AstroChemical Newsletter #17

March 2017

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

Exploring molecular complexity with ALMA (EMoCA): Simulations of branched carbon-chain chemistry in Sgr B2(N)

R. T. Garrod, A. Belloche, H. S. P. Mueller, K. M. Menten

Using mm-wavelength data from ALMA, the EMoCA spectral line survey revealed the presence of both the straight-chain and branched forms of propyl cyanide (C3H7CN) toward the Galactic Center star-forming source Sgr B2(N2). This was the first interstellar detection of a branched aliphatic molecule. Through computational methods, we seek to explain the observed i:n ratio for propyl cyanide, and to predict the abundances of the four different forms of the homologous nitrile, butyl cyanide (C4H9CN). We also investigate whether other molecules will show a similar degree of branching, by modeling alkanes up to pentane (C5H12). We use a coupled three-phase chemical kinetics model to simulate the chemistry of Sgr B2(N2), using an updated chemical network that includes grain-surface/ice-mantle formation routes for branched nitriles and alkanes. We use the EMoCA survey data to search for the straight-chain form of butyl cyanide toward Sgr B2(N2). The observed i:n ratio for propyl cyanide is reproduced by the models. Butyl cyanide is predicted to show similar abundances to propyl cyanide, and to exhibit strong branching, with the sec form clearly dominant over all others. The addition of CN to acetylene and ethene is found to be important to the production of vinyl, ethyl, propyl, and butyl cyanide. We report a non-detection of n-C4H9CN toward Sgr B2(N2), with an abundance at least 1.7 times lower than that of n-C3H7CN. This value is within the range predicted by the chemical models. The models indicate that the degree of branching rises with increasing molecular size. The efficiency of CN addition to unsaturated hydrocarbons boosts the abundances of nitriles in the model, and enhances the ratio of straight-to-branched molecule production. The predicted abundance of s-C4H9CN makes it a good candidate for future detection toward Sgr B2(N2).

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CO2 infrared emission as a diagnostic of planet-forming regions of disks

Arthur D. Bosman, Simon Bruderer, Ewine F. van Dishoeck

[Abridged] The infrared ro-vibrational emission lines from organic molecules in the inner regions of protoplanetary disks are unique probes of the physical and chemical structure of planet forming regions and the processes that shape them. The non-LTE excitation effects of carbon dioxide (CO2) are studied in a full disk model to evaluate: (i) what the emitting regions of the different CO2 ro-vibrational bands are; (ii) how the CO2 abundance can be best traced using CO2 ro-vibrational lines using future JWST data and; (iii) what the excitation and abundances tell us about the inner disk physics and chemistry. CO2 is a major ice component and its abundance can potentially test models

with migrating icy pebbles across the iceline. A full non-LTE CO2 excitation model has been built. The characteristics of the model are tested using non-LTE slab models. Subsequently the CO2 line formation has been modelled using a two-dimensional disk model representative of T-Tauri disks. The CO2 gas that emits in the 15 µm and 4.5 µm regions of the spectrum is not in LTE and arises in the upper layers of disks, pumped by infrared radiation. The v2 15 µm feature is dominated by optically thick emission for most of the models that fit the observations and increases linearly with source luminosity. Its narrowness compared with that of other molecules stems from a combination of the low rotational excitation temperature (~250 K) and the inherently narrower feature for CO2. The inferred CO2 abundances derived for observed disks are more than two orders of magnitude lower than those in interstellar ices (~10^5), similar to earlier LTE disk estimates. Line-to-continuum ratios are low, of order a few %, thus high signal-to-noise (S/N > 300) observations are needed for individual line detections. Prospects of accurate abundance retrieval with JWST-MIRI and JWST-NIRSpec are discussed.

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A study of singly deuterated cyclopropenylidene c-C3HD in protostar IRAS 16293-2422

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Cyclic-C3HD (c-C3HD) is a singly deuterated isotopologue of c-C3H2, which is one of the most abundant and widespread molecules in our Galaxy. We observed IRAS 16293-2422 in the 3 mm band with a single frequency setup using the EMIR heterodyne 3 mm receiver of the IRAM 30m telescope. We observed seven lines of c-C3HD and three lines of c-C3H2. Observed abundances are compared with astrochemical simulations using the NAUTILUS gas-grain chemical model. Our results clearly show that c-C3HD can be used as an important supplement for studying chemistry and physical conditions for cold environments. Assuming that the size of the protostellar envelope is 3000 AU and same excitation temperatures for both c-C3H2 and c-C3HD, we obtain a deuterium fraction of 14 (+4, −3)%.

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Experimental and theoretical investigations of the ion-neutral reaction of C2H2N+ with C2H6 and implications on chain elongation processes in Titan’s atmosphere

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In this study we report theoretical and experimental evidence for the formation of ionic products by the ion-neutral reaction of C2H2N+ with C2H6. Our investigations consist of laboratory measurements using a guided ion beam mass spectrometer together with complementary ab initio quantum chemical computations, at the MP2/6-311++G(d,p) level of theory, in order to elucidate the energetics and geometries of the intermediates and transition states that are involved in the production of the observed productions. This study also provides insights on the isomeric nature of the observed product ions, their formation pathways together with collision energy and pressure dependences. The experimental data agrees well with the predictions of the ab initio calculations. Despite data provides evidence for the occurrence of C2H5+ as the most salient product ion, the production of CH3+, C2H3+, C3H5+, C3H7+ and C2H4N+ is also evident. A reaction scheme was proposed to elucidate the mechanisms responsible for the formation of the observed product ions. These processes might be intermediate

steps in the generation of long chain carbon and nitrogen-bearing compounds in Titan's ionosphere, the interstellar medium or circumstellar envelopes.

International Journal of Mass Spectrometry Volume 411, 10 December 2016, Pages 1–13
DOI: 10.1016/j.ijms.2016.10.003
Full-text URL: http://www.sciencedirect.com/science/article/pii/S1387380616302068?np=y&npKey=72e45897909464320bf21cf11ec07d9ef51515d8597c45bd5e1bd1d86b533814

Decrease of the organic deuteration during the evolution of Sun-like protostars: the case of SVS13-A

E. Bianchi, C. Codella, C. Ceccarelli, F. Fontani, L. Testi, R. Bachiller, B. Lefloch, L. Podio, V. Taquet

We present the results of formaldehyde and methanol deuteration measurements towards the Class I low-mass protostar SVS13-A, in the framework of the IRAM 30-m ASAI (Astrochemical Surveys At IRAM) project. We detected emission lines of formaldehyde, methanol, and their deuterated forms (HDCO, D2CO, CHD2OH, CH3OD) with Eup up to 276 K. The formaldehyde analysis indicates Tkin = 15 - 30 K, n (H2) >= 10^6 cm^-3, and a size of about 1200 AU suggesting an origin in the protostellar envelope. For methanol we find two components: (i) a high temperature (Tkin = 80 K) and very dense (> 10^8 cm^-3) gas from a hot corino (radius about 35 AU), and (ii) a colder Tkin <= 70 K) and more extended (radius about 350 AU) region. The deuterium fractionation is 9 10^-2 for HDCO, 4 10^-3 for D2CO, and 2 - 7 10^-3 for CH2DOH, up to two orders of magnitude lower than the values measured in Class 0 sources. We derive also formaldehyde deuteration in the outflow: 4 10^-3, in agreement with what found in the L1157-B1 protostellar shock. Finally, we estimate [CH2DOH]/[CH3OD] about 2. The decrease of deuteration in the Class I source SVS13-A with respect to Class 0 sources can be explained by gas-phase processes. Alternatively, a lower deuteration could be the effect of a gradual collapse of less deuterated external shells of the protostellar evelope. The present measurements fill in the gap between prestellar cores and protoplanetary disks in the context of organics deuteration measurements.

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Weakly bound molecular complexes in the laboratory and in the interstellar medium: A lost interest?

Alexey Potapov

Weakly bound molecular complexes have been studied in the laboratory for more than 40 years. Interest in them was heightened when they were predicted to be important species in the chemistry of the atmosphere and the interstellar medium (ISM) and also because of their unusual rotational dynamics, described in some cases by nearly free rotation of monomers within the complex. About 15 years ago the interest was heated by the observation of microscopic superfluidity in small helium clusters. On the other hand, a number of unsuccessful tries to detect weakly bound complexes in the ISM considerably lowered the interest in their further investigations for astrophysicists. With this short review I would like to show a perspective for future studies of astrophysically relevant weakly bound molecular complexes in the laboratory and for their potential search in the ISM.

Molecular Astrophysics, Volume 6, March 2017, Pages 16–21
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Full-text URL: http://www.sciencedirect.com/science/article/pii/S2405675816300343

The turbulent life of dust grains in the supernova-driven, multi-phase interstellar medium

Thomas Peters, Svitlana Zhukovska, Thorsten Naab, Philipp Girichidis, Stefanie Walch, Simon C. O. Glover, Ralf S. Klessen, Paul C. Clark, Daniel Seifried

Dust grains are an important component of the interstellar medium (ISM) of galaxies. We present the first direct measurement of the residence times of interstellar dust in the different ISM phases, and of the transition rates between these phases, in realistic hydrodynamical simulations of the multi-phase ISM. Our simulations include a time-dependent chemical network that follows the abundances of H+, H, H2, C+ and CO and take into account self-shielding by gas and dust using a tree-based radiation transfer method. Supernova explosions are injected either at random locations, at density peaks, or as a mixture of the two. For each simulation, we investigate how matter circulates between the ISM phases and find more sizeable transitions than considered in simple mass exchange schemes in the literature. The derived residence times in the ISM phases are characterised by broad distributions, in particular for the molecular, warm and hot medium. The most realistic simulations with random and mixed driving have median residence times in the molecular, cold, warm and hot phase around 17, 7, 44 and 1 Myr, respectively. The transition rates measured in the random driving run are in good agreement with observations of Ti gas-phase depletion in the warm and cold phases in a simple depletion model. ISM phase definitions based on chemical abundance rather than temperature cuts are physically more meaningful, but lead to significantly different transition rates and residence times because there is no direct correspondence between the two definitions.

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Nitrogen Fractionation in Protoplanetary Disks from the H13CN/HC15N Ratio

V.V. Guzmán, K.I. Öberg, J. Huang, R. Loomis and C. Qi

Nitrogen fractionation is commonly used to assess the thermal history of Solar System volatiles. With ALMA it is for the first time possible to directly measure 14N/15N ratios in common molecules during the assembly of planetary systems. We present ALMA observations of the H13CN and HC15N J=3-2 lines at 0".5 angular resolution, toward a sample of six protoplanetary disks, selected to span a range of stellar and disk structure properties. Adopting a typical 12C/13C ratio of 70, we find comet-like 14N/15N ratios of 80-160 in 5/6 of the disks (3 T Tauri and 2 Herbig Ae disks) and lack constraints for one of the T Tauri disks (IM Lup). There are no systematic differences between T Tauri and Herbig Ae disks, or between full and transition disks within the sample. In addition, no correlation is observed between disk-averaged D/H and 14N/15N ratios in the sample. One of the disks, V4046 Sgr, presents unusually bright HCN isotopologue emission, enabling us to model the radial profiles of H13CN and HC15N. We find tentative evidence of an increasing 14N/15N ratio with radius, indicating that selective photodissociation in the inner disk is important in setting the 14N/15N ratio during planet formation.

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Diffusion and Clustering of Carbon Dioxide on non-porous Amorphous Solid Water

J. He, S. Emtiaz, G. Vidali

Observations by ISO and Spitzer towards young stellar objects (YSOs) showed that CO2 segregates in the icy mantles covering dust grains. Thermal processing of ice mixture was proposed as responsible for the segregation. Although several laboratory studied thermally induced segregation, a satisfying quantification is still missing. We propose that the diffusion of CO2 along pores inside water ice is the key to quantify segregation. We combined Temperature Programmed Desorption (TPD) and Reflection Absorption InfraRed Spectroscopy (RAIRS) to study how CO2 molecules interact on a non-porous amorphous solid water (np-ASW) surface. We found that CO2 diffuses significantly on a np-ASW surface above 65 K and clusters are formed at well below one monolayer. A simple rate equation simulation finds that the diffusion energy barrier of CO2 on np-ASW is 2150+-50 K, assuming a diffusion pre-exponential factor of 10^12 s^-1. This energy should also apply to the diffusion of CO2 on wall of pores. The binding energy of CO2 from CO2 clusters and CO2 from H2O ice have been found to be 2415+-20 and 2250+-20 K, respectively, assuming the same prefactor for desorption. CO2-CO2 interaction is stronger than CO2-H2O interaction, in agreement with the experimental finding that CO2 does not wet np-ASW surface. For comparison, we carried out similar experiments with CO on np-ASW, and found that the CO-CO interaction is always weaker than CO-H2O. As a result, CO wets np-ASW surface. This study should be of help to uncover the thermal history of CO2 on the icy mantles of dust grains.

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Full-text URL: https://arxiv.org/abs/1611.02182

Water isotopologues in the circumstellar envelopes of M-type AGB stars

Taïssa Danilovich, R. Lombaert, L. Decin, A. Karakas, M. Maercker, H. Olofsson

AIM: In this study we examine rotational emission lines of two isotopologues of water: H_2 17O and H_2 18O. By determining the abundances of these molecules, we aim to use the derived isotopologue --- and hence oxygen isotope --- ratios to put constraints on the masses of a sample of M-type AGB stars that have not been classified as OH/IR stars. METHODS: We use detailed radiative transfer analysis based on the accelerated lambda iteration method to model the circumstellar molecular line emission of H_2 17O and H_2 18O for IK Tau, R Dor, W Hya, and R Cas. The emission lines used to constrain our models come from Herschel/HIFI and Herschel/PACS observations and are all optically thick, meaning that full radiative transfer analysis is the only viable method of estimating molecular abundance ratios. RESULTS: We find generally low values of the 17O/18O ratio for our sample, ranging from 0.15 to 0.69. This correlates with relatively low initial masses, in the range ~1.0 to 1.5 M⊙ for each source, based on stellar evolutionary models. We also find ortho-to-para ratios close to 3, which are expected from warm formation predictions. CONCLUSIONS: The 17O/18O ratios found for this sample are at the lower end of the range predicted by stellar evolutionary models, indicating that the sample chosen had relatively low initial masses.

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Inelastic cross sections and rate coefficients for collisions between CO and H2

Christina Castro, Kyle Doan, Michael Klemka, Robert C. Forrey, Benhui Yang, Phillip C. Stancil, N. Balakrishnan

A five-dimensional coupled states (5D-CS) approximation is used to compute cross sections and rate coefficients for CO+H2 collisions. The 5D-CS calculations are benchmarked against accurate six-dimensional close-coupling (6D-CC) calculations for transitions between low-lying rovibrational states. Good agreement between the two formulations is found for collision energies greater than 10 cm−1. The 5D-CS approximation is then used to compute two separate databases which include highly excited states of CO that are beyond the practical limitations of the 6D-CC method. The first database assumes an internally frozen H2 molecule and allows rovibrational transitions for $v \leq 5$ and $j \leq 30$, where v and j are the vibrational and rotational quantum numbers of the initial state of the CO molecule. The second database allows H2 rotational transitions for initial CO states with $v \leq 5$ and $j \leq 10$. The two databases are in good agreement with each other for transitions that are common to both basis sets. Together they provide data for astrophysical models which were previously unavailable.

Molecular Astrophysics, Volume 6, March 2017, Pages 47–58
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The Possibility of Forming Propargyl Alcohol in the Interstellar Medium

Prasanta Gorai, Ankan Das, Liton Majumdar, Sandip Kumar Chakrabarti, Bhalamurugan Sivaraman, Eric Herbst

Propargyl alcohol (HC2CH2OH, PA) has yet to be observed in the interstellar medium (ISM) although one of its stable isomers, propenal (CH2CHCHO), has already been detected in Sagittarius B2(N) with the 100-meter Green Bank Telescope in the frequency range 18−26 GHz. In this paper, we investigate the formation of propargyl alcohol along with one of its deuterated isotopomers, HC2CH2OD (OD-PA), in a dense molecular cloud. Various pathways for the formation of PA in the gas and on ice mantles surrounding dust particles are discussed. We use a large gas-grain chemical network to study the chemical evolution of PA and its deuterated isotopomer. Our results suggest that gaseous HC2CH2OH can most likely be detected in hot cores or in collections of hot cores such as the star-forming region Sgr B2(N). A simple LTE (Local thermodynamic equilibrium) radiative transfer model is employed to check the possibility of detecting PA and OD-PA in the millimeter-wave regime. In addition, we have carried out quantum chemical calculations to compute the vibrational transition frequencies and intensities of these species in the infrared for perhaps future use in studies with the James Webb Space Telescope (JWST).

Molecular Astrophysics, Volume 6, March 2017, Pages 36–46
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Hydrogen atom mobility, kinetic isotope effects and tunneling on interstellar ices (Ih and ASW)

Bethmini Senevirathne, Stefan Andersson, Francois Dulieu, Gunnar Nyman

Transitions of a single H atom between local minima on the surfaces of crystalline ice (Ih) and amorphous solid water (ASW) are studied theoretically in the temperature range 4–25 K. Binding energies, barrier heights, transition rate constants and the kinetic isotope effect (KIE) with and without tunneling are calculated. Harmonic transition state theory is used to obtain the transition rate constants and tunneling is treated with the Wigner tunneling correction, Eckart barrier correction and harmonic quantum transition state theory (HQTST). The classical binding energies are smaller on

Ih (<47 meV) than on ASW (<89 meV). Also the classical barrier heights are smaller on Ih (<14 meV) than on ASW (<69 meV) and distributed over a range of energies, in line with previous experimental observations. Similarly the vibrationally adiabatic ground state (VAG) barrier heights are smaller on Ih (< 7 meV) than on ASW (<54 meV). The surface morphology strongly influences the well depths. Tunneling increases some of the transition rate constants substantially but has a much smaller effect on others. The average KIE for Ih is higher than for ASW for the same range of barrier heights.

Molecular Astrophysics, Volume 6, March 2017, Pages 59–69
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Full-text URL: http://www.sciencedirect.com/science/article/pii/S2405675816300318

The growth of carbon chains in IRC+10216 mapped with ALMA

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Linear carbon chains are common in various types of astronomical molecular sources. Possible formation mechanisms involve both bottom-up and top-down routes. We have carried out a combined observational and modeling study of the formation of carbon chains in the C-star envelope IRC+10216, where the polymerization of acetylene and hydrogen cyanide induced by ultraviolet photons can drive the formation of linear carbon chains of increasing length. We have used ALMA to map the emission of 3 mm rotational lines of the hydrocarbon radicals C2H, C4H, and C6H, and the CN-containing species CN, C3N, HC3N, and HC5N with an angular resolution of 1". The spatial distribution of all these species is a hollow, 5-10" wide, spherical shell located at a radius of 10-20" from the star, with no appreciable emission close to the star. Our observations resolve the broad shell of carbon chains into thinner sub-shells which are 1-2" wide and not fully concentric, indicating that the mass loss process has been discontinuous and not fully isotropic. The radial distributions of the species mapped reveal subtle differences: while the hydrocarbon radicals have very similar radial distributions, the CN-containing species show more diverse distributions, with HC3N appearing earlier in the expansion and the radical CN extending later than the rest of the species. The observed morphology can be rationalized by a chemical model in which the growth of polyynes is mainly produced by rapid gas-phase chemical reactions of C2H and C4H radicals with unsaturated hydrocarbons, while cyanopolyynes are mainly formed from polyynes in gas-phase reactions with CN and C3N radicals.

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Thermochemical modelling of brown dwarf disks

A.J. Greenwood, I. Kamp, L.B.F.M. Waters, P. Woitke, W.-F. Thi, Ch. Rab, G. Aresu, M. Spaans

The physical properties of brown dwarf disks, in terms of their shapes and sizes, are still largely unexplored by observations. To what extent brown dwarf disks are similar to scaled-down T Tauri disks is poorly known, and this work is a step towards understanding these differences. We use observations of the brown dwarf disk ρ Oph 102 to infer a fiducial model around which we build a small grid of brown dwarf disk models, in order to model the CO, HCN, and HCO+ line fluxes and the chemistry which drives their abundances. These are the first brown dwarf models to be published which relate detailed, 2D radiation thermochemical disk models to observational data. We predict that moderately extended ALMA antenna configurations will spatially resolve CO line emission around brown dwarf disks, and that HCN and HCO+ will be detectable in integrated flux, following our conclusion that the flux ratios of these molecules to CO

emission are comparable to that of T Tauri disks. These molecules have not yet been observed in sub-mm wavelengths in a brown dwarf disk, yet they are crucial tracers of the warm surface-layer gas and of ionization in the outer parts of the disk. We present the prediction that if the physical and chemical processes in brown dwarf disks are similar to those that occur in T Tauri disks -- as our models suggest -- then the same diagnostics that are used for T Tauri disks can be used for brown dwarf disks (such as HCN and HCO+ lines that have not yet been observed in the sub-mm), and that these lines should be observable with ALMA. Through future observations, either confirmation (or refutation) of these ideas about brown dwarf disk chemistry will have strong implications for our understanding of disk chemistry, structure, and subsequent planet formation in brown dwarf disks.

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Modification of ices by cosmic rays and solar wind

Hermann Rothard, Alicja Domaracka, Philippe Boduch, Maria Elisabetta Palumbo, Giovanni Strazzulla, Enio F da Silveira, Emmanuel Dartois

Astrophysical ices are exposed to different radiation fields including photons, electrons and ions. The latter stem from interstellar cosmic rays (CR), the solar and stellar winds, shock waves or are trapped in the magnetospheres of giant planets. We briefly discuss the physics of energy deposition by ion ir radiation in condensed matter and experimental methods to study the induced effects. We then present results on radiation effects such as sputtering, amorphisation and compaction, dissociation of molecules, formation of new molecular species after radiolysis and by implantation of ions. The formation and radio-resistance of organic molecules, related to the question of the initial conditions for the emergence of life, are briefly discussed. This review is not meant to be comprehensive, but rather focusses on recent findings, with special emphasis on experiments with heavy multiply charged ion beams. These experiments aim in particular at simulating the effects of CRs on icy grains in dense molecular clouds, and on the formation of molecules on icy bodies in the Solar System.

J. Phys. B: At. Mol. Opt. Phys. 50 (2017) 062001 (Topical Review)
DOI: 10.1088/1361-6455/50/6/062001
Full-text URL: https://doi.org/10.1088/1361-6455/50/6/062001

Complex Organic Molecules Formation in Space Through Gas Phase Reactions: A Theoretical Approach

P. Redondo, C. Barrientos, and A. Largo

Chemistry in the interstellar medium (ISM) is capable of producing complex organic molecules (COMs) of great importance to astrobiology. Gas phase and grain surface chemistry almost certainly both contribute to COM formation. Amino acids as building blocks of proteins are some of the most interesting COMs. The simplest one, glycine, has been characterized in meteorites and comets and, its conclusive detection in the ISM seems to be highly plausible. In this work, we analyze the gas phase reaction of glycine and to establish the role of this process in the formation of alanine or other COMs in the ISM. Formation of protonated α- and β-alanine in spite of being exothermic processes is not viable under interstellar conditions because the different paths leading to these isomers present net activation energies. Nevertheless, glycine can evolve to protonated 1-imide-2, 2-propanediol, protonated amino acetone, protonated hydroxyacetone, and protonated propionic acid. However, formation of acetic acid and protonated methylamine is also a favorable process and therefore will be a competitive channel with the evolution of glycine to COMs.

ApJ, 836:240, 2017
DOI: 10.3847/1538-4357/aa5ca4
Full-text URL: http://iopscience.iop.org/article/10.3847/1538-4357/aa5ca4

Announcements

Molecules in space: Linking the interstellar medium to (exo)planets

Fall National Meeting of the American Chemical Society 20-24th August, 2017, Washington DC, USA Organizers: Prof. Alexander Tielens (Leiden University) and Dr. Partha P. Bera (NASA Ames Research Center) http://ism2planets.strw.leidenuniv.nl/ Molecules from simple to as complex as fullerenes have been identified in various astrophysical environments such as the interstellar media, dark clouds, hot cores, outflows of carbon stars, protoplanetary disks, and in the atmospheres of (exo)planets. We are only beginning to understand by sustained laboratory experimental, spectroscopic, computational, modeling, and observational efforts how these molecules are synthesized in the gas phase and on grain surfaces, evolve in those exotic conditions, and become incorporated in to planetary bodies. With the advent of new and upcoming capabilities such as the Atacama Large Millimeter Array (ALMA) and the James Webb Space Telescope (JWST), the scope of molecular exploration will increase many folds over the next decade. We are organizing a five-day symposium “Molecules in Space: Linking the Interstellar Medium to (exo)planets” at the American Chemical Society’s Fall National Meeting to be held in Washington DC from 20-24th August, 2017 to address the exploration of the molecular universe. The symposium will cover a wide breadth of subjects that will include organic inventory of the gas phase, the chemistry of the dark clouds, interplay of gas and dust, hot-cores and corinos, organic inventory of proto-planetary disks, high-resolution spectroscopy, the diffuse interstellar bands, the chemistry of atmospheres of stars and planets, and present and future opportunities such as ALMA, SOFIA, and JWST. Each session will begin with an overview talk by an eminent scholar in the field, followed by talks on astronomical observation, laboratory experiment, quantum chemistry calculations, and modeling. The sessions will be introduced by overview talks followed by invited talks on specific aspects of the session and contributed papers. In addition, there are poster sessions. Abstracts can be submitted for consideration for contributed talks and posters through the ACS Fall 2017 National Meeting webpage between the following dates. Abstract submission window open on 23rd January, 2017. Abstract submission window closes on 6th April, 2017. Session Titles Session I: Organic inventory of the gas phase: from small molecules to PAHs Session II: Chemistry of dark clouds: the interplay of gas and dust Session III: Hot cores and corinos: Observations, theory and experiments Session IV: Organic inventory of protoplanetary disks Session V: Spectroscopy: Meeting the needs of astronomers with experiments and theory Session VI: The DIBs: solving a century old problem Session VII: Chemistry of atmospheres of stars and planets

Fundamentals of Life in the Universe

Fundamentals of Life in the Universe Groningen, August 31 & September 1, 2017 Registration and deadlines: http://www.origins-symposium.nl/ The origin of life, on Earth and elsewhere, is a topic which fascinates the public, and which is ideally suited to bring together scientists from various disciplines. In Summer 2017, we will organize a two-day conference called “Fundamentals of Life in the Universe”, covering a wide spectrum of interests, from planetary evolution to the fabrication of synthetic cells. Besides invited talks, the conference includes a keynote speech by Ben Feringa (2016 Nobel laureate in chemistry), and a public lecture by Charley Lineweaver. The topics of the meeting are: 1. The origin of the Earth and of life 2. Predicting the evolution of life 3.

Building and directing life from molecule to biosphere 4. Life in extraterrestrial environments 5. Emergence and bridging of temporal and spatial scales

Job opening for a 2 yr post-doctoral position in exoplanet atmosphere modelling

At the Leuven University (Belgium), we seek an excellent candidate for a post-doctoral research position, ready to play a key role in our interdisciplinary project focusing on exoplanet atmosphere modelling. The goal of the project is to understand the intricate host star - exoplanet interaction, both in terms of dynamics and chemistry. We seek a post-doctoral researcher with expertise in theoretical modelling and/or retrieval algorithms. We aim to further develop our in-house developed dynamical + chemistry exoplanet modelling tools and to confront the model observables with new exoplanet spectra which will be obtained with the James Webb Space Telescope (JWST, launch in 2018). More information can be found at http://fys.kuleuven.be/ster/vacancies/2-yr-post-doctoral-position-in-the-field-of-exoplanets DEADLINE for the application: 1 April 2017 http://fys.kuleuven.be/ster/vacancies/2-yr-post-doctoral-position-in-the-field-of-exoplanets