AstroChemical Newsletter #54

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Abstracts

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

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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.

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Benzonitrile as a Proxy for Benzene in the Cold ISM: Low-temperature Rate Coefficients for CN + C6H6

I. Cooke, D. Gupta, J. Messinger and I. Sims

The low-temperature reaction between CN and benzene (C6H6) is of significant interest in the astrochemical community due to the recent detection of benzonitrile, the first aromatic molecule identified in the interstellar medium (ISM) using radio astronomy. Benzonitrile is suggested to be a low-temperature proxy for benzene, one of the simplest aromatic molecules, which may be a precursor to polycyclic aromatic hydrocarbons. In order to assess the robustness of benzonitrile as a proxy for benzene, low-temperature kinetics measurements are required to confirm whether the reaction remains rapid at the low gas temperatures found in cold dense clouds. Here, we study the C6H6 + CN reaction in the temperature range 15–295 K, 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. We obtain rate coefficients, k(T), in the range (3.6–5.4) × 1e−10 cm^3 s^−1 with no obvious temperature dependence between 15 and 295 K, confirming that the CN + C6H6 reaction remains rapid at temperatures relevant to the cold ISM.

2020 ApJL 891 L41
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Full-text URL: https://arxiv.org/abs/2003.02101

Sensitivity of gas-grain chemical models to surface reaction barriers: Effect from a key carbon-insertion reaction, C + H2 → CH2

Matjaž Simončič, Dmitry Semenov, Serge Krasnokutski, Thomas Henning, Cornelia Jäger

The feasibility of contemporary gas-grain astrochemical models depends on the availability of accurate kinetics data, in particular, for surface processes. We study the sensitivity of gas-grain chemical models to the energy barrier Ea of the important surface reaction between some of the most abundant species: C and H2 (surface C + surface H2 = surface CH2). We used the gas-grain code ALCHEMIC to model the time-dependent chemical evolution over a 2D grid of densities (nH: 10^{3} - 10^{12}cm^{-3}) and temperatures (T: 10 - 300 K), assuming UV-dark (Av = 20 mag) and partly UV-irradiated (Av = 3 mag) conditions that are typical of the dense interstellar medium. We considered two values for the energy barrier of the surface reaction, Ea = 2500 K (as originally implemented in the networks) and Ea = 0 K (as measured in the laboratory and computed by quantum chemistry simulations). We find that if the C + H2 = CH2 surface reaction is barrierless, a more rapid conversion of the surface carbon atoms into methane ice occurs. Overproduction of the CHn hydrocarbon ices affects the surface formation of more complex hydrocarbons, cyanides and nitriles, and CS-bearing species at low temperatures < 10-15 K. The surface hydrogenation of CO and hence the synthesis of complex (organic) molecules become affected as well. As a result, important species whose abundances may change by more than a factor of two at 1 Myr include atomic carbon,

small mono-carbonic (C1) and di-carbonic (C2) hydrocarbons, CO2, CN, HCN, HNC, HNCO, CS, H2CO, H2CS, CH2CO, and CH3OH (in either gas and/or ice). The abundances of key species, CO, H2O, and N2 as well as O, HCO+, N2H+, NH3, NO, and most of the S-bearing molecules, remain almost unaffected. Further accurate laboratory measurements and quantum chemical calculations of the surface reaction barriers will be crucial to improve the accuracy of astrochemical models.

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Theoretical Rovibrational Characterization of th cis/trans-HCSH and H2SC Isomers of the Known Interstellar Molecule Thioformaldehyde

N. Inostroza-Pino, C. Z. Palmer, T. J. Lee, and R. C. Fortenberry

The missing sulfur of the interstellar medium may be hiding in molecules for which there are no spectral data yet available for any astrophysical observation, molecules like isomers of H2CS a known interstellar compound. Every known interstellar molecule is a pointer to the presence and detectability of related molecules in the ISM. This quantum chemical study provides the necessary spectral data for the observation of cis-, trans-, and 3A HCSH as well as for 1A1 and 3A" H2SC. Benchmarks of the CCSD(T)-F12/cc-pVTZ-F12 quartic force field for the known thioformaldehyde provide anharmonic vibrational frequencies of with an average of 1.9 cm−1 of gas-phase experiment demonstrating reliability for the computed fundamental frequencies. The 1A1 H2SC form has bright spectral features in the infrared and millimeter-wave regimes, but is the highest-energy species of this set. The trans-HCSH isomer is the lowest-energy (43.69 kcal/mol or 1.90 eV) isomer next to thioformaldehyde, but the slightly higher cis-HCSH isomer has greater intensities for its brightest fundamental frequencies and a larger dipole moment making it potentially more likely to be observed. These data determined here may also assist in laboratory characterization of these molecules and how their chemistry will likely progress.

J. Molec. Spectrosc., 2020, 369(111273)
DOI: 10.1016/j.jms.2020.111273
Full-text URL: https://www.sciencedirect.com/science/article/abs/pii/S0022285220300412?via

Chemical equilibrium in AGB atmospheres: successes, failures, and prospects for small molecules, clusters, and condensates

M. Agundez, J. I. Martinez, P. L. de Andres, J. Cernicharo, J. A. Martin-Gago

Chemical equilibrium has proven extremely useful to predict the chemical composition of AGB atmospheres. Here we use a recently developed code and an updated thermochemical database, including gaseous and condensed species involving 34 elements, to compute the chemical equilibrium composition of AGB atmospheres of M-, S-, and C-type stars. We include for the first time TixCy clusters, with x = 1-4 and y = 1-4, and selected larger clusters ranging up to Ti13C22, for which thermochemical data is obtained from quantum chemical calculations. We find that in general chemical equilibrium reproduces well the observed abundances of parent molecules in circumstellar envelopes of AGB stars. There are however severe discrepancies, of various orders of magnitude, for some parent molecules: HCN, CS, NH3, and SO2 in M-type stars, H2O and NH3 in S-type stars, and the hydrides H2O, NH3, SiH4, and PH3 in C-type stars. Several molecules not yet observed in AGB atmospheres, like SiC5, SiNH, SiCl, PS, HBO, and the metal-containing molecules MgS, CaS, CaOH, CaCl, CaF, ScO, ZrO, VO, FeS, CoH, and NiS, are good candidates for detection with observatories like ALMA. The first condensates predicted are carbon, TiC, and SiC in C-rich atmospheres and Al2O3 in O-rich outflows. The most probable gas-phase precursors of dust are acetylene, atomic carbon, and/or C3 for carbon dust, SiC2 and Si2C for SiC dust, and atomic Al and AlOH, AlO, and Al2O for Al2O3 dust. In the case of TiC dust, atomic Ti is probably the main supplier of titanium. However, chemical equilibrium predicts that clusters like Ti8C12 and Ti13C22 become the major reservoirs of titanium at the expense of atomic Ti in the region where condensation of TiC is expected to occur, suggesting that the assembly of large TixCy clusters could be related to the formation of the first condensation nuclei of TiC.

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Characterizing irradiated surfaces using IR spectroscopy

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Solar wind ion irradiation continuously modifies the optical properties of unprotected surfaces of airless bodies in the Solar System. This alteration induces significant biases in the interpretation of the spectral data obtained through remote sensing, and it impedes a correct estimation of the composition of the sub-surface pristine materials. However, as the alteration of the surface is a function of time, an in-depth understanding of the phenomenon may provide an original way to estimate the weathering age of a surface. Laboratory experiments show that mid- and far-IR bands are very sensitive to space weathering, as they are significantly modified upon irradiation. These bands can thus constitute a reliable proxy of the time-bound effects of irradiation on an object. We show that the detection of irradiation effects is within the reach of IR spectral resolution of the OSIRIS-REx mission and of the future James Webb Space Telescope. Our results provide a possible evidence for space weathering effects in the IR spectrum of asteroid 101955 Bennu measured by OTES/OSIRIS-REx.

2020, Icarus, Volume 345, article id. 113722.
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Full-text URL: https://www.sciencedirect.com/science/article/abs/pii/S0019103520301135?via%3Dihub

An experimental study of the surface formation of methane in interstellar molecular clouds

D. Qasim, G. Fedoseev, K.-J. Chuang, J. He, S. Ioppolo, E.F. van Dishoeck, H. Linnartz

Methane is one of the simplest stable molecules that is both abundant and widely distributed across space. Observational surveys of CH4 ice towards low- and high-mass young stellar objects showed that much of the CH4 is expected to be formed by the hydrogenation of C on dust grains, and that CH4 ice is strongly correlated with solid H2O. However, this has not been investigated under controlled laboratory conditions. Here, we successfully demonstrate with a C-atom beam implemented in an ultrahigh vacuum apparatus the formation of CH4 ice in two separate co-deposition experiments: C + H on a 10 K surface to mimic CH4 formation directly before H2O ice is formed on the dust grain, and C + H + H2O on a 10 K surface to mimic CH4 formed simultaneously with H2O ice. We confirm that CH4 can be formed by the reaction of atomic C and H, and that the CH4 formation rate is twice as high when CH4 is formed within a H2O-rich ice. This is in agreement with the observational finding that interstellar CH4 and H2O form together in the polar ice phase. The conditions that lead to interstellar CH4 (and CD4) ice formation are reported, and can be incorporated into astrochemical models to further constrain CH4 chemistry in the interstellar medium and in other regions where CH4 is inherited.

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A cryogenic ice setup to simulate carbon atom reactions in interstellar ices

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The design, implementation, and performance of a customized carbon atom beam source for the purpose of investigating solid-state reaction routes in interstellar ices in molecular clouds are discussed. The source is integrated into an existing ultrahigh vacuum setup, SURFace REaction SImulation DEvice (SURFRESIDE2), which extends this double atom (H/D, O, and N) beamline apparatus with a third atom (C) beamline to a unique system that is fully suited to explore complex organic molecule solid-state formation under representative interstellar cloud conditions. The parameter space for this system is discussed, which includes the flux of the carbon atoms hitting the ice sample, their temperature, and the potential impact of temperature on ice reactions. Much effort has been put into constraining the beam size to within the limits of the sample size with the aim to reduce carbon pollution inside the setup. How the C-atom beam performs is quantitatively studied through the example experiment, C + 18O2, and supported by computationally-derived activation barriers. The potential for this source to study the solid-state formation of interstellar complex organic molecules through C-atom reactions is discussed.

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Molecule formation in dust-poor irradiated jets I. Stationary disk winds

Tabone, B.; Godard, B.; Pineau des Forêts, G.; Cabrit, S.; van Dishoeck, E. F.

Recent ALMA observations suggest that the highest velocity part of molecular protostellar jets are launched from the dust-sublimation regions of the accretion disks (<0.3 au). However, formation and survival of molecules in inner protostellar disk winds, in the presence of a harsh FUV radiation field and the absence of dust, remain unexplored. We aim at determining if simple molecules can be synthesized and spared in fast and collimated dust-free disk winds or if a fraction of dust is necessary to explain the observed molecular abundances. This work is based on the Paris-Durham shock code designed to model irradiated environments. Fundamental properties of the dust-free chemistry are investigated from single point models. A laminar 1D disk wind model is then built using a parametric flow geometry. This model includes time-dependent chemistry and the attenuation of the radiation field by gas-phase photoprocesses. We show that a small fraction of H2 (< 1e-2), primarily formed through the H- route, can efficiently initiate molecule synthesis such as CO and SiO above TK ~ 800 K. The attenuation of the radiation field by atomic species (eg. C, Si, S) proceeds through continuum self-shielding. This process ensures efficient formation of CO, OH, SiO, H2O through neutral-neutral reactions, and the survival of these molecules. Class 0 dust-free winds with high mass-loss rates (> 2e-6 Msun/yr) are predicted to be rich in molecules if warm (TK > 800 K). The molecular content of disk winds is very sensitive to the presence of dust and a mass-fraction of surviving dust as small as 1e-5 significantly increases the H2O and SiO abundances. Chemistry of high-velocity jets is a powerful tool to probe their content in dust and uncover their launching point. Models of internal shocks are required to fully exploit the current (sub-)millimeter observations and prepare future JWST observations.

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Chemical desorption versus energy dissipation: insights from ab-initio molecular dynamics of HCO formation.

Stefano Pantaleone, Joan Enrique-Romero, Cecilia Ceccarelli, Piero Ugliengo, Nadia Balucani and Albert Rimola

Molecular clouds are the cold regions of the Milky Way where stars form. They are enriched by rather complex molecules. Many of these molecules are believed to be synthesized on the icy surfaces of the interstellar submicron-sized dust grains that permeate the Galaxy. At 10 K thermal desorption is ineffcient and, therefore, why these molecules are found in the cold gas has tantalized astronomers for years. The assumption of the current models, called chemical desorption, is that the molecule formation energy released by the chemical reaction at the grain surface is partially absorbed by the grain and the remaining one causes the ejection of the newly formed molecule into the gas. Here we report an accurate ab-initio molecular dynamics simulations aimed to study the fate of the energy released by the first reaction of the H addition chain on CO, CO + H -> HCO, occurring on a crystalline ice surface model. We show that about 90% of the HCO formation energy is injected towards the ice in the first picosecond, leaving HCO with an energy content (10-15 kJ mol-1) more than a factor two lower than its adsorption energy (30 kJ mol-1). As a result, in agreement with laboratory experiments, we conclude that chemical desorption is ineffcient for this specific system, namely H + CO on crystalline ice. We suspect this behavior to be quite general when dealing with hydrogen bonds, which are responsible of both the cohesive energy of the ice mantle and the interaction with adsorbates, as the HCO radical, even though ad hoc simulations are needed to draw specific conclusions on other systems.

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Detection of deuterated molecules, but not of lithium hydride, in the z=0.89 absorber toward PKS1830-211

Muller, S.; Roueff, E.; Black, J. H.; Gerin, M.; Guelin, M.; Menten, K. M.; Henkel, C.; Aalto, S.; Combes, F.; Martin, S.; Marti-Vidal, I.

Deuterium and lithium are light elements of high cosmological and astrophysical importance. In this work we report the first detection of deuterated molecules and a search for lithium hydride, 7LiH, at redshift z=0.89 in the spiral galaxy intercepting the line of sight to the quasar PKS1830-211. We used ALMA to observe several submillimeter lines of ND, NH2D, and HDO, and their related isotopomers NH2, NH3, and H2^18O, in absorption against the southwest image of the quasar, allowing us to derive XD/XH abundance ratios. The absorption spectra mainly consist of two distinct narrow velocity components for which we find remarkable differences. One velocity component shows XD/XH abundances that is about 10 times larger than the primordial elemental D/H ratio, and no variability of the absorption profile during the time span of our observations. [...] The second component has XD/XH abundances that are 100 times larger than the primordial D/H ratio, a deepening of the absorption by a factor of two within a few months, and a rich chemical composition, with relative enhancements of N2H+, CH3OH, SO2, and complex organic molecules. We therefore speculate that this component is associated with the analog of a Galactic dark cloud, while the first component is likely more diffuse. Our search for the 7LiH (1--0) line was unsuccessful and we derive an upper limit 7LiH/H2 = 4 x 10^-13 (3sigma) in the z=0.89 absorber toward PKS1830-211. Besides, with ALMA archival data, we could not confirm the previous tentative detections of this line in the z=0.68 absorber toward B0218+357; we derive an upper limit 7LiH/H2 = 5 x 10^-11 (3sigma), although this is less constraining than our limit toward PKS1830-211. We conclude that, as in the Milky Way, only a tiny fraction of lithium nuclei are possibly bound in LiH in these absorbers at intermediate redshift.

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Modelling thermochemical processes in protoplanetary disks I: numerical methods

T. Grassi, B. Ercolano, L. Szűcs, J. Jennings, G. Picogna

The dispersal phase of planet-forming disks via winds driven by irradiation from the central star and/or magnetic fields in the disk itself is likely to play an important role in the formation and evolution of planetary systems. Current theoretical models lack predictive power to adequately constrain observations. We present PRIZMO, a code for evolving thermochemistry in protoplanetary disks capable of being coupled with hydrodynamical and multi-frequency radiative transfer codes. We describe the main features of the code, including gas and surface chemistry, photochemistry, microphysics, and the main cooling and heating processes. The results of a suite of benchmarks, which include photon-dominated regions, slabs illuminated by radiation spectra that include X-ray, and well-established cooling functions evaluated at different temperatures show good agreement both in terms of chemical and thermal structures. The development of this code is an important step to perform quantitative spectroscopy of disk winds, and ultimately the calculation of line profiles, which is urgently needed to shed light on the nature of observed disk winds.

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Unusually High CO Abundance of the First Active Interstellar Comet

Cordiner, M. A., Milam, S. N., Biver, N., Bockelée-Morvan, D., Roth, N. X., Bergin, E. A., Jehin, E., Remijan, A. J., Charnley, S. B., Mumma, M. J., Boissier, J., Crovisier, J., Paganini, L., Kuan, Y.-J., Lis, D. C

Comets spend most of their lives at large distances from any star, during which time their interior compositions remain relatively unaltered. Cometary observations can therefore provide direct insight into the chemistry that occurred during their birth at the time of planet formation. To-date, there have been no confirmed observations of parent volatiles (gases released directly from the nucleus) of a comet from any planetary system other than our own. Here we present high-resolution, interferometric observations of 2I/Borisov, the first confirmed interstellar comet, obtained using the Atacama Large Millimeter/submillimeter Array (ALMA) on 15th-16th December 2019. Our observations reveal emission from hydrogen cyanide (HCN), and carbon monoxide (CO), coincident with the expected position of 2I/Borisov's nucleus, with production rates Q(HCN)=(7.0±1.1)×10^23 s^−1 and Q(CO)=(4.4±0.7)×10^26 s^−1. While the HCN abundance relative to water (0.06-0.16%) appears similar to that of typical, previously observed comets in our Solar System, the abundance of CO (35-105%) is among the highest observed in any comet within 2 au of the Sun. This shows that 2I/Borisov must have formed in a relatively CO-rich environment - probably beyond the CO ice-line in the very cold, outer regions of a distant protoplanetary accretion disk, as part of a population of small, icy bodies analogous to our Solar System's own proto-Kuiper Belt.

Nature Astronomy
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CAB: Towards the RNA-world in the interstellar medium – detection of urea, and search of 2-amino-oxazole and simple sugars

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In the past decade, Astrochemistry has witnessed an impressive increase in the number of detections of complex organic molecules. Some of these species are of prebiotic interest such as glycolaldehyde, the simplest sugar, or amino acetonitrile, a possible precursor of glycine. Recently, we have reported the detection of two new nitrogen-bearing complex organics, glycolonitrile and Z-cyanomethanimine, known to be intermediate species in the formation process of ribonucleotides within theories of a primordial ribonucleic acid (RNA)-world for the origin of life. In this paper, we present deep and high-sensitivity observations toward two of the most chemically rich sources in the Galaxy: a Giant Molecular Cloud in the center of the Milky Way (G+0.693-0.027) and a proto-Sun (IRAS16293-2422 B). Our aim is to explore whether the key precursors considered to drive the primordial RNA-world chemistry, are also found in space. Our high-sensitivity observations reveal that urea is present in G+0.693-0.027 with an abundance of about 5x10-11. This is the first detection of this prebiotic species outside a star-forming region. Urea remains undetected toward the proto-Sun IRAS16293-2422 B (upper limit to its abundance of less than 2x10-11). Other precursors of the RNA-world chemical scheme such as glycolaldehyde or cyanamide are abundant in space, but key prebiotic species such as 2- amino-oxazole, glyceraldehyde or dihydroxyacetone are not detected in either source. Future more sensitive observations targeting the brightest transitions of these species will be needed to disentangle whether these large prebiotic organics are certainly present in space.

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High-resolution rovibrational spectroscopy of c-C3H2+: The v7 C–H antisymmetric stretching band

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The antisymmetric C–H stretching fundamental of c-C3H2+ has been characterized in a cryogenic 22-pole ion trap by a novel type of action spectroscopy, in which the rovibrational excitation of c-C3H2+ is detected as a slowing down of the low-temperature reaction c-C3H2+ + H2 -> C3H3+ + H2. Ninety-one rovibrational transitions with partly resolved fine structure doublets were measured in high resolution. Supported by high-level quantum chemical calculations, spectroscopic parameters were determined by fitting the observed lines with an effective Hamiltonian for an asymmetric rotor in a doublet electronic ground state, X 2A1 , yielding a band origin at 3113.6400(3) cm−1. Based on these spectroscopic parameters, the rotational spectrum of this astronomically important molecule is predicted.

2020 J. Mol. Struct. 1214, 128023
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Full-text URL: https://www.sciencedirect.com/science/article/pii/S0022286020303483

Mechanism and kinetics of astrophysically relevant gas-phase stereoinversion in glutamic acid: A computational study

Namrata Rani, Vikas

Enantiomeric excess of amino acids observed in the meteoritic samples of carbonaceous chondrites has incited many

researchers to search for an extra-terrestrial origin of life on prebiotic Earth. However, in a non-catalytic environment, only racemic amino acids are synthesized. This computational quantum-mechanical study explores non-catalytic mechanistic pathways for stereoinversion in proteinogenic L-glutamic acid, which may be observable under gas-phase conditions of interstellar medium (ISM). The multi-step stereoinversion pathways proposed in this study are traced through a global reaction route mapping (GRRM) strategy utilizing density-functional and coupled-cluster theories. Notably, a few of the pathways are observed to proceed through simultaneous intramolecular hydrogen atom and proton transfer as well as through a proton-coupled electron transfer mechanism. The intermediates explored along the stereoinversion pathways resemble ammonium ylide and imine, the key ingredients in Strecker synthesis of amino acids. The thermodynamic and kinetic analysis of the stereoinversion pathways in different temperature regions of ISM are also carried out, predicting the streoinversion to proceed over any dissociation of intermediates and conformers of glutamic acid along the pathways. However, initial step of the pathways involves an unsurmountable energy barrier though the key step responsible for stereoinversion has a very low energy barrier and is predicted to proceeds with significant rates. The work suggests the possibility of observing stereoinversion of glutamic acid in the warmer regions of ISM.

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The case for gas-phase astrochemistry without carbon

Ryan C. Fortenberry

Most carbon in the Universe is tied up in carbon monoxide or in polycyclic aromatic hydrocarbons. Even so, a vast majority of the molecules detected in various astrophysical media contain at least one carbon atom in them. These could nearly all be classified as hydrocarbons. However, only a fraction of the atoms in the Universe heavier than helium are actually carbon. This review will explore the past astronomical detections of molecules that do not contain carbon and will discuss the present workings and future outlooks of pure, inorganic astrochemistry. Such molecules have bonding structures that are often “atypical,” have notable spectroscopic intensities, and open the door for new chemical insights. Asking novel questions can lead to novel insights, and inorganic astrochemistry provides a strong motivation for asking the most creative chemical questions.

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On the possibility of electronically excited states in stable amine anions: Dicyanoamine, cyanoethynylamine, and diethynylamine

Taylor J. Santaloci, Ryan C. Fortenberry

Of the dicyanomine anion (NCNCN-), cyanoethynylamine anion (NCNC2H-), and diethynylamine anion (HC2NC2H-), only the mixed, CsNCNC2H- anion has are large enough dipole moment to support an electronically excited state at 3.0323 eV. This quantum chemical study shows that this value lies 0.0051 eV below the electron binding energy (eBE) and may have correlation to early-onset diffuse interstellar bands. None of these three anions possess further valence excited electronic states beyond the singlet ground states, and triplet excited states are all beyond their respective eBEs.

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Announcements

PhD positions in the CHAMELEON ITN: Virtual Laboratories for Exoplanets and Planet-Forming Disks

We invite applicants to join the European Marie Sklodowska-Curie Innovative Training Network (ITN) entitled ”CHAMELEON” for two PhD positions in modelling the chemistry and grain charges in planet-forming disks. Our disk models are based on chemical rate networks that are to be expanded to include the relevant processes in the warm inner disk (ESR 8) and the size-dependent statistical charging of grains that may cause lightning in disks (ESR 7). Details about the individual projects can be found here: http://chameleon.wp.st-andrews.ac.uk/recruitment/. This European ITN will hire 15 PhD students altogether and combines the expertise from the Universities of St Andrews, Antwerp, Copenhagen, Groningen, Leuven and Edinburgh, the Netherlands Institute for Space Research and the Max-Planck Institute in Heidelberg to cover all physical, chemical, radiative and numerical aspects for modelling planetary atmospheres and planet-forming disks, including data analysis, machine learning and interpretation. Virtual laboratories play an essential role in simulating yet unexplored physico-chemical environments of the diverse exoplanet population known so far, and they are key find out whether our Solar System is unique and how life emerged.
We seek excellent students with a strong background in numerical modelling and astrochemistry. Successful candidates must hold a Masters degree or equivalent. Previous research experience on aspects of exoplanet atmospheres, planet-forming disks, analysis of astronomical spectra, and/or astrochemistry and astrobiology, scientific coding and a track record

of team work/mobility will be important criteria for the selection. For further questions please contact P. Woitke (pw31@st-andrews.ac.uk) or I. Kamp (kamp@astro.rug.nl).

PhD Fellowship at IPAG (Grenoble, FR) & MPE (Garching, GE)

We are pleased to announce the availability of one Early Stage Researchers (ESRs) position.
Thesis title: A new model of the Proto Solar Nebula: organic and molecular fractionation chemistry.
Supervisor: Prof. C. Ceccarelli (University Grenoble Alpes - IPAG)
Co-Supervisors: Prof. P. Caselli (Max Planck institute for Extraterrestrial Studies) and Dr. P. Beck (University Grenoble Alpes – IPAG) Recruitment Institutions: the first 18 months at University Grenoble Alpes, Grenoble (France); the second 18 months at Max Planck institute for Extraterrestrial Studies, Garching (Germany)
Doctoral School: University Grenoble Alpes, Grenoble (France)
Mobility: The ESR will spend the first 18 months at University Grenoble Alpes (Grenoble, France) and the second 18 months at Max Planck institute for Extraterrestrial Studies (Garching, Germany).

Eligibility: European and non-European students who have not resided or carried out their main activity (work, studies, ect.) in France for more than 12 months in the 3 years immediately before the recruitment date.

Thesis description:
The formation of the Solar System has left traces in the chemical composition of early-accreted bodies. Particularly rich in this information are the so-called small bodies: comets, asteroids, and their fragments that reach the Earth as meteorites, Interplanetary Dust Particles (IDPs), Trans-Neptunians Objects (TNOs)... Specifically, their content in complex organics as well as the so-called isotopic anomalies turns out to be an extremely useful testimony of what happened to the Solar System at its birth. The goal of the thesis is to construct a model of the early phases of the Proto Solar Nebula (PSN) based on the chemical link between the Solar System small bodies and the currently forming Solar-like planetary systems. To this end, the thesis will develop a model coupling the dynamic evolution of the first phases of the collapse with a dedicated astrochemical model to predict the evolution of organic matter and the molecular fractionation during the earliest phases the Solar System, namely up to the hot corino and the onset of disk phase. The student will include the new reactions studied by the ACO project and make use of the comparison between the model predictions and the observations obtained by ACO members to constrain the model.
The thesis is part of the ACO network, whose ultimate goal is to reconstruct the early history of the Solar System by comparing the chemical composition of presently forming Solar-like planetary systems with that of small bodies in our Solar System. The comparison will be based on the most advanced astrochemical knowledge, which will be developed by the interdisciplinary ACO team.
Requested background:
The successful applicant must have a Master’s degree in Physics or Astrophysics or Computer Science or similar by the time of enrollment and be highly motivated. Knowledge of relevant program languages and/or previous experience in astrochemistry and modeling will be appreciated.
Excellent Master's degree grades are expected as well as a high level of written and spoken English. Team work ability is essential.
Salary: The gross amount of the Research fellowship is paid as follows:
- for the first 18 months: € 2708/month (living allowance) + € 430/month (mobility allowance) = € 3138 (monthly gross amount) plus possible Family Allowance in addition to coverage of study and research relates expenses;
- for the last 18 months: € 2599/month.
Social security is fully covered.
See details on the financial aspects of Marie Sklodowska-Curie-ITN in the Guide for applicants Marie Sklodowska-Curie Actions Innovative Training Networks (ITN) 2018, published at
http://ec.europa.eu/research/participants/data/ref/h2020/other/guides_for_applicants/h2020-guide-appl-msca-itn_en.pdf.
How to apply:
Send the application in pdf format to the address aco-esr17@univ-grenoble-alpes.fr.
The application should include a letter of interest, a CV with the marks of the Master year, and at least one recommendation letter, which could also be sent separately to the same e-mail address.

Closing date for application: 2 June 2020
Selection announcement: by 15th June 2020
Expected date of recruitment: within 1 October and 1 December 2020.

Selection procedure
A short list of candidate will be selected by the 4th June. The short listed candidates will be interviewed the following week and the final selection will be announced by the 15th June.

EAS 2020 VIRTUAL meeting: Abstract Submission Reopened, deadline May 3rd

Due to the COVID-19 pandemic, the European Astronomical Society (EAS) 2020 meeting (https://eas.unige.ch/EAS2020/) will move to a virtual meeting with attendance fees of 80 EUR (50 EUR for one-day attendance).
The Abstract Portal (https://eas.unige.ch/EAS2020/abstract_submission.jsp) has been re-opened to collect new submissions both for Virtual Talk Contribution and e-posters, with deadline May 3rd and notification of acceptance by Mid May. With this, we would like to invite submissions for our Special Session "The Molecular Journey: from stars to disks" (https://eas.unige.ch/EAS2020/session.jsp?id=SS11)

AIM & SCOPE.
In this special session we will focus on the study of molecules and their isotopologues and what they can teach us about the journey of molecules in our Galaxy. The scope is to bring the community together to showcase molecular insights in the evolution of matter from old stars to the ISM and into newly formed planets, to highlight recent advances in molecular astrophysics, to design strategies to best exploit the new astronomical facilities, and to provide fertile ground for future, interdisciplinary collaborations.

TOPICS
Molecules & Stellar Ejecta
The molecular ISM & Star Formation
Molecules & Protoplanetary Disks (and exoplanets)

Limited financial support may be available for early career researchers (PhD students and postdocs). For information and/or question: a.candian@uva.nl
On behalf of the SOC
Alessandra Candian (UvA)
Annemieke Petrignani (UvA)
Marie Van de Sande (KULeuven)
Serena Viti (UCL/Leiden)
Tom Millar (QUB)
Francesco Fontani (INAF)