AstroChemical Newsletter #49

December 2019

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

Detection of Phosphorus-bearing Molecules toward a Solar-type Protostar

Jennifer Bergner , Karin Öberg, Salma Walker, Viviana Guzmán , Thomas Rice, and Edwin Bergin

Phosphorus is a key ingredient in terrestrial biochemistry, but is rarely observed in the molecular interstellar medium and therefore little is known about how it is inherited during the star and planet formation sequence. We present observations of the phosphorus-bearing molecules PO and PN toward the Class I low-mass protostar B1-a using the IRAM 30 m telescope, representing the second detection of phosphorus carriers in a solar-type star-forming region. The P/H abundance contained in PO and PN is ∼1e-10−1e−9 depending on the assumed source size, accounting for just 0.05%–0.5% of the solar phosphorus abundance and implying significant sequestration of phosphorus in refractory material. Based on a comparison of the PO and PN line profiles with the shock tracers SiO, SO2, and CH3OH, the phosphorus molecule emission seems to originate from shocked gas and is likely associated with a protostellar outflow. We find a PO/PN column density ratio of ∼1–3, which is consistent with the values measured in the shocked outflow of the low-mass protostar L1157, the massive star-forming regions W51 and W3(OH), and the galactic center GMC G+0.693-0.03. This narrow range of PO/PN ratios across sources with a range of environmental conditions is surprising, and likely encodes information on how phosphorus carriers are stored in grain mantles.

2019, ApJL 884:L36
DOI: 10.3847/2041-8213/ab48f9
Full-text URL: https://arxiv.org/abs/1910.04539

The first steps of Interstellar Phosphorus Chemistry

J. Chantzos, V. M. Rivilla, A. Vasyunin, E. Redaelli, L. Bizzocchi, F. Fontani, P. Caselli

Phosphorus-bearing species are an essential key to form life on Earth, however they have barely been detected in the interstellar medium. Since only PN and PO have been identified so far towards star-forming regions, the chemical formation pathways of P-bearing molecules are not easy to constrain and are thus highly debatable. An important factor still missing in the chemical models is the initial elemental abundance of phosphorus, i.e. the depletion level of P. In order to overcome this problem, we study P-bearing species in diffuse/translucent clouds. In these objects phosphorus is mainly in the gas phase and therefore the elemental initial abundance needed in our chemical simulations corresponds to the cosmic one and is thus well constrained. An advanced chemical model with an updated P-chemistry network has been used. Single-pointing observations were performed with the IRAM 30m telescope towards the line of sight to the blazar B0355+508 aiming for the (2-1) transitions of PN, PO, HCP and CP. This line of sight incorporates five diffuse/translucent clouds. The (2-1) transitions of the PN, PO, HCP and CP were not detected. We report detections of the (1-0) lines of 13CO, HNC and CN along with a first detection of C34S. We have reproduced the observations of HNC, CN, CS and CO in every cloud by applying typical conditions for diffuse/translucent clouds. According to our best-fit model, the most abundant P-bearing species are HCP and CP (~1e-10), followed by PN, PO and PH3 (~1e-11). We show that the production of P-bearing species is favoured towards translucent rather than diffuse clouds, where the environment provides a stronger shielding from the interstellar radiation. Based on our improved model, the (1-0) transitions of HCP, CP, PN and PO are expected to be detectable with estimated intensities up to ~200 mK.

Accepted in A&A
DOI: 10.1051/0004-6361/201936531
Full-text URL: https://arxiv.org/abs/1910.13449

Fingerprinting the effects of hyperfine structure on CH and OH far infrared spectra using Wiener filter deconvolution

Arshia M. Jacob, Karl M. Menten, Helmut Wiesemeyer, Min-Young Lee, Rolf Güsten, and Carlos A. Durán

In this paper, we investigate the influence of hyperfine splitting on complex spectral lines, with the aim of evaluating canonical abundances by decomposing their dependence on hyperfine structures. This is achieved from first principles through deconvolution. We present high spectral resolution observations of the rotational ground state transitions of CH near 2 THz seen in absorption toward the strong FIR-continuum sources AGAL010.62-00.384, AGAL034.258+00.154, AGAL327.293-00.579, AGAL330.954-00.182, AGAL332.826-00.549, AGAL351.581-00.352 and SgrB2(M). These were observed with the GREAT instrument on board SOFIA. The observed line profiles of CH were deconvolved from the imprint left by the lines' hyperfine structures using the Wiener filter deconvolution, an optimised kernel acting on direct deconvolution. The quantitative analysis of the deconvolved spectra first entails the computation of CH column densities.

Reliable N(CH) values are of importance owing to the status of CH as a powerful tracer for H2 in the diffuse regions of the interstellar medium. The N(OH)/N(CH) column density ratio is found to vary within an order of magnitude with values ranging from one to 10, for the individual sources that are located outside the Galactic centre. Using CH as a surrogate for H2, we determined the abundance of the OH molecule to be X(OH)=1.09x1e-7 with respect to H2. The radial distribution of CH column densities along the sightlines probed in this study, excluding SgrB2(M), showcase a dual peaked distribution peaking between 5 and 7 kpc. The similarity between the correspondingly derived column density profile of H2 with that of the CO-dark H2 gas traced by the cold neutral medium component of [CII] 158um emission across the Galactic plane, further emphasises the use of CH as a tracer for H2.

Astronomy & Astrophysics, Volume 632, December 2019, A60
DOI: 10.1051/0004-6361/201936037
Full-text URL: https://arxiv.org/abs/1911.00393

Efficient Production of S8 in Interstellar Ices: The effects of cosmic ray-driven radiation chemistry and non-diffusive bulk reactions

Christopher N. Shingledecker, Thanja Lamberts, Jacob C. Laas, Anton Vasyunin, Eric Herbst, Johannes Kaestner, Paola Caselli

In this work, we reexamine sulfur chemistry occurring on and in the ice mantles of interstellar dust grains, and report the effects of two new modifications to standard astrochemical models; namely, (a) the incorporation of cosmic ray-driven radiation chemistry and (b) the assumption of fast, non-diffusive reactions for key radicals in the bulk. Results from our models of dense molecular clouds show that these changes can have a profound influence on the abundances of sulfur-bearing species in ice mantles, including a reduction in the abundance of solid-phase H2S and HS, and a significant increase in the abundances of OCS, SO2, as well as pure allotropes of sulfur, especially S8. These pure-sulfur species - though nearly impossible to observe directly - have long been speculated to be potential sulfur reservoirs and our results represent possibly the most accurate estimates yet of their abundances in the dense ISM. Moreover, the results of these updated models are found to be in good agreement with available observational data. Finally, we examine the implications of our findings with regard to the as-yet-unknown sulfur reservoir thought to exist in dense interstellar environments.

ApJ, accepted
Full-text URL: https://arxiv.org/abs/1911.01239

Understanding H2 Formation on Hydroxylated Pyroxene Nanoclusters: Ab Initio Study of the Reaction Energetics and Kinetics

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The rate constants of H2 formation on five models of silicate nanoclusters with varying degrees of hydroxylation, (Mg4Si4O12)(H2O)N, were computed over a wide temperature range [180–2000 K]. We tested nine combinations of density functional methods and basis sets for their suitability for calculating reaction energies and barrier heights, and we computed the minimum energy H + H → H2 reaction paths on each nanocluster. Subsequently, we computed the rate constants employing three semiclassical approaches that take into account tunneling and nonclassical reflection effects by means of the zero curvature tunneling (ZCT), the small curvature tunneling (SCT), and the one-dimensional semiclassical transition state theory (SCTST) methods, which all provided comparable results. Our investigations show that the H2 formation process following the Langmuir–Hinshelwood (LH) mechanism is more efficient on the hydroxylated (N = 1–4) nanoclusters than on the bare (N = 0) one due to relatively higher reaction barrier height on the latter. H2 formation is found to have the smallest barrier and the most exothermic reaction for the moderately hydroxylated (Mg4Si4O12)(H2O)2 nanocluster for all nine considered methods. Overall, we conclude that all the considered nanoclusters are very efficient catalyzing grains for H2 formation in the physical conditions of the interstellar medium (ISM) with pyroxene nanosilicates having moderate to high hydroxylation being more efficient than bare nanograins.

J. Phys. Chem. A 2019, 123, 43, 9282-9291
DOI: 10.1021/acs.jpca.9b06713
Full-text URL: https://pubs.acs.org/doi/10.1021/acs.jpca.9b06713

Chemical and kinematic structure of extremely high-velocity molecular jets in the Serpens Main star-forming region

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The fastest molecular component to the protostellar outflows -- extremely high-velocity (EHV) molecular jets -- are still puzzling since they are seen only rarely. The first aim is to analyze the interaction between the EHV jet and the slow outflow by comparing their outflow force content. The second aim is to analyze the chemical composition of the different outflow velocity components and to reveal the spatial location of molecules. ALMA 3 mm and 1.3 mm observations of five outflow sources at 130 – 260 au resolution in the Serpens Main cloud are presented. Observations of CO, SiO, H2CO and HCN reveal the kinematic and chemical structure of those flows. Three velocity components are distinguished: the slow and the fast wing, and the EHV jet. Out of five sources, three have the EHV component. Comparison of outflow forces reveals that only the EHV jet in the youngest source Ser-emb 8 (N) has enough momentum to power the slow outflow. The SiO abundance is generally enhanced with velocity, while HCN is present in the slow and the fast wing, but disappears in the EHV jet. For Ser-emb 8 (N), HCN and SiO show a bow-shock shaped structure surrounding one of the EHV peaks suggesting sideways ejection creating secondary shocks upon interaction with the surroundings. Also, the SiO abundance in the EHV gas decreases with distance from this protostar, whereas that in the fast wing increases. H2CO is mostly associated with low-velocity gas but also appears surprisingly in one of the bullets in the Ser-emb 8 (N) EHV jet. The high detection rate suggests that the presence of the EHV jet may be more common than previously expected. The origin and temporal evolution of the abundances of SiO, HCN and H2CO through high-temperature chemistry are discussed. The data are consistent with a low C/O ratio in the EHV gas versus high C/O ratio in the fast and slow wings.

Accepted for publication in A&A
DOI: 10.1051/0004-6361/201935409
Full-text URL: https://arxiv.org/abs/1910.07857

The absolute photoionization cross section of the mercapto radical (SH) from threshold up to 15.0 eV

Helgi Rafn Hrodmarsson, Gustavo A. Garcia, Laurent Nahon, Jean-Christophe Loison and Bérenger Gans

We present the absolute photoionization cross-section of the mercapto radical, SH, recorded from its first ionization energy at 10.4 eV up to a photon energy of 15 eV. The absolute scale was calibrated at the fixed photon energy of 11.2 eV using the known values of H2S and S as references. SH and S were produced in a microwave discharge flow-tube reactor by hydrogen abstraction of the H2S precursor. The measured photoionization cross-section of SH dramatically differs from the one currently employed to model the presence of this species in a number of astronomical environments, where SH along with its ionic counterpart SH+ have been detected. The cation spectroscopy and fragmentation of H2S, SH and S in the 9.2–15.0 eV energy range obtained using threshold photoelectron techniques is also presented and discussed in the context of existing literature.

Physical Chemistry Chemical Physics, 2019, DOI: 10.1039/C9CP05809E
DOI: 10.1039/C9CP05809E
Full-text URL: https://pubs.rsc.org/en/content/articlelanding/2019/CP/C9CP05809E#!divAbstract

Rovibrational Spectral Analysis of CO3 and C2O3: Potential Sources for O2 Observed in Comet 67P/Churyumov–Gerasimenko

Ryan C. Fortenberry, Daniel Peters, Brian C. Ferrari, and Christopher J. Bennett

The recent ROSETTA mission to comet 67P/Churyumov–Gerasimenko detected surprisingly high levels of molecular oxygen (O2; hypervolatile species) in the coma. Current models predict that considerable levels of other hypervolatiles (such as molecular nitrogen, N2, methane, CH4, and Argon) should be found at similar levels, whereas they are more depleted. One explanation explored here is that larger (less volatile) parent molecules may have been formed during radiolysis of cometary ices and, upon sublimation, are subsequently broken down within the coma into smaller, more volatile fragments. In support of this hypothesis, this work employs reliable quantum chemical techniques to provide the spectral data necessary for the detection of two candidate precursor "parent" molecules, cyclic carbon trioxide (c-CO3), and cyclic dicarbon trioxide (c-C2O3). Benchmark computations performed for gas-phase CO2 give vibrational frequencies to within 1.5 cm−1 or better for the three fundamentals. Both c-CO3 and c-C2O3 have strong infrared features in the 4.5–5.5 μm (1800–2200 cm−1) range and other notable infrared features closer to 1100 cm−1 (9.10 μm). These molecules are both rotationally active, unlike CO2, and are therefore potentially observable and present new targets for radio telescope observations. Due to the stronger dipole moment, c-CO3 should be more easily detectable than the nearly non-polar c-C2O3. These data may help observations of these molecules and can provide insights as to how radiation-driven derivatization of CO/CO2 precursors could contribute to the generation of higher-mass parent species that subsequently degrade to produce more volatile species, such as O2, observed in cometary comae.

2019 ApJL 886 L10
DOI: 10.3847/2041-8213/ab53e8
Full-text URL: https://iopscience.iop.org/article/10.3847/2041-8213/ab53e8

Low Temperature Kinetics of the Reaction Between Methanol and the CN Radical

D. Gupta, S. Cheikh Sid Ely, I. R. Cooke, T. Guillaume, O. Abdelkader Khedaoui, T. S. Hearne, B. M Hays, I. R. Sims

Methanol (CH3OH) is considered by astronomers to be the simplest complex organic molecule (COM) and has been detected in various astrophysical environments, including protoplanetary disks, comets, and the interstellar medium (ISM). Studying the reactivity of methanol at low temperatures will aid our understanding of the formation of other complex and potentially prebiotic molecules. A major destruction route for many neutral COMs, including methanol, is via their reactions with radicals such as CN, which is ubiquitous in space. Here, we study the kinetics of the reaction between methanol and the CN radical using the well-established CRESU technique (a French acronym standing for Reaction Kinetics in Uniform Supersonic Flow) combined with Pulsed-Laser Photolysis–Laser-Induced Fluorescence (PLP-LIF). Electronic structure calculations were also performed to identify the exothermic channels through which this reaction can proceed. Our results for the rate coefficient are represented by the modified Arrhenius equation, k(T) = 1.26 × 10^−11(T/300 K)^−0.7 exp(−5.4 K/T), and display a negative temperature dependence over the temperature range 16.7—296 K, which is typical of what has been seen previously for other radical-neutral reactions that do not possess potential energy barriers. The rate coefficients obtained at room temperature strongly disagree with a previous kinetics study, which is currently available in the Kinetics Database for Astrochemistry (KIDA) and therefore used in some astrochemical models.

2019 J. Phys. Chem. A. (accepted)
DOI: 10.1021/acs.jpca.9b08472
Full-text URL: https://hal.archives-ouvertes.fr/hal-02360549

Threshold dissociation of the 1-ethynylpyrene cation at internal energies relevant to H I regions

G. Rouillé, M. Steglich, P. Hemberger, C. Jäger, T. Henning

Photoelectron photoion coincidence spectroscopy has been used to measure the threshold photoelectron spectrum of 1-ethynylpyrene and to obtain the breakdown graph describing the dissociation of the 1-ethynylpyrene cation. The threshold photoelectron measurement has allowed us to improve the determination of the ionization energy of 1-ethynylpyrene at 7.391 +/- 0.005 eV. Concerning the main dissociation channels, the analysis of the breakdown graph has given 3.70 +/- 0.60 eV as the activation energy for the loss of one H atom and 2.98 +/- 1.80 eV for the loss of a second independent H atom. The corresponding entropies of activation are affected by large errors as observed in similar studies of other polycyclic aromatic hydrocarbon cations. Minor dissociation channels were also detected and identified as the loss of the C2H group and the loss of a C2H2 unit and/or that of an H atom plus the C2H group. The activation energies and the entropies of activation of these minor pathways could not be derived from the measurements. It is found that the cation of 1-ethynylpyrene behaves like the cation of pyrene and is consequently more photostable than the cation of 1-methylpyrene. We conclude that photodissociation is not the leading cause of the low abundance, if not the absence, of ethynyl-substituted polycyclic aromatic hydrocarbon species in the interstellar medium.

2019 The Astrophysical Journal, 885, 21
DOI: 10.3847/1538-4357/ab4418
Full-text URL: https://arxiv.org/abs/1909.05718

Temperature profiles of young disk-like structures: The case of IRAS 16293A

Merel L.R. van 't Hoff, Ewine F. van Dishoeck, Jes K. Jørgensen, & Hannah Calcutt

Temperature is a crucial parameter in circumstellar disk evolution and planet formation because it governs the resistance of the gas to gravitational instability and sets the chemical composition of the planet-forming material. We set out to determine the gas temperature of the young disk-like structure around the Class 0 protostar IRAS 16293-2422A. We used Atacama Large Millimeter/submillimeter Array (ALMA) observations of multiple H2CS J=7-6 and J=10-9 lines from the Protostellar Interferometric Line Survey (PILS) to create a temperature map for the inner ~200 AU of the disk-like structure. This molecule is a particularly useful temperature probe because transitions between energy levels with different Ka quantum numbers operate only through collisions. Based on the H2CS line ratios, the temperature is between ~100-175 K in the inner ~150 AU, and drops to ~75 K at ~200 AU. At the current resolution (0.5" ~ 70 AU), no jump is seen in the temperature at the disk-envelope interface. The temperature structure derived from H2CS is consistent with envelope temperature profiles that constrain the temperature from 1000 AU scales down to ~100 AU, but does not follow the temperature rise seen in these profiles at smaller radii. Higher angular resolution observations of optically thin temperature tracers are needed to establish whether cooling by gas-phase water, the presence of a putative disk, or the dust optical depth influences the gas temperature at ~100 AU scales. The temperature at 100 AU is higher in IRAS 16293A than in the embedded Class 0/I disk L1527, consistent with the higher luminosity of the former.

Accepted in A&A
DOI: 10.1051/0004-6361/201936839
Full-text URL: https://arxiv.org/abs/1911.03495

Prevalence of non-aromatic carbonaceous molecules in the inner regions of circumstellar envelopes

L. Martínez, G. Santoro, P. Merino, M. Accolla, K. Lauwaet, J. Sobrado, H. Sabbah, R. J. Peláez, V. J. Herrero, I. Tanarro, M. Agúndez, A. Martín-Jimenez, R. Otero, G. J. Ellis, C. Joblin, J. Cernicharo & J. A. Martín-Gago

Evolved stars are foundries of chemical complexity, gas and dust that provide the building blocks of planets and life, and dust nucleation first occurs in their photosphere. The circumstellar regions enveloping these stars, despite their importance, remain hidden to many observations, and dust formation processes are therefore still poorly understood. Laboratory astrophysics provides complementary routes to unveil these chemical processes, but most experiments rely on combustion or plasma decomposition of molecular precursors under physical conditions far removed from those in space. To reproduce and characterize the bottom-up dust formation process, we have built an ultra-high vacuum machine combining atomic gas aggregation with advanced in situ characterization techniques. We show that carbonaceous dust analogues that formed from low-pressure gas-phase condensation of carbon atoms in a hydrogen atmosphere, in a ratio of carbon to molecular hydrogen similar to that reported for evolved stars, lead to the formation of amorphous carbon nanograins and aliphatic carbon clusters. Aromatic species and fullerenes do not form effectively under these conditions, raising implications for a revision of the chemical mechanisms taking place in circumstellar envelopes.

Nature Astronomy (Published 21 October 2019)

DOI: 10.1038/s41550-019-0899-4
Full-text URL: https://www.nature.com/articles/s41550-019-0899-4

The 3D structure of CO depletion in high-mass prestellar regions

S. Bovino, S. Ferrada-Chamorro, A. Lupi, G. Sabatini, A. Giannetti, D. R. G. Schleicher

Disentangling the different stages of the star-formation process, in particular in the high-mass regime, is a challenge in astrophysics. Chemical clocks could help alleviating this problem, but their evolution strongly depends on many parameters, leading to degeneracy in the interpretation of the observational data. One of these uncertainties is the degree of CO depletion. We present here the first self-consistent magneto-hydrodynamic simulations of high-mass star-forming regions at different scales, fully coupled with a non-equilibrium chemical network, which includes C-N-O bearing molecules. Depletion and desorption processes are treated time-dependently. The results show that full CO-depletion (i.e. all gas-phase CO frozen-out on the surface of dust grains), can be reached very quickly, in one third or even smaller fractions of the free-fall time, whether the collapse proceeds on slow or fast timescales. This leads to a high level of deuteration in a short time both for typical tracers like N2H+, as well as for the main ion H+3, the latter being in general larger and more extended. N2 depletion is slightly less efficient, and no direct effects on N-bearing molecules and deuterium fractionation are observed. We show that CO depletion is not the only driver of deuteration, and that there is a strong impact on Dfrac when changing the grain-size. We finally apply a two-dimensional gaussian Point Spread Function to our results to mimic observations with single-dish and interferometers. Our findings suggest that the low-values observed in high-mass star-forming clumps are in reality masking a full-depletion stage in the inner 0.1 pc region.

accepted in ApJ
Full-text URL: https://arxiv.org/abs/1910.13981

Influence of phyllosilicates on the hydrothermal alteration of organic matter in asteroids: Experimental perspectives

V. Vinogradoff, C. Le Guillou, S. Bernard, J.C. Viennet, M. Jaber, L. Remusat

The origin of the diverse organic compounds present in carbonaceous chondrites (CC) remains uncertain. We aim at investigating the role that hydrothermal alteration may have had on the molecular evolution of organic matter (OM). In particular, within CC matrices, OM is intimately embedded within phyllosilicates down to the nanometer scale, which raises the question of the influence of phyllosilicates on OM transformation during hydrothermal alteration on parent bodies. We conducted hydrothermal experiments at 150 C and alkaline pH, using a well-known molecule present in processed interstellar ice analogues, the hexamethylenetetramine (HMT), in the presence of Al- and Fe-rich smectites. Experimental products were characterized by gas chromatography mass spectrometry, infrared spectroscopy, X-ray diffraction and synchrotron-based X-ray absorption near edge structure spectroscopy. Within 31 days, the HMT + smectites + H2O system leads to (1) the formation of a diverse suite of soluble organic compounds, yet less abundant and less complex than in the absence of smectite, (2) carbon-rich smectite residues (3.8 wt.% and 2.6 wt.% of carbon for the Al- and Fe-rich smectite residues, respectively). In addition, the abundance and molecular composition of the final organic compounds depend on the nature of the phyllosilicate (Al vs. Fe-smectite). Various and complex interaction mechanisms could occur between OM and smectite. Physisorption, chemisorption and intercalation processes have likely entrapped a significant portion of the organic compounds, thereby altering their chemical evolution. The present work demonstrates that the presence and the nature of phyllosilicates influences the reaction pathways of organic compounds during hydrothermal alteration and that the presence of organic compounds may impact the mineral assemblage. This could have had significant importance for the co-evolution of OM and mineral phases in primitive bodies during hydrothermal alteration.

Geochimica Cosmochimica Acta, Volume 269, 15 January 2020, Pages 150-166
DOI: 10.1016/j.gca.2019.10.029
Full-text URL: https://www.sciencedirect.com/science/article/pii/S0016703719306830?via%3Dihub

Astrochemistry as a tool to follow the protostellar evolution: the Class I stage

E. Bianchi, C. Ceccarelli, C. Codella, J. Enrique-Romero, C. Favre, B. Lefloch

The latest developments in astrochemistry have shown how some molecular species can be used as a tool to study the early stages of the solar-type star formation process. Among them, the more relevant species are the interstellar complex organic molecules (iCOMs) and the deuterated molecules. Their analysis give us information on the present and past history of protostellar objects. Among the protostellar evolutionary stages, Class I protostars represent a perfect laboratory in which to study the initial conditions for the planet formation process. Indeed, from a physical point of view, the Class I stage is the bridge between the Class 0 phase, dominated by the accretion process, and the protoplanetary disk phase, when planets form. Despite their importance, few observations of Class I protostars exist and very little is known about their chemical content. In this paper we review the (few) existing observations of iCOMs and deuterated species in Class I protostars. In addition, we present new observations of deuterated cyanoacetylene and thioformaldehyde towards the Class I protostar SVS13-A. These new observations allow us to better understand the physical and chemical structure of SVS13-A and compare the cyanoacetylene and thioformaldehyde deuteration with other sources in different evolutionary phases.

accepted in ACS Earth and Space Chemistry
DOI: 10.1021/acsearthspacechem.9b00158
Full-text URL: http://arxiv.org/abs/1911.08991

Measurements of Low Temperature Rate Coefficients for the Reaction of CH with CH2O and Application to Dark Cloud and AGB Stellar Wind Models.

Niclas A. West, Tom J. Millar, Marie Van de Sande, Edward Rutter, Mark A. Blitz, Leen Decin, and Dwayne E. Heard

Rate coefficients have been measured for the reaction of CH radicals with formaldehyde, CH2O, over the temperature range 31 - 133 K using a pulsed Laval nozzle apparatus combined with pulsed laser photolysis and laser induced fluorescence spectroscopy. The rate coefficients are very large and display a distinct decrease with decreasing temperature below 70 K, although classical collision rate theory fails to reproduce this temperature dependence. The measured rate coefficients have been parameterized and used as input for astrochemical models for both dark cloud and AGB stellar outflow scenarios. The models predict a distinct change (up to a factor of two) in the abundance of ketene, H2CCO, which is the major expected molecular product of the CH + CH2O reaction.

The Astrophysical Journal 885, 134, November 2019
DOI: 10.3847/1538-4357/ab480e
Full-text URL: https://arxiv.org/abs/1910.07996

Infrared Complex Refractive Index of N-containing astrophysical ices free of water processed by cosmic-ray simulated in laboratory

W.R.M.Rocha, S.Pilling, A.Domaracka, H.Rothard, P.Boduch

Several nitrogen-containing molecules have been unambiguously identified in the Solar System and in the Interstellar Medium. It is believed that such a rich inventory of species is a result of the energetic processing of astrophysical ices during the interaction with ionizing radiation. An intrinsic parameter of matter, the complex refractive index, stores all the “chemical memory” triggered by energetic processing, and therefore might be used to probe ice observations in the infrared. In this study, four N-containing ices have been condensed in an ultra-high vacuum chamber and processed by heavy ions (O and Ni) with energies between 0.2 and 15.7 MeV at the Grand Accélérateur National d’Ions Lourds (GANIL), in Caen, France. All chemical changes were monitored in situ by Infrared Absorption Spectroscopy. The complex refractive index was calculated directly from the absorbance spectrum, by using the Lambert-Beer and Kramers-Kroning relations, and the values are available in an online database: https://www1.univap.br/gaa/nkabs-database/data.htm. As a result, other than the database, it was observed that non-polar ices are more destroyed by sputtering than polar ones. Such destruction and chemical evolution lead to variation in the IR albedo of samples addressed in this paper.

Accepted in Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy
DOI: 10.1016/j.saa.2019.117826
Full-text URL: https://www.sciencedirect.com/science/article/abs/pii/S1386142519312168?via%3Dihub

Announcements

Dynamics of Electrons in Atomic and Molecular Nanoclusters

The workshop will take place July 10-16, 2020 at the Ettore Majorana Centre in beautiful Erice, Sicily.
Co-directors V. Kresin (USC) and K. Hansen (Gothenburg & Tianjin).
The topics covered include:
Metallic, molecular and ionic clusters,
Optical properties and spectroscopy,
Storage rings, traps, laser cooling,
Collisions, scattering, reactions,
Excited states and relaxation,
Attachment and evaporation.

The workshop will include time for discussions. A good deal of the topics concern gas phase properties and reactions. The ambition of the workshop is to connect people from different fields working on adjacent subjects, and the workshop is a good chance for astrochemists and -physicists to connect with molecular beam workers that may be outside their immediate contact circles.

For more information and registration, please go to http://physics.usc.edu/deamn20/index.html

2 PhD Positions in Laboratory Astrophysics in the OU Astrochemistry Group

Two positions are available starting Oct 2020 for PhD studentships in the group of Dr Helen Fraser.
2 PhD Studentships in Laboratory Astrophysics - Deadline Feb 21st 2020
If you would like to apply send a completed application form - home and EU students or application form - overseas students, an up to date CV, list of individual courses taken and grades obtained (or full course transcript), a personal statement of why you are interested in the particular project and how your skills match the research area, together with IETLS score (non UK nationals) to STEM-SPS-Phd@open.ac.uk by Feb 21st 2020. You are encouraged to contact the Dr Helen Fraser (helen.fraser@open.ac.uk) prior to your application and to discuss the projects in more detail.

PhD 1:-Light-Field Motion Tracking in Laboratory Studies of Planet Formation

Overarching aim:- One of our key scientific drivers in the OU Astrochemistry group is to describe qualitatively and quantitatively the collisions that dominate the earliest stages of icy planetesimal-formation, to answer “how do planets form?”. We aim to be the first in the world to develop and exploit an experimental payload to address this challenge, taking advantage of the high-quality, medium-duration microgravity environments in sub-orbital flight, to study sub-cm/s collisions between ensembles of ~nm-sized icy grains, forming µm-mm sized fluffy ice aggregates, that stick to form cm-sized icy pebbles. Without these specific microgravity conditions, our particles sediment (at the low velocities), the aggregates fall apart or compact (weight effects), and there is insufficient time to collide and aggregate all the particles. The ability to attempt such collision experiments is only just emerging as sub-orbital flight providers commence operating, making this studentship timely for developing the underpinning technology ‘just in time’ to realize our scientific ambitions. This scientific aim is reliant on the deployment of appropriate video camera technology capable of operating in low pressure (< 10-4 mBar), temperature (< 180 K) and microgravity conditions, to record, track, and subsequently compute, the 3D motion of every particle in the ensemble, accounting for appropriate illumination, adapting to opacity changes as the aggregation progresses, accounting for dynamic changes in particle orientation, occlusion, shadowing and range as a function of time, and ensuring rapid data storage (no lost frames at a high frame rate > 500 fps) over a sustained (> 240 s) period, in a field of view not smaller than ~ 100 cm3. Consequently, the aim of this studentship is to develop this capability in a single, light-field camera with micro-lens array, and produce the associated software processing tools (with industrial partner DIAL). The methodology involves bread-boarding a prototype camera to a flight-ready model through two evolutions, at each step benchmarking, testing, and space-qualifying the camera technology by employing it in a range of scientifically-motivated laboratory and microgravity experiments, focused on icy-grain aggregation relevant to planet-formation processes, exploiting existing experimental set-ups at the academic partner (OU). The major technological outcome of the studentship will be to demonstrate that 3D motion tracking of an ensemble of icy particles undergoing aggregating collisions in simulated planet-forming environments can be performed using a single light-field camera operating in video mode, concurrently addressing our scientific outcome; to enhance our empirical understanding of the processes that dominate the earliest stages of exoplanets, exomoon and exocomet formation. Qualifications required: Masters in Physics or Engineering with significant experimental / instrumentational project work / research projects / internships in image technology / signal processing preferred. May suit Engineering students as much as those with a strong Physics background. With involve working with an industrial partner.

PhD 2:- Unveiling the Structure and Reactivity of Interstellar Ice with Neutron Scattering Studies Overarching aim:- Another key scientific driver in the Astrochemistry group is to describe qualitatively and quantitatively the structure of the condensed materials found on tiny dust grains in star- and planet- forming regions. It is the “ice” structure that governs chemical reactivity, diffusion rates and consequently the degree to which molecular complexity can arise in star-formation environments, and form the bridge between diatomic species and those pre-biotic complex organic molecules that are required somewhere in the biosphere of a habitable planet such that life can emerge. As the porous, amorphous ices are metastable and must be formed at low pressure and temperature, it is very difficult to produce and study the materials chemistry in a traditional sense. Therefore we have developed methods in the last few years to exploit novel neutron scattering techniques to understand the ice nano- micro- and macro- porosity. Our experiments have enabled us to see not only how water ice “grows” in space, but also how its structure is destroyed and modified by very low energy processes. This experimental work has been backed up by extensive molecular dynamics modelling. Since our work to date has only focused on water-ice, the obvious next step in this research is to look at multi-molecular ice systems, from binary to mixed ices, more akin to those envisaged to form in interstellar star-forming regions. The second obvious step is to look at not the bulk ice growth, but those interactions right at the start – where water is aggregating on the nano-scale on the silicaceous and carbonaceous surfaces of the dust grains. Both of these next steps can be probed with neutron scattering techniques available at RAL-ISIS and ILL. Therefore the aims of this PhD are two-fold:-
a. to study the dynamics of water adsorption and transport on model ISM surfaces of silicates and carbon, to look at the kinetic evolution of the water nano-clusters as a function of time and temperature
b. to study two model binary ice systems, CO-H2O and CH3OH-H2O using NIMROD and SANS2D instruments at ISIS. The experiments will involve dynamics studies of the ice growth and restructuring as a function of time and temperature, as well as the thermal evolution of the systems upon heating to destruction.
The student will be encouraged to link the work back to others in the research group working on surface dynamics, molecular dynamics, ice observations and place the resultant scientific data in both chemistry / physics and astronomy publications.
Qualifications required: Masters in Physics or Chemistry with significant experimental project work / research projects / internships condensed matter chemistry or physics. Previous beam-time or large scale facilities experience is welcome but not essential.

Bell Burnell Graduate Scholarship Fund - potential PhD Studentship Funding in Astrochemistry at the OU

We welcome expressions of interest from candidates interested in applying for the Bell Burnell Graduate Scholarship Fund, administered by the IOP. This is a fund donated by Prof Dame Jocelyn Bell Burnell (former OU Head of Physics) to support full or part-time graduates who wish to study towards a doctorate in physics and are from groups that are currently under-represented in physics. If you are interested in applying, please read the Guidance Notes. For the purpose of this fund the definition* of under-represented groups in physics refers to: women, students of Black-Caribbean, Black-African and other minority ethnic (BAME) heritage, students with disabilities, or who require additional funding to support inclusive learning, LGBT+ students and students from disadvantaged backgrounds who may struggle to find the levels of funding needed to complete their studies. People with qualifying refugee status who meet the above criteria are also encouraged to apply.
*This definition will be reviewed annually and amended in line with available data.

If you wish to apply and work in the field of Astrochemistry, please contact Dr Helen Fraser in the OU School of Physical Sciences, not later than Dec 11th 2019, in order to devise a project proposal – this can be in any area of observational, theoretical or laboratory astrophysics. Application forms for the fund (and for PhD applications at the OU) should be completed by the applicant and by the proposed supervisor(s) then submitted to STEM-SPS-PHD by Monday 6th January 2020. The School will then submit up to two applications to the IOP for consideration.