-chemical structure of deeply embedded protostars: IRAS 16293-2422 versus VLA 1623-2417

Nadia M. Murillo, Ewine F. van Dishoeck, Matthijs H. D. van der Wiel, Jes K. Jørgensen, Maria N. Drozdovskaya, Hannah Calcutt, and Daniel Harsono

Much attention has been placed on the dust distribution in protostellar envelopes, but there are still many unanswered questions regarding the structure of the gas. We aim to start identifying the factors that determine the chemical structure of protostellar regions, by studying and comparing low-mass embedded systems in key molecular tracers. The cold and warm chemical structures of two embedded Class 0 systems, IRAS16293 and VLA1623 are characterized through interferometric observations. DCO+, N2H+ and N2D+ are used to trace the spatial distribution and physics of the cold regions of the envelope, while c-C3H2 and C2H from models of the chemistry are expected to trace the warm (UV-irradiated) regions. Both sources show a number of striking similarities and differences. DCO+ consistently traces the cold material at the disk-envelope interface, where gas and dust temperatures are lowered due to disk shadowing. N2H+ and N2D+, also tracing cold gas, show low abundances towards VLA1623, but for IRAS16293, the distribution of N2D+ is consistent with the same chemical models that reproduce DCO+. c-C3H2 and C2H show different spatial distributions for the two systems. For IRAS16293, c-C3H2 traces the outflow cavity wall, while C2H is found in the envelope material but not the outflow cavity wall. In contrast, toward VLA1623 both molecules trace the outflow cavity wall. Finally, hot core molecules are abundantly observed toward IRAS16293 but not toward VLA1623. We identify temperature as one of the key factors in determining the chemical structure of protostars as seen in gaseous molecules. More luminous protostars, such as IRAS16293, will have chemical complexity out to larger distances than colder protostars, such as VLA1623. Additionally, disks in the embedded phase have a crucial role in controlling both the gas and dust temperature of the envelope, and consequently the chemical structure.

Accepted for publication in A&A
Full-text URL: https://arxiv.org/abs/1805.05205

Complex cyanides as chemical clocks in hot cores

V. Allen, F. F. S. van der Tak, C. Walsh

In the high-mass star-forming region G35.20-0.74N, small scale (~ 800 AU) chemical segregation has been observed in which complex organic molecules containing the CN group are located in a small location. We aim to determine the physical origin of the large abundance difference (about 4 orders of magnitude) in complex cyanides within G35.20-0.74 B, and we explore variations in age, gas and dust temperature, and gas density. We performed gas-grain astrochemical modeling experiments with exponentially increasing (coupled) gas and dust temperature rising from 10 to 500 K at constant H2 densities of 10^7, 10^8, and 10^9 cm^−3. We tested the effect of varying the initial ice composition, cosmic-ray ionization rate, warm-up time (over 50, 200, and 1000 kyr), and initial (10, 15, and 25 K) and final temperatures (300 and 500 K). Varying the initial ice compositions within the observed and expected ranges does not noticeably affect the modeled abundances indicating that the chemical make-up of hot cores is determined in the warm-up stage. Complex cyanides vinyl and ethyl cyanide (CH2CHCN and C2H5CN, respectively) cannot be produced in abundances (versus H2) greater than 5e−10 for CH2CHCN and 2e−10 for C2H5CN with a fast warm-up time (52 kyr), while the lower limit for the observed abundance of C2H5CN toward source B3 is 3.4e−10. Complex cyanide abundances are reduced at higher initial temperatures and increased at higher cosmic-ray ionization rates. Reproducing the observed abundances toward G35.20-0.74 Core B3 requires a fast warm-up at a high cosmic-ray ionization rate (1x10^−16 s^−1) at a high gas density (>10^9 cm^−3). G35.20-0.74 source B3 only needs to be about 2000 years older than B1/B2 for the observed chemical difference to be present. (This abstract has been shortened)

Forthcoming on A&A. Available on arXiv
DOI: 10.1051/0004-6361/201732553
Full-text URL: https://arxiv.org/abs/1804.02041

The Charge State of Polycyclic Aromatic Hydrocarbons across a Reflection Nebula, an H II Region, and a Planetary Nebula

C. Boersma, J. Bregman, L.J. Allamandola

Low-resolution Spitzer-IRS spectral map data of a reflection nebula (NGC 7023), H II region (M17), and planetary nebula (NGC 40), totaling 1417 spectra, are analyzed using the data and tools available through the NASA Ames PAH IR Spectroscopic Database. The polycyclic aromatic hydrocarbon (PAH) emission is broken down into PAH charge and size subclass contributions using a database-fitting approach. The resulting charge breakdown results are combined with those derived using the traditional PAH band strength ratio approach, which interprets particular PAH band strength ratios as proxies for PAH charge. Here the 6.2/11.2 µm PAH band strength ratio is successfully calibrated against its database equivalent: the nPAH+/nPAH0 ratio. In turn, this ratio is converted into the PAH ionization parameter, which relates it to the strength of the radiation field, gas temperature, and electron density. Population diagrams are used to derive the H2 density and temperature. The bifurcated plot of the 8.6 versus 11.2 µm PAH band strength for the northwest photo dissociation region in NGC 7023 is shown to be a robust diagnostic template for the nPAH+/nPAH0 ratio in all three objects. Template spectra for the PAH charge and size subclasses are determined for each object and shown to favorably compare. Using the determined template spectra from NGC 7023 to fit the emission in all three objects yields, upon inspection of the Structure SIMilarity maps, satisfactory results. The choice of extinction curve proves to be critical.

Concluding, the distinctly different astronomical environments of a reflection nebula, H II region, and planetary nebula are reflected in their PAH emission spectra.

2018, The Astrophysical Journal, 858, 67
DOI: 10.3847/1538-4357/aabcbe
Full-text URL: http://iopscience.iop.org/article/10.3847/1538-4357/aabcbe

The chemistry of disks around T Tauri and Herbig Ae/Be stars

Marcelino Agundez, Evelyne Roueff, Franck Le Petit, Jacques Le Bourlot

Infrared and (sub-)mm observations of disks around T Tauri and Herbig Ae/Be stars point to a chemical differentiation between both types of disks, with a lower detection rate of molecules in disks around hotter stars. To investigate the potential underlying causes we perform a comparative study of the chemistry of T Tauri and Herbig Ae/Be disks, using a model that pays special attention to photochemistry. The warmer disk temperatures and higher ultraviolet flux of Herbig stars compared to T Tauri stars induce some differences in the disk chemistry. In the hot inner regions, H2O, and simple organic molecules like C2H2, HCN, and CH4 are predicted to be very abundant in T Tauri disks and even more in Herbig Ae/Be disks, in contrast with infrared observations that find a much lower detection rate of water and simple organics toward disks around hotter stars. In the outer regions, the model indicates that the molecules typically observed in disks, like HCN, CN, C2H, H2CO, CS, SO, and HCO+, do not have drastic abundance differences between T Tauri and Herbig Ae disks. Some species produced under the action of photochemistry, like C2H and CN, are predicted to have slightly lower abundances around Herbig Ae stars due to a narrowing of the photochemically active layer. Observations indeed suggest that these radicals are somewhat less abundant in Herbig Ae disks, although in any case the inferred abundance differences are small, of a factor of a few at most. A clear chemical differentiation between both types of disks concerns ices, which are expected to be more abundant in Herbig Ae disks. The global chemical behavior of T Tauri and Herbig Ae/Be disks is quite similar. The main differences are driven by the warmer temperatures of the latter, which result in a larger reservoir or water and simple organics in the inner regions and a lower mass of ices in the outer disk.

A&A, accepted.
DOI: 10.1051/0004-6361/201732518
Full-text URL: http://adsabs.harvard.edu/abs/2018arXiv180309450A

Formation of interstellar methanol ice prior to the heavy CO freeze-out stage

D. Qasim, K.-J. Chuang, G. Fedoseev, S. Ioppolo, A.C.A. Boogert, and H. Linnartz

The formation of methanol (CH3OH) on icy grain mantles during the star formation cycle is mainly associated with the CO freeze-out stage. Yet there are reasons to believe that CH3OH also can form at an earlier period of interstellar ice evolution in CO-poor and H2O-rich ices. This work focuses on CH3OH formation in a H2O-rich interstellar ice environment following the OH-mediated H-abstraction in the reaction, CH4 + OH. Experimental conditions are systematically varied to constrain the CH3OH formation yield at astronomically relevant temperatures. CH4, O2, and hydrogen atoms are co-deposited in an ultrahigh vacuum chamber at 10-20 K. OH radicals are generated by the H + O2 surface reaction. Temperature programmed desorption - quadrupole mass spectrometry (TPD-QMS) is used to characterize CH3OH formation, and is complemented with reflection absorption infrared spectroscopy (RAIRS) for CH3OH characterization and quantitation. CH3OH formation is shown to be possible by the sequential surface reaction chain, CH4 + OH -> CH3 + H2O and CH3 + OH -> CH3OH at 10-20 K. This reaction is enhanced by tunneling, as noted in a recent theoretical investigation (Lamberts et al. 2017). The CH3OH formation yield via the CH4 + OH route versus the CO + H route is approximately 20 times smaller for the laboratory settings studied. The astronomical relevance of the new formation channel investigated here is discussed.

A&A 612, A83 (2018)
DOI: 10.1051/0004-6361/201732355
Full-text URL: https://www.aanda.org/articles/aa/abs/2018/04/aa32355-17/aa32355-17.html

The ALMA-PILS survey: Complex nitriles towards IRAS 16293-2422

H. Calcutt, J. K. Jørgensen, H. S. P. Müller, L. E. Kristensen, A. Coutens, T. L. Bourke, R. T. Garrod, M. V. Persson, M. H. D. van der Wiel, E. F. van Dishoeck, S. F. Wampfler

Complex organic molecules are readily detected in the inner regions of the gaseous envelopes of forming protostars. In particular, molecules that contain nitrogen are interesting due to the role nitrogen plays in the development of life and the compact scales such molecules have been found to trace around forming protostars. The goal of this work is to determine the inventory of one family of nitrogen-bearing organic molecules, complex nitriles (molecules with a −CN functional group) towards two hot corino sources in the low-mass protostellar binary IRAS 16293−2422. This work explores the abundance differences between the two sources, the isotopic ratios, and the spatial extent derived from molecules containing the nitrile functional group. Using data from the Protostellar Interferometric Line Survey (PILS) obtained with ALMA we determine abundances and excitation temperatures for the detected nitriles. We also present a new method for determining the spatial structure of sources with high line density and large velocity gradients − Velocity-corrected INtegrated emission (VINE) maps. We detect methyl cyanide (CH3CN) as well as 5 of its isotopologues, including the detection of CHD2CN which is the first detection in the ISM. We also detect ethyl cyanide (C2H5CN), vinyl cyanide (C2H3CN), and cyanoacetylene (HC3N). We find that abundances are similar between IRAS 16293A and IRAS 16293B on small scales except for vinyl cyanide which is only detected towards the latter source. This suggests an important difference between the sources either in their evolutionary stage or warm-up timescales. We also detect a spatially double-peaked emission for the first time in molecular emission in the A source, suggesting that this source is showing structure related to a rotating toroid of material.

Accepted in A&A
DOI: 10.1051/0004-6361/201732289
Full-text URL: https://arxiv.org/abs/1804.09210

Announcements

Laboratory Astrophysics Meeting at the IAU General Assembly in Vienna in August

Dear Colleagues, The IAU Commission on Laboratory Astrophysics is holding an event at the upcoming IAU General Assembly meeting in Vienna in August. Two 1.5 hour-long sessions devoted to the progress in laboratory astrophysics are scheduled. The program is listed below: Monday, August 27, 2018: Session 4b parallel session 10:30 – 12:00 Reports Commission B5 – Laboratory Astrophysics: from Observations to Interpretation (Part 1) 10:30 – 11:00: Commission B5 Business Meeting – Farid Salama CB5 Triennial report and CB5 Working Group reports OC Elections; Plans for the future, 2019 IAUS 350: Laboratory Astrophysics non-GA Symposium; Q&As 11:00 – 11:20: Progress report of the Working Group Spectroscopic and Radiative Data for Molecules – Steve Federman 11:20 – 11:40: The ESO Diffuse Interstellar Band Large Exploration Survey: First Results – Jan Cami 11:40 – 12:00: The Virtual Atomic and Molecular Data Centre (VAMDC). A Resource for Atomic and Molecular Data – Marie-Lise Dubernet Session 5b parallel session 13:30 – 15:00 Reports Commission B5 – Laboratory Astrophysics: from Observations to Interpretation (Part 2) 13:30 – 13:50: A progress report of the Working Group High-Accuracy Stellar Spectroscopy – Tanya Ryabchikova 13:50 – 14:10: Searching for the sources of meteorites in the asteroid belt – Peter Jenniskens 14:10 – 14:30: Laboratory Astrophysics in the era of JWST – Stefanie Milam 14:30 – 14:50: Cosmic Dust: Laboratory Experiments – Lisseth Gavilan 14:50 – 15:00: Open Discussion: Summary and Conclusions – All Link to IAU Commission B5: https://www.iau.org/science/scientific_bodies/commissions/B5/ Link to IAU GA Program: http://astronomy2018.univie.ac.at/division-days/ddb/

PhD position

PhD studentship in Theoretical Physical Chemistry Type of employment: Fixed-term employment, 4 years Extent: 100 % Location: Department of Chemistry and Molecular Biology, Gothenburg First day of employment: Flexible Application deadline 26 June 2018. Research and graduate education at the department of chemistry and molecular biology comprises a wide scientific field from the atomic and molecular levels all the way through cells to entire organisms. Much of the phenomena studied here impact on our natural environment and living systems. We participate in undergraduate programs in chemistry, molecular biology, medicinal chemistry, biology, marine sciences, and pharmacy. A third cycle education at our department will lead to a Ph.D. in Natural sciences, or Natural sciences with a specialisation in Chemistry, Biology or Biophysics. Ph.D. studies comprises four years at the post graduate level. The time period can be extended to 5 years in total through teaching and/or other departmental duties Information about the research group: The group develops theory and implements it on computers in order to study chemical processes in the gas phase and in condensed phase. We are interested in chemical kinetics, spectroscopy and dynamics in general, but focus on processes that are relevant to astrochemistry, e.g. radiative association and diffusion on and in interstellar ice particles. We often collaborate with other research groups, nationally and internationally. In particular it would be possible to collaborate with Martin Rahm, who heads a group in theoretical chemistry (rahmlab.com) at Chalmers exploring the formation of macromolecules in the solar system and their relevance to the origin of life. Another possible project would be carried out in collaboration with AstraZeneca in Mölndal. See also https://cmb.gu.se/english/about_us/staff?userId=xnymgu for information about the research group. The focus of the present project will be decided together with the student. Job assignments: Taking part in the development of theoretical methods and the implementation of these in computer programs. Run the programs and analyze the results for publication in international journals. Informal inquiries may be sent to Professor Gunnar Nyman: Nyman at chem.gu.se Further information and on-line application is found at: https://www.gu.se/english/about_the_university/job-opportunities/vacancies-details/?id=2605

Conference: Our Astro-Chemical History: Past, Present, and Future

"Our Astro-Chemical History: Past, Present and Future": the final conference of our COST Action CM1401 Sept 10th -14th 2018 Assen, Netherlands Key dates: - registration closes June 15th 2018 - accommodation booking required by July 1st 2018 The main aim of this final conference of the EU COST action CM1401 is to discuss the scientific results from our action, focusing on the areas covered by our working groups (a) the chemistry in cold diluted gases, (b) icy grain surface chemistry, (c) UV and X-ray photochemistry and (d) isotopic fractionation. We plan to have a strong focus on new collaborations and projects originating from our funded short term scientific missions. Additional invited talks will highlight the most recent discoveries and upcoming missions/facilities related to astrochemistry. The conference is also meant to look into the future and define the key areas where progress needs to be made to move the field ahead. An overview of the preliminary program and the scheduled sessions can be found at our website http://cost.obs.ujf-grenoble.fr/conference2018/program The conference will take place in Assen (Netherlands) at the Hof van Saksen from 10-14 September 2018. The deadline for registration is June 15 http://www.open.ac.uk/science/physical-science-conferences/cm1401-conference-our-astro-%C2%ADchemical-history-past-present-and-future After completing registration, you will receive the contact details to book your accomodation package (5 days, 4 nights including board and lodging) with the Hof van Saksen in Assen. The last management meeting of the action will take place on Wednesday afternoon. We are looking forward to seeing as many of you as possible there! The SOC Inga Kamp, Jean-Hugues Fillion, Helen Fraser, Octavio Roncero, Dmitry Semenov, Yury Suleymanov, Charlotte Vastel, Laurent Wiesenfeld

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