AstroChemical Newsletter #28

February 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

Survey Observations to Study Chemical Evolution from High-Mass Starless Cores to High-Mass Protostellar Objects I: HC3N and HC5N

Kotomi Taniguchi, Masao Saito, T. K. Sridharan, Tetsuhiro Minamidani

We carried out survey observations of HC3N and HC5N in the 42−45 GHz band toward 17 high-mass starless cores (HMSCs) and 35 high-mass protostellar objects (HMPOs) with the Nobeyama 45 m radio telescope. We have detected HC3N from 15 HMSCs and 28 HMPOs, and HC5N from 5 HMSCs and 14 HMPOs, respectively. The average values of the column density of HC3N are found to be (5.7±0.7)×1e12 and (1.03±0.12)×1e13 cm−2 in HMSCs and HMPOs, respectively. The average values of the fractional abundance of HC3N are derived to be (6.6±0.8)×1e−11 and (3.6±0.5)×1e−11 in HMSCs and HMPOs, respectively. We find that the fractional abundance of HC3N decreases from HMSCs to HMPOs using the Kolmogorov-Smirnov test. On the other hand, its average value of the column density slightly increases from HMSCs to HMPOs. This may imply that HC3N is newly formed in dense gas in HMPO regions. We also investigate the relationship between the column density of HC3N in HMPOs and the luminosity-to-mass ratio (L/M), a physical evolutional indicator. The column density of HC3N tends to decrease with increasing the L/M ratio, which suggests that HC3N is destroyed by the stellar activities.

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Unveiling the chemistry of interstellar CH: Spectroscopy of the 2 THz N = 2←1 ground state line

H. Wiesemeyer, R. Güsten, K.M. Menten, C.A. Durán, T. Csengeri, A.M. Jacob, R. Simon, J. Stutzki, F. Wyrowski

The methylidyne radical CH is commonly used as a proxy for molecular hydrogen in the cold, neutral phase of the interstellar medium. The optical spectroscopy of CH is limited by interstellar extinction, whereas far-infrared observations provide an integral view through the Galaxy. While the HF ground state absorption, another H2 proxy in diffuse gas, frequently suffers from saturation, CH remains transparent both in spiral-arm crossings and high-mass star forming regions, turning this light hydride into a universal surrogate for H2. However, in slow shocks and in regions dissipating turbulence its abundance is expected to be enhanced by an endothermic production path, and the idea of a “canonical” CH abundance needs to be addressed. The N=2←1 ground state transition of CH at λ149 µm has become accessible to high-resolution spectroscopy thanks to GREAT, the German Receiver for Astronomy at Terahertz Frequencies aboard the Stratospheric Observatory for Infrared Astronomy, SOFIA. Its unsaturated absorption and the absence of emission from the star forming regions makes it an ideal candidate for the determination of column densities with a minimum of assumptions. Here we present an analysis of four sightlines towards distant Galactic star forming regions, whose hot cores emit a strong far-infrared dust continuum serving as background signal. Moreover, if combined with the sub-millimeter line of CH at λ560 µm, environments forming massive stars can be analyzed. For this we present a case study on the “proto-Trapezium” cluster W3 IRS5. While we confirm the global correlation between the column densities of HF and those of CH, both in arm and interarm regions, clear signposts of an over-abundance of CH are observed towards lower densities. However, a significant correlation between the column densities of CH and HF remains. A characterization of the hot cores in the W3 IRS5 proto-cluster and its envelope demonstrates that the sub-millimeter/far-infrared lines of CH reliably trace not only diffuse but also dense, molecular gas. In diffuse gas, at lower densities a quiescent ion-neutral chemistry alone cannot account for the observed abundance of CH. Unlike the production of HF, for CH+ and CH, vortices forming in turbulent, diffuse gas may be the setting for an enhanced production path. However, CH remains a valuable tracer for molecular gas in environments reaching from diffuse clouds to sites of high-mass star formation.

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CO Diffusion and Desorption Kinetics in CO2 Ices

Ilsa R. Cooke, Karin I. Öberg, Edith C. Fayolle, Zoe Peeler, and Jennifer B. Bergner

The diffusion of species in icy dust grain mantles is a fundamental process that shapes the chemistry of interstellar regions; yet, measurements of diffusion in interstellar ice analogs are scarce. Here we present measurements of CO diffusion into CO2 ice at low temperatures (T = 11–23 K) using CO2 longitudinal optical phonon modes to monitor the level of mixing of initially layered ices. We model the diffusion kinetics using Fick's second law and find that the temperature-dependent diffusion coefficients are well fit by an Arrhenius equation, giving a diffusion barrier of 300 ± 40 K. The low barrier along with the diffusion kinetics through isotopically labeled layers suggest that CO diffuses through CO2 along pore surfaces rather than through bulk diffusion. In complementary experiments, we measure the desorption energy of CO from CO2 ices deposited at 11–50 K by temperature programmed desorption and find that the desorption barrier ranges from 1240 ± 90 K to 1410 ± 70 K depending on the CO2 deposition temperature and resultant ice porosity. The measured CO–CO2 desorption barriers demonstrate that CO binds equally well to CO2 and H2O ices when both are compact. The CO–CO2 diffusion–desorption barrier ratio ranges from 0.21 to 0.24 dependent on the binding environment during diffusion. The diffusion–desorption ratio is consistent with the above hypothesis that the observed diffusion is a surface process and adds to previous experimental evidence on diffusion in water ice that suggests surface diffusion is important to the mobility of molecules within interstellar ices.

2018, ApJ, 852, 75
DOI: 10.3847/1538-4357/aa9ce9
Full-text URL: https://arxiv.org/abs/1711.09967

Imaging the water snowline in a protostellar envelope with H13CO+

Merel L.R. van 't Hoff, Magnus V. Persson, Daniel Harsono, Vianney Taquet, Jes K. Jørgensen, Ruud Visser, Edwin A. Bergin, Ewine F. van Dishoeck

Snowlines are key ingredients for planet formation. Providing observational constraints on the locations of the major snowlines is therefore crucial for fully connecting planet compositions to their formation mechanism. Unfortunately, the most important snowline, that of water, is very difficult to observe directly in protoplanetary disks due to its close proximity to the central star. Based on chemical considerations, HCO+ is predicted to be a good chemical tracer of the water snowline, because it is particularly abundant in dense clouds when water is frozen out. This work maps the optically thin isotopologue H13CO+ (J=3-2) toward the envelope of the low-mass protostar NGC1333-IRAS2A (observed with NOEMA at ~0.9" resolution), where the snowline is at larger distance from the star than in disks. The H13CO+ emission peaks ~2" northeast of the continuum peak, whereas the previously observed H2-18O shows compact emission on source. Quantitative modeling shows that a decrease in H13CO+ abundance by at least a factor of six is needed in the inner ~360 AU to reproduce the observed emission profile. Chemical modeling predicts indeed a steep increase in HCO+ just outside the water snowline; the 50% decrease in gaseous H2O at the snowline is not enough to allow HCO+ to be abundant. This places the water snowline at 225 AU, further away from the star than expected based on the 1D envelope temperature structure for NGC1333-IRAS2A. In contrast, DCO+ observations show that the CO snowline is at the expected location, making an outburst scenario unlikely. The spatial anticorrelation of the H13CO+ and H2-18O emission provide a proof of concept that H13CO+ can be used as a tracer of the water snowline.

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CO and dust properties in the TW Hya disk from high-resolution ALMA observations

Jane Huang, Sean M. Andrews, L. Ilsedore Cleeves, Karin I. Oberg, David J. Wilner, Xuening Bai, Til Birnstiel, John Carpenter, A. Meredith Hughes, Andrea Isella, Laura M. Perez, Luca Ricci, Zhaohuan Zhu

We analyze high angular resolution ALMA observations of the TW Hya disk to place constraints on the CO and dust properties. We present new, sensitive observations of the 12CO J=3−2 line at a spatial resolution of 8 AU (0.14"). The CO emission exhibits a bright inner core, a shoulder at r≈70 AU, and a prominent break in slope at r≈90 AU. Radiative transfer modeling is used to demonstrate that the emission morphology can be reasonably reproduced with a 12CO column density profile featuring a steep decrease at r≈15 AU and a secondary bump peaking at r≈70 AU. Similar features have been identified in observations of rarer CO isotopologues, which trace heights closer to the midplane. Substructure in the underlying gas distribution or radially varying CO depletion that affects much of the disk's vertical extent may explain the shared emission features of the main CO isotopologues. We also combine archival 1.3 mm and 870 μm continuum observations to produce a spectral index map at a spatial resolution of 2 AU. The spectral index rises sharply at the continuum emission gaps at radii of 25, 41, and 47 AU. This behavior suggests that the grains within the gaps are no larger than a few millimeters. Outside the continuum gaps, the low spectral index values of α≈2 indicate either that grains up to centimeter size are present, or that the bright continuum rings are marginally optically thick at millimeter wavelengths.

Huang, J. et al. 2018, ApJ, 852, 2
DOI: 10.3847/1538-4357/aaa1e7
Full-text URL: http://iopscience.iop.org/article/10.3847/1538-4357/aaa1e7/meta

Evolution of interstellar organic compounds under asteroidal hydrothermal conditions

V.Vinogradoff ; S.Bernard ; C.Le Guillou ; L.Remusat

Carbonaceous chondrites (CC) contain a diversity of organic compounds. No definitive evidence for a genetic relationship between these complex organic molecules and the simple organic molecules detected in the interstellar medium (ISM) has yet been reported. One of the many difficulties arises from the transformations of organic compounds during accretion and hydrothermal alteration on asteroids. Here, we report results of hydrothermal alteration experiments conducted on a common constituent of interstellar ice analogs, Hexamethylenetetramine (HMT – C6H12N4). We submitted HMT to asteroidal hydrothermal conditions at 150°C, for various durations (up to 31 days) and under alkaline pH. Organic products were characterized by gas chromatography mass spectrometry, infrared spectroscopy and synchrotron-based X-ray absorption near edge structure spectroscopy. Results show that, within a few days, HMT has evolved into (1) a very diverse suite of soluble compounds dominated by N-bearing aromatic compounds (> 150 species after 31 days), including for instance formamide, pyridine, pyrrole and their polymers (2) an aromatic and N-rich insoluble material that forms after only 7 days of experiment and then remains stable through time. The reaction pathways leading to the soluble compounds likely include HMT dissociation, formose and Maillard-type reactions, e.g. reactions of sugar derivatives with amines. The present study demonstrates that, if interstellar organic compounds such as HMT had been accreted by chondrite parent bodies, they would have undergone chemical transformations during hydrothermal alteration, potentially leading to the formation of high molecular weight insoluble organic molecules. Some of the diversity of soluble and insoluble organic compounds found in CC may thus result from asteroidal hydrothermal alteration.

2017, Icarus, in press
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Full-text URL: https://www.sciencedirect.com/science/article/pii/S0019103517305109

Detection of the aromatic molecule benzonitrile (c-C6H5CN) in the interstellar medium

Brett A. McGuire, Andrew M. Burkhardt, Sergei Kalenskii, Christopher N. Shingledecker, Anthony J. Remijan, Eric Herbst, and Michael C. McCarthy

Polycyclic aromatic hydrocarbons and polycyclic aromatic nitrogen heterocycles are thought to be widespread throughout the Universe, because these classes of molecules are probably responsible for the unidentified infrared bands, a set of emission features seen in numerous Galactic and extragalactic sources. Despite their expected ubiquity, astronomical identification of specific aromatic molecules has proven elusive. We present the discovery of benzonitrile (c-C_6H_5CN), one of the simplest nitrogen-bearing aromatic molecules, in the interstellar medium. We observed hyperfine-resolved transitions of benzonitrile in emission from the molecular cloud TMC-1. Simple aromatic molecules such as benzonitrile may be precursors for polycyclic aromatic hydrocarbon formation, providing a chemical link to the carriers of the unidentified infrared bands.

Science (2018) 359, 202
DOI: 10.1126/science.aao4890
Full-text URL: https://arxiv.org/abs/1801.04228

H2 Formation on Cosmic Grain Siliceous Surfaces Grafted with Fe+ : A Silsesquioxanes-Based Computational Model

Fioroni Marco, DeYonker Nathan J.

Cosmic siliceous dust grains are involved in the synthesis of H_2 in the inter-stellar medium. In this work, the dust grain siliceous surface is represented by a hydrogen Fe-metalla-silsesquioxane model of general formula: $[Fe(H_7 Si_7 O_{12-n})(OH)_n]^+$ (n=0,1,2) where Fe^+ behaves like a single-site heterogeneous catalyst grafted on a siliceous surface synthesizing H_2 from H. A computational analysis is performed using two levels of theory (B3LYP-D3BJ and MP2-F12) to quantify the thermodynamic driving force of the reaction: $[Fe\text{-}T_7H_7]^+ + 4H \rightarrow [Fe\text{-}T_7H_7(OH)_2]^+ + H_2$. The general outcomes are: 1) H_2 synthesis is thermodynamically strongly favored; 2) Fe-H / Fe-H_2 barrier-less formation potential; 3) chemisorbed H-Fe leads to facile H_2 synthesis at $20 \leq T \leq 100$ K; 4) relative spin energetics and thermodynamic quantities between the B3LYP-D3BJ and MP2-F12 levels of theory are in qualitative agreement. The metalla-silsesquioxane model shows how Fe^+ fixed on a siliceous surface can potentially catalyze H_2 formation in space.

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Full-text URL: http://onlinelibrary.wiley.com/doi/10.1002/cphc.201600607/abstract

Methanol ice co-desorption as a mechanism to explain cold methanol in the gas-phase

N. F. W. Ligterink, C. Walsh, R.G. Bhuin, S. Vissapragada, J. Terwisscha van Scheltinga, H. Linnartz

Methanol is formed via surface reactions on icy dust grains. Methanol is also detected in the gas-phase at temperatures below its thermal desorption temperature and at levels higher than can be explained by pure gas-phase chemistry. The process that controls the transition from solid state to gas-phase methanol in cold environments is not understood. The goal of this work is to investigate whether thermal CO desorption provides an indirect pathway for methanol to co-desorb at low temperatures. Mixed CH_3OH:CO/CH_4 ices were heated under UHV (ultra-high vacuum) conditions and ice contents are traced using RAIRS (reflection absorption IR spectroscopy), while desorbing species were detected mass spectrometrically. An updated gas-grain chemical network was used to test the impact of the results of these experiments. The physical model used is applicable for TW Hya, a protoplanetary disk in which cold gas-phase methanol has recently been detected. Methanol release together with thermal CO desorption is found to be an ineffective process in the experiments, resulting in an upper limit of <7.3e-7 CH_3OH molecules per CO molecule over all ice mixtures considered. Chemical modelling based on the upper limits shows that co-desorption rates as low as 1E-6 CH_3OH molecules per CO molecule are high enough to release substantial amounts of methanol to the gas-phase at and around the location of the CO thermal desorption front in a protoplanetary disk. The impact of thermal co-desorption of CH_3OH with CO as a grain-gas bridge mechanism is compared with that of UV induced photodesorption and chemisorption.

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Characterization of methanol as a magnetic field tracer in star-forming regions

Boy Lankhaar, Wouter Vlemmings, Gabriele Surcis, Huib Jan van Langevelde, Gerrit C. Groenenboom, Ad van der Avoird

Magnetic fields play an important role during star formation. Direct magnetic field strength observations have proven specifically challenging in the extremely dynamic protostellar phase. Because of their occurrence in the densest parts of star forming regions, masers, through polarization observations, are the main source of magnetic field strength and morphology measurements around protostars. Of all maser species, methanol is one of the strongest and most abundant tracers of gas around high-mass protostellar disks and in outflows. However, as experimental determination of the magnetic characteristics of methanol has remained largely unsuccessful, a robust magnetic field strength analysis of these regions could hitherto not be performed. Here we report a quantitative theoretical model of the magnetic properties of methanol, including the complicated hyperfine structure that results from its internal rotation. We show that the large range in values of the Landé g-factors of the hyperfine components of each maser line lead to conclusions which differ substantially from the current interpretation based on a single effective g-factor. These conclusions are more consistent with other observations and confirm the presence of dynamically important magnetic fields around protostars. Additionally, our calculations show that (non-linear) Zeeman effects must be taken into account to further enhance the accuracy of cosmological electron-to-proton mass ratio determinations using methanol.

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Infrared spectra of complex organic molecules in astronomically relevant ice matrices. I. Acetaldehyde, ethanol, and dimethyl ether

J. Terwisscha van Scheltinga, N.F.W. Ligterink, A.C.A. Boogert, E.F. van Dishoeck, H. Linnartz

Context. The number of identified complex organic molecules (COMs) in inter- and circumstellar gas-phase environments is steadily increasing. Recent laboratory studies show that many such species form on icy dust grains. At present only smaller molecular species have been directly identified in space in the solid state. Accurate spectroscopic laboratory data of frozen COMs, embedded in ice matrices containing ingredients related to their formation scheme, are still largely lacking. Aims. This work provides infrared reference spectra of acetaldehyde (CH3CHO), ethanol (CH3CH2OH), and dimethyl ether (CH3OCH3) recorded in a variety of ice environments and for astronomically relevant temperatures, as needed to guide or interpret astronomical observations, specifically for upcoming James Webb Space Telescope observations. Methods. Fourier transform transmission spectroscopy (500-4000 cm−1 / 20-2.5 µm, 1.0 cm−1 resolution) was used to investigate solid acetaldehyde, ethanol and dimethyl ether, pure or mixed with water, CO, methanol, or CO:methanol. These species were deposited on a cryogenically cooled infrared transmissive window at 15K. A heating ramp was applied, during which IR spectra were recorded until all ice constituents were thermally desorbed. Results. We present a large number of reference spectra that can be compared with astronomical data. Accurate band positions and band widths are provided for the studied ice mixtures and temperatures. Special efforts have been put into those bands of each molecule that are best suited for identification. For acetaldehyde the 7.427 and 5.803 µm bands are recommended, for ethanol the 11.36 and 7.240 µm bands are good candidates, and for dimethyl ether bands at 9.141 and 8.011 µm can be used. All spectra are publicly available in the Leiden Database for Ice.

Astronomy & Astrophysics, accepted
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Full-text URL: https://www.aanda.org/component/article?access=doi&doi=10.1051/0004-6361/201731998

Probing Episodic Accretion in Very Low Luminosity Objects

Tien-Hao Hsieh, Nadia M. Murillo, Arnaud Belloche, Naomi Hirano, Catherine Walsh, Ewine F. van Dishoeck, Shih-Ping Lai

Episodic accretion has been proposed as a solution to the long-standing luminosity problem in star formation; however, the process remains poorly understood. We present observations of line emission from N2H+ and CO isotopologues using the Atacama Large Millimeter/submillimeter Array (ALMA) in the envelopes of eight Very Low Luminosity Objects (VeLLOs). In five of the sources the spatial distribution of emission from N2H+ and CO isotopologues shows a clear anti-correlation. It is proposed that this is tracing the CO snow line in the envelopes: N2H+ emission is depleted toward the center of these sources in contrast to the CO isotopologue emission which exhibits a peak. The positions of the CO snow lines traced by the N2H+ emission are located at much larger radii than those calculated using the current luminosities of the central sources. This implies that these five sources have experienced a recent accretion burst because the CO snow line would have been pushed outwards during the burst due to the increased luminosity of the central star. The N2H+ and CO isotopologue emission from DCE161, one of the other three sources, is most likely tracing a transition disk at a later evolutionary stage. Excluding DCE161, five out of seven sources (i.e., ∼70%) show signatures of a recent accretion burst. This fraction is larger than that of the Class 0/I sources studied by Jørgensen et al. (2015) and Frimann et al. (2016) suggesting that the interval between accretion episodes in VeLLOs is shorter than that in Class 0/I sources.

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An efficient statistical method to compute molecular collisional rate coefficients

Jérôme Loreau, François Lique, Alexandre Faure

Our knowledge about the "cold" Universe often relies on molecular spectra. A general property of such spectra is that the energy level populations are rarely at local thermodynamic equilibrium. Solving the radiative transfer thus requires the availability of collisional rate coefficients with the main colliding partners over the temperature range 10-1000 K. These rate coefficients are notoriously difficult to measure and expensive to compute. In particular, very few reliable collisional data exist for inelastic collisions involving reactive radicals or ions. Here we explore the use of a fast quantum statistical method to determine molecular collisional excitation rate coefficients. The method is benchmarked against accurate (but costly) close-coupling calculations. For collisions proceeding through the formation of a strongly-bound complex, the method is found to be highly satisfactory up to room temperature. Its accuracy decreases with decreasing potential well depth and with increasing temperature, as expected. This new method opens the way to the determination of accurate inelastic collisional data involving key reactive species such as H3+, H2O+, and H3O+ for which exact quantum calculations are currently not feasible.

ApJL 853 L5 (2018)
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Full-text URL: http://iopscience.iop.org/article/10.3847/2041-8213/aaa5fe/meta

Circumstellar environment of the M-type AGB star R Doradus. APEX spectral scan at 159.0 - 368.5 GHz

E. De Beck and H. Olofsson

Our current insights into the circumstellar chemistry of asymptotic giant branch (AGB) stars are largely based on studies of carbon-rich stars and stars with high mass-loss rates. In order to expand the current molecular inventory of evolved stars we present a spectral scan of the nearby, oxygen-rich star R Dor, a star with a low mass-loss rate (~2x10^{-7} Msun/yr). We carried out a spectral scan in the frequency ranges 159.0-321.5 GHz and 338.5-368.5 GHz (wavelength range 0.8-1.9 mm) using the SEPIA/Band-5 and SHeFI instruments on the APEX telescope and we compare it to previous surveys, including one of the oxygen-rich AGB star IK Tau, which has a high mass-loss rate (~5x10^{-6} Msun/yr). The spectrum of R Dor is dominated by emission lines of SO2 and the different isotopologues of SiO. We also detect CO, H2O, HCN, CN, PO, PN, SO, and tentatively TiO2, AlO, and NaCl. Sixteen out of approximately 320 spectral features remain unidentified. Among these is a strong but previously unknown maser at 354.2 GHz, which we suggest could pertain to H2SiO, silanone. With the exception of one, none of these unidentified lines are found in a similarly sensitive survey of IK Tau performed with the IRAM 30m telescope. We present radiative transfer models for five isotopologues of SiO (28SiO, 29SiO, 30SiO, Si17O, Si18O), providing constraints on their fractional abundance and radial extent. We derive isotopic ratios for C, O, Si, and S and estimate that, based on our results for 17O/18O, R Dor likely had an initial mass in the range 1.3-1.6 Msun, in agreement with earlier findings based on models of H2O line emission. From the presence of spectral features recurring in many of the measured thermal and maser emission lines we tentatively identify up to five kinematical components in the outflow of R Dor, indicating deviations from a smooth, spherical wind.

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Announcements

B1.3 at COSPAR2018 "Growing Up: the Long Journey of Planetary Systems from Interstellar Volatiles and Refractories to Asteroids, Comets, and Planets"

Dear Colleagues, We wish to invite you to attend event B1.3: "Growing Up: the Long Journey of Planetary Systems from Interstellar Volatiles and Refractories to Asteroids, Comets, and Planets", jointly organized by Commission B "Space Studies of the Earth-Moon System, Planets, and Small Bodies of the Solar System" and Commission E "Research in Astrophysics from Space" at the 42nd COSPAR Scientific Assembly (https://www.cospar-assembly.org) that will be held in Pasadena, California, USA, on 14-22 July 2018. *********************IMPORTANT DATE***************************** ABSTRACT SUBMISSION DEADLINE is 9 FEBRUARY 2018 *** Scientific Rationale: The path starting from interstellar materials and leading to the formation of planetary systems is complex and still not completely understood. To advance our understanding, the history of the different planetary bodies needs to be studied together with their evolving surroundings. The initial interstellar volatile composition, its chemical evolution and the growth of refractory particles into the primordial planetesimals are tightly coupled to the emergence of a star-disc system from a prestellar core. The evolution of the star-disc system, in turn, deeply affects the growth of the planetesimals into planets and the composition of their cores and atmospheres. Finally, the physical and compositional characteristics of the different planetary bodies are influenced by the evolution of the planetary system as a whole. The aim of this COSPAR event, co-organized by Commissions B and E, is to provide researchers studying prestellar cores and protoplanetary discs, small bodies and meteorites, the Solar System and exoplanets with an interdisciplinary venue for presenting and comparatively discussing new data and results to advance our understanding of the long journey interstellar materials undertake to form the rich variety of planetary systems orbiting the Sun and other stars. This scientific event is sponsored by the Center for Space and Habitability of the University of Bern (www.csh.unibe.ch). Main Scientific Organizers: Diego Turrini (INAF-IAPS; Italy) & Maria Drozdovskaya (University of Bern; Switzerland) Deputy Organizers: Martin Rubin (University of Bern; Switzerland) & Sho Sasaki (Osaka University; Japan) Scientific Organizing Committee: Francesca Altieri (INAF-IAPS; Italy) Daniel Angerhausen (Center for Space and Habitability, University of Bern; Switzerland) Nicolas Biver (Observatoire Paris-Site de Meudon, LESIA; France) Ilse Cleeves (Harvard-Smithsonian Center for Astrophysics; U.S.A.) Gennaro D'Angelo (Los Alamos National Laboratory; U.S.A.) Björn Davidsson (JPL, Caltech; U.S.A.) Lucas Ellerbroek (Anton Pannekoek Institute for Astronomy, University of Amsterdam; The Netherlands) Kenji Furuya (Center for Computational Sciences, University of Tsukuba; Japan) Sebastiaan Krijt (Department of the Geophysical Sciences, University of Chicago; U.S.A.) Francesco Marzari (Department of Physics and Astronomy, University of Padova; Italy) Paola Pinilla (Department of Astronomy, University of Arizona; U.S.A.) Motohide Tamura (University of Tokyo; Astrobiology Center, NINS; Japan) Mark Wyatt (Institute of Astronomy, University of Cambridge; U.K.) Hajime Yano (Department of Interdisciplinary Space Sciences, JAXA-ISAS; Japan) Confirmed Invited Speakers: Yuri Aikawa (University of Tokyo; Japan) Adrian Brunini (FCAG/UNLP; Argentina) Duncan Forgan (University of St Andrews; U.K.) Meredith Hughes (Wesleyan University; U.S.A.) Masahiro Ikoma (University of Tokyo; Japan) Karen Meech (University of Hawaii; U.S.A.) Laura Pérez (NRAO; U.S.A.) Caroline Smith (The Natural History Museum; U.K.) Akira Tsuchiyama (Kyoto University; Japan) Diana Valencia (MIT; U.S.A.) We look forward to seeing many of you in Pasadena this summer!

2018 NASA Laboratory Astrophysics Workshop

Announcing the 2018 NASA Laboratory Astrophysics Workshop (LAW) to be held April 8-11, 2018, at the University of Georgia, Athens, GA, USA. See www.physast.uga.edu/workshops/law *** Important Deadlines *** Hotel: March 11, 2018 Registration: March 16, 2018 Abstracts: March 22, 2018 *** Confirmed Invited Speakers *** Keith Arnaud (NASA GSFC) Peter Bernath (Old Dom. U.) Adam Foster (SAO) Robert Petre (NASA GSFC) Klaus Pontoppidan (STScI) Farid Salama (NASA Ames) Frank Timmes (Ariz. State U.) The purpose of NASA LAW 2018 is focused on identifying and prioritizing critical laboratory astrophysics data needs to meet the demands of NASA's current and near- term astrophysics missions. The meeting will also provide a forum within which the community can present and review the current state of knowledge in laboratory astrophysics and identify challenges and opportunities for the field. The agenda will include 17 invited talks, posters, panel discussions, and break-out sessions. Registration is $250 with a reduced rate of $125 for students and those who received their Ph.D. after April 1, 2016. With best wishes from the co-chairs, Phillip Stancil (UGA) Doug Hudgins (NASA HQ) Scientific Organizing Committee: Gary Ferland (U. Kentucky) Bill Latter (NASA HQ) Stefanie Milam (NASA GSFC) David Neufeld (Johns Hopkins U.) Ella Sciamma-O'Brien (NASA Ames) Alan Smale (NASA GSFC) Randall Smith (SAO) Artemis Spyrou (Michigan State U.) Lisa Storrie-Lombardi (JPL) Glenn Wahlgren (STScI)

PAHs in the ISM: observational, experimental, and computational tools

Venue: Les Houches Time: April 2-April 6: Arrival on Sunday evening April 1st, departure on Friday April 6 after lunch. Theme: This session will give a comprehensive view of the role of PAHs in space with thorough introductions to astronomical observations & theory, experimental & quantum chemical techniques relevant for the study of PAHs in the interstellar medium of galaxies, and observing opportunities from the ground and with the to-be-launched James Webb Space telescope. Topics: The molecular Universe; Interstellar PAHs; Observations of PAHs; Laboratory studies of PAHs; Quantum chemical studies of PAHs; Observing from the ground and from JWST; PAH data bases Lecturers: Tom Millar, Christine Joblin, Liv Hornekaer, Giacomo Mulas, Els Peeters, Olivier Berne, Alessandra Candian, Christiaan Boersma Organized on behalf of the Marie Curie Initial Training Network, EUROPAH, and the Dutch Astrochemistry Network, DAN-II by Antoine Gusdorf (LERMA, Observatoire de Paris), Xander Tielens (Leiden Observatory) Website: http://pahschool2018.strw.leidenuniv.nl/index.html Description and objectives: Interstellar polycyclic aromatic hydrocarbons PAHs are ubiquitous and lock up close to 15% of the elemental carbon in space. They play a key role in the ionization balance and heating of the interstellar gas and thus control the phase structure of the interstellar medium (ISM) of galaxies and regulate star formation. PAHs are also central to the chemical complexity of space and the organic inventory of regions of star and planet formation. Understanding PAHs and their role in the Universe is thus a key question in astrophysics. On Earth, PAHs are predominantly known as carcinogenic pollutants, as found, for example, in motor vehicle exhaust fumes and petroleum-related pollution. However, in astrochemistry PAHs play much more benign roles: 1) They act as probes of astrophysical and astrochemical conditions both in the Milky Way and in other galaxies, even at high redshift. 2) They act as catalysts for H2 formation as well as for increasing molecular complexity and possibly even the chemical evolution of life. 3) They interact with interstellar nano-scale dust grains and control their surface properties. 4) They are found in comets and meteorites along with other organic molecules including amino acids - thus forging a strong link between interstellar and solar system chemistry. The session will provide the students with a thorough training in astronomical observations and their analysis and laboratory techniques & quantum theoretical methods relevant to PAHs in space. Introductory lectures will ensure that the students can place interstellar PAHs in the wider context of astronomy and astrochemistry. The school will consist of a mixture of lectures and practical sessions. The lectures are intended to provide the students with the background of relevant topics, while the practical sessions will give the students hands-on experience in the reduction and interpretation of IR astronomical data, the use of quantum chemical computer codes such as Gaussian, and the exploration of astronomical and PAH data bases.

PhD position in The Surface Chemistry of Complex Organic Molecules in Space

A Ph.D. studentship (42 months) is available from September 2018 under the supervision of Prof Wendy Brown, Department of Chemistry, School of Life Sciences, University of Sussex, UK This PhD project will use a combination of experimental and theoretical surface science techniques to investigate the adsorption, processing (thermally and by electrons and photons) and formation of complex organic molecules (COMs) in conditions relevant to interstellar space and to cometary and planetary ices. This research is particularly timely because of the upcoming launch of the James Webb Space Telescope (JWST) in 2019, which will allow the detection of molecules in space with much higher sensitivity than previously possible. There will hence be the chance for this PhD student to be involved in laboratory and theoretical work directly relevant to observational astronomy. COMs are currently a hot topic in Astrochemistry, with new species being found all of the time in a range of different environments, including stars, planets and comets. Their importance stems from the fact that many COMs are pre-biotic i.e. they act as precursors to the formation of biologically relevant species such as simple amino acids. Further information about the work in the Brown research group can be found at http://www.sussex.ac.uk/lifesci/brownlab/ Please submit a formal application using our online application system at http://www.sussex.ac.uk/study/phd/apply, including a CV, degree transcripts and certificates, statement of interest (clearly stating supervisor’s name and the project title) and names of two academic referees. Programme of Study is PhD Chemistry. Applicants will have an excellent academic record and should have received or be expected to receive a relevant first or upper-second class honours degree in a relevant subject. The full award is available to UK and to EU students who have been ordinarily resident in the UK for the previous 3 years. EU candidates who do not meet this criteria will be eligible for a fee waiver only and Overseas (non EU) students are not eligible to apply. The EPSRC award covers Home/EU PhD fees, a tax-free living allowance at Research Council UK rates (currently £14,553 per annum) and research/training expenses for 3.5 years Contact Anna Izykowska for application enquiries (a.izykowska@sussex.ac.uk) Contact Prof Wendy Brown (W.A.Brown@sussex.ac.uk) for enquiries about the project

PDRA and PhD positions in Lab / Observational Astrochemistry

2 PDRAs (Laboratory Astrophysics) and 2 PhDs (Observational Astrochemistry & Laboratory Astrophysics) in the OU Astrochemistry Group (with Dr. H J Fraser) The School of Physical Sciences at the Open University, UK, is seeking to fill 2 STFC-funded PDRA positions and 2 PhD positions in the Astrochemistry Group in collaboration with Dr. Helen Jane Fraser. The overarching aim of this group is to understand the role of ices in star- and planet-formation processes, through observational and laboratory activities. For further information on any of these positions, please contact Dr. Helen Jane Fraser helen.fraser@open.ac.uk . PDRA – (Laboratory Astrophysics: Ice Aggregation Studies) 2 year fixed term, until 31st March 2020 [Ref: 14377] £29,799 - £38,833 (based on experience) Closing date 28th Feb 2018 (12 noon) [Interviews between March 8th and 13th 2018] This project aims to understand how ensembles of icy interstellar grains aggregate to form ‘pebbles’ in the regions around the snowline in proto-planetary disks, and to establish if this process can generate gas-phase water in the same regions. The successful candidate will continue the development of a novel instrument, designed to study the aggregation of ensembles of icy grains. They will be expected to lead the day-to-day experimental work, data analysis and resulting scientific publications. The experiments will focus on the aggregation of solid mm-sized icy grains, and porous-mm to cm-sized icy grains, as well as quantifying the collision induced outgassing of water. Some of the experiments will be conducted in microgravity environments in addition to the OU Astrochemistry Laboratories. Applicants will have a PhD in Experimental Physics, Physical Chemistry or Laboratory Astrochemistry or a directly related experimental field, and will be experienced in working with at least two of the following techniques: ultra-high vacuum, mass spectroscopy, cryogenics, ultra-fast video imaging. Additionally, they will have experience of experiment development and experimental computer control and data analysis. The successful candidate will also have excellent communication skills and be able to evidence strong teamwork in scientific or engineering projects, as well as demonstrating an emerging track record of peer-reviewed publications in international scientific journals. PDRA – (Laboratory Astrophysics: Ice Aggregation Studies) 1 year fixed term, starting between April 1st 2018 and Oct 1st 2018 [Ref: 14379] £29,799 - £38,833 (based on experience) Closing date 28th Feb 2018 (12 noon) [Interviews between March 8th and 13th 2018] This project applies fundamental condensed matter physics and neutron scattering techniques to our understanding of the materials involved in planet aggregation processes. The PDRA will be expected to design and lead experiments to form, manipulate and store the small amorphous icy particles, which will then subsequently be exploited in aggregation studies. The bulk and surface structure of the particles will be characterized using neutron-scattering techniques at a variety of nano- and micrometre length scales, exploiting the ISIS neutron facility at Rutherford Appleton Laboratories, UK. Subsequently the thermal and temporal evolution of these particles will also be investigated. By the time of taking up the post, the successful applicant will have a PhD in Neutron Science, Condensed Matter, Experimental Physics, Physical Chemistry or Laboratory Astrochemistry or a directly related experimental field. They will be experienced in working at large-scale neutron facilities and have experience with at least two of the following techniques: condensed molecular material (ice), cryogens, particle handing, particle characterization methods (e.g. mass distribution, size distribution, spectroscopic analysis). Additionally, they will have experience of neutron scattering experiments and the associated data analysis and necessary coding experience. The successful candidate will also have excellent communication skills and be able to evidence strong teamwork in scientific or engineering projects, as well as demonstrating an emerging track record of peer-reviewed publications in international scientific journals. For detailed information on how to apply follow the respective hyperlinks to each position above. You will need to complete an online application and also provide a full academic CV (including names and contact details for three academic referees), a publication list and a cover letter explaining why this project is of interest, how a PDRA fits with your longer-term career aspirations and how you meet the person specifications for the role. PhD– (Observational Astrochemistry: Ice-Mapping in the JWST Era) 3.5 year fixed term, commencing October 1st 2018 [Ref: A5] up to £14,533 (tax free stipend per annum) plus fees (terms & conditions apply) Applications will be considered from Feb 16th 2018, with initial interviews March 14th & 15th 2018, followed by a further round of interviews in late March until all positions are filled. Early application is advised. This PhD will build on our legacy of ice-mapping with the AKARI satellite to pave the way for the next generation of space- and ground-based facilities, which are set to revolutionize the “icy” astronomy world – JWST and E-ELT (Metis). The PhD will involve software and simulation preparations for JWST cycle 1 observations, particularly NIRCAM slitless spectroscopy of star-forming regions. The observations have been awarded time as part of the JWST ERS “Ice Age” programme (on which HJF is a Co-I) and the PhD student will be involved in the ERS data reduction and analysis. Subsequently the student will be involved in NIRSPEC MSA ice-mapping of pre-stellar cores, in JWST Cycle 1 and 2, as

well as having the opportunity for planning and simulating future ice observations possible with E-ELT Metis. In addition, this PhD will exploit archival data to generate combined ice-dust-gas maps of up to 12 pre-stellar cores, for which data from AKARI, Spitzer, Herschel, JCMT, Nobeyama and IRAM are already in hand. The analysis will not only produce beautiful imagery, but decipher for the first time, how water, CO and CO2 ices (as well as methanol and ammonia) are interrelated, and how ice chemistry can be linked to deuteration processes (or other isotopic differentiation), as well as dust abundances and the gas-phase abundances of key chemical and physical tracers in star-forming regions, such as CO, HCO+, H2D+ and CH3OH. There will be scope to apply for telescope observing time on VLT (KMOS), Subaru, Keck and JCMT / IRAM / NOEMA / ALMA, to obtain new gas- dust- and ice- observations to extend our chemical picture. Applicants require a Masters Degree in Physics or Astronomy, with evidence of extended observational or computing-based project work. PhD– (Laboratory Astrochemistry: Experimenting with the Earliest Stages of Planet Formation) 3.5 year fixed term, commencing October 1st 2018 [Ref: A4] up to £14,533 (tax free stipend per annum) plus fees (terms & conditions apply) Applications will be considered from Feb 16th 2018, with initial interviews March 14th & 15th 2018, followed by a further round of interviews in late March until all positions are filled. Early application is advised. This PhD will focus on laboratory work to produce and characterize the porous amorphous icy particles required for collision experiments, testing the earliest stages of planet formation. Our scientific goal is to describe, qualitatively and quantitatively, the collisions that dominate the earliest stages of icy planetesimal-formation, to answer, “how do planets form?” We use laboratory experiments to test icy grain collisions, taking advantage of the microgravity duration and quality in parabolic and sub-orbital flight, to study cm to sub-cm s-1 collisions between ensembles of micrometre-sized icy grains, forming micron – mm sized ‘fluffy’ ice aggregates, that stick to form cm-sized icy ‘pebbles’. These “ingredients” form the basis of material that aggregates in protoplanetary disks (including our own pre-solar nebula) to form the cores of planets, comets and asteroids. The PhD work will move from coarse proof of concept experiments in the laboratory, to large-scale reproducible production of icy grains, which will be characterized through neutron scattering experiments, and IR spectroscopy, and whose behavior will be tested in drop tower and parabolic flight experiments. The PhD includes significant facilities use requiring week(s) on “in situ” experimentation away from the OU. There is also an opportunity to apply the research to understanding of mission data (e.g. Rosetta, OSIRIS-Rex, Phobos sample return), and astronomical observations (e.g. JWST and ALMA). Applicants require a good quality pass in an undergraduate degree in Physics or Materials or Engineering, with evidence of extended laboratory based project work potentially involving image analysis, Labview programming, and handling of cryogens. An understanding of atomic and molecular physics is desirable. For detailed information on how to apply for either of these PhDs go to; http://www.open.ac.uk/science/physical-science/job-and-studentshipopportunities/studentshipsphd-opportunities You will need send a completed an application form (available at the link above), full CV (including names and contact details for two academic referees), full transcript of courses studied and grades awarded, and a cover letter explaining why this project is of interest, how a PhD fits with your longer-term career aspirations to STEM-SPS-PhD-admin@open.ac.uk as soon as possible. Please state the PhD project reference number on your application. Both PhD projects are also open to students worldwide with personal fellowship funding or those eligible for SEPNET scholarships. Please look at ; http://www.sepnet.ac.uk/sepnet-phd-scholarships-2018/ for further details of the SEPNET scholarship application process, which closes on Feb 14th 2018.