AstroChemical Newsletter #30

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Abstracts

Thermal desorption of formamide and methylamine from graphite and amorphous water ice surfaces

Henda Chaabouni, Stephan Diana, Thanh Nguyen, François Dulieu

Formamide (NH2CHO) and methylamine (CH3NH2) are known to be the most abundant amine-containing molecules in many astrophysical environments. The presence of these molecules in the gas phase may result from thermal desorption of interstellar ices. The aim of this work is to determine the values of the desorption energies of formamide and methylamine from analogues of interstellar dust grain surfaces and to understand their interaction with water ice. TPD experiments of formamide and methylamine ices were performed in the submonolayer and monolayer regimes on graphite (HOPG) and non-porous amorphous solid water ice surfaces at 40-240 K. The desorption energy distributions of these two molecules were calculated from TPD measurements using a set of independent Polanyi-Wigner equations. The maximum of the desorption of formamide from both graphite and ASW ice surfaces occurs at 176 K after the desorption of H2O molecules, whereas the desorption profile of methylamine depends strongly on the substrate. Solid methylamine starts to desorb below 100 K from the graphite surface. Its desorption from the water ice surface occurs after 120 K and stops during the water ice sublimation around 150 K. It continues to desorb from the graphite surface at temperatures higher than 160 K. More than 95 % of NH2CHO diffuses through the water ice surface towards the graphitic substrate and is released into the gas phase with a desorption energy distribution (7460-9380 K), which is measured with the best-fit pre-exponential factor A=10^18 s-1. However, the desorption energy distribution of methylamine from the np-ASW ice surface (3850-8420 K) is measured with the best-fit pre-exponential factor A=10^12 s-1. A fraction of solid methylamine monolayer of roughly 0.15 diffuses through the water ice surface towards the HOPG substrate. This small amount desorbs later with higher binding energies (5050-8420 K).

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Full Dimension Potential Energy Surface and Low Temperature Dynamics of the H2CO + OH -> HCO + H2O reaction

A. Zanchet, P. Del-Mazo, A. Aguado, O. Roncero, E. Jiménez, A. Canosa, M. Agúndez, and J. Cernicharo

A new method is proposed to analytically represent the potential energy surface of reactions involving polyatomic molecules capable of accurately describing long-range interactions and saddle points, needed to describe low-temperature collisions. It is based on two terms, a reactive force field term and a manybody term. The reactive force field term accurately describes the fragments, long-range interactions among them and the saddle points for reactions. The many-body term increases the desired accuracy everywhere else. This method has been applied to the OH + H2CO -> H2O + HCO reaction, giving a barrier of 27.4 meV. The simulated classical rate constants with this potential are in good agreement with recent experimental results [Ocaña et al., Astrophys. J., 2017, submitted], showing an important increase at temperatures below 100 K. The reaction mechanism is analyzed in detail here, and explains the observed behavior at low energy by the formation of long-lived collision complexes, with roaming trajectories, with a capture observed for very long impact parameters, 4100 a.u., determined by the long-range dipole–dipole interaction.

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http://pubs.rsc.org/en/Content/ArticleLanding/2018/CP/C7CP05307J#!divAbstract

Gas Phase Kinetics of the OH + CH3CH2OH Reaction at Temperatures of the Interstellar Medium (T = 21 - 107 K)

A.J. Ocaña, S. Blázquez, B. Ballesteros, A. Canosa, M. Antiñolo, J. Albaladejo, and E. Jiménez

Abstract: Ethanol, CH3CH2OH, has been unveiled in the interstellar medium (ISM) by radioastronomy and it is thought to be released into the gas phase after the warm-up phase of the grain surface, where it is formed. Once in the gas phase, it can be destroyed by different reactions with atomic and radical species, such as hydroxyl (OH) radicals. The knowledge of the rate coefficients of all these processes at temperatures of the ISM is essential in the accurate interpretation of the observed abundances. In this work, we have determined the rate coefficient for the reaction of OH with CH3CH2OH (k(T)) between 21 and 107 K by employing the pulsed and continuous CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme, which means Reaction Kinetics in a Uniform Supersonic Flow) technique. The pulsed laser photolysis technique was used for generating OH radicals, whose time evolution was monitored by laser induced fluorescence. An increase of approximately 4 times was observed for k(21 K) with respect to k(107 K). With respect to k(300 K), the OH-reactivity at 21 K is enhanced by two orders of magnitude. The obtained T-expression in the investigated temperature range is k(T) = (2.1± 0.5) 10^-11 (T/300 K)^-(0.71±0.10) cm3 molecule-1 s-1. In addition, the pressure dependence of k(T) has been investigated at several temperatures between 21 K and 90 K. No pressure dependence of k(T) was observed in the investigated ranges. This may imply that this reaction is purely bimolecular or that the high-pressure limit is reached at the lowest total pressure experimentally accessible in our system. From our results, k(T) at usual IS temperatures (˜10–100 K) is confirmed to be very fast. Typical rate coefficients can be considered to range within about 4 10^-11 cm3 molecule-1 s-1 at 100 K and around 1 10^-10 cm3 molecule-1 s-1 at 20 K. The extrapolation of k at the lowest temperatures of the dense molecular clouds of ISM is also discussed in this paper.

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Nitrogen isotope fractionation in protoplanetary disks

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Aims: The two stable isotopes of nitrogen, 14N and 15N, exhibit a range of abundance ratios both inside and outside the solar system. The elemental ratio in the solar neighborhood is 440. Recent ALMA observations showed HCN/HC15N ratios from 83 to 156 in six T Tauri and Herbig disks and a CN/C15 N ratio of 323 +/- 30 in one T Tauri star. We aim to determine the dominant mechanism responsible for these enhancements of 15N: low-temperature exchange reactions or isotope-selective photodissociation of N2. Methods: Using the thermochemical code DALI, we model the nitrogen isotope chemistry in circumstellar disks with a 2D axisymmetric geometry. Our chemical network is the first to include both fractionation mechanisms for nitrogen. The model produces abundance profiles and isotope ratios for several key N-bearing species. We study how these isotope ratios depend on various disk parameters. Results: The formation of CN and HCN is closely coupled to the vibrational excitation of H2 in the UV-irradiated surface layers of the disk. Isotope fractionation is completely dominated by isotope-selective photodissociation of N2. The column density ratio of HCN over HC15N in the disk's inner 100 au does not depend strongly on the disk mass, the flaring angle or the stellar spectrum, but it is sensitive to the grain size distribution. For larger grains, self-shielding of N2 becomes more important relative to dust extinction, leading to stronger isotope fractionation. Between disk radii of ~50 and 200 au, the models predict HCN/HC15N and CN/C15N abundance ratios consistent with observations of disks and comets. The HCN/HC15N and CN/C15N column density ratios in the models are a factor of 2-3 higher than those inferred from the ALMA observations.

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Low temperature kinetics and theoretical studies of the reaction CN + CH3NH2: a potential source of cyanamide and

methyl cyanamide in the interstellar medium

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The reaction between cyano radicals (which are ubiquitous in interstellar clouds) and methylamine (a molecule detected in various interstellar sources) has been investigated in a synergistic experimental and theoretical study. The reaction has been found to be very fast in the entire range of temperatures investigated (23–297 K) by using a CRESU apparatus coupled to pulsed laser photolysis – laser induced fluorescence. The global experimental rate coefficient is given by k(T) = (3.18 ± 0.27) x 10^-10 (T/300)^(-0.42±0.11) exp(-(15±6)/T) cm3 molec-1s-1 In addition, dedicated electronic structure calculations of the underlying potential energy surface have been performed, together with capture theory and RRKM calculations. The experimental data have been interpreted in the light of the theoretical calculations and the product branching ratio has been established. According to the present study, in the range of temperatures investigated the title reaction is an efficient interstellar route of formation of cyanamide, NH2CN, another interstellar species. The second most important channel is the one leading to methyl cyanamide, CH3NHCN (an isomer of aminoacetonitrile), via a CN/H exchange mechanism with a yield of 12% of the global reaction in the entire range of temperatures explored. For a possible inclusion in future astrochemical models we suggest, by referring to the usual expression k(T) = α (T/300)^β exp(-γ/T) the following values: α = 3.68 10^-12 cm3 molec-1 s-1, β = 1.80, γ = 7.79 K for the channel leading to NH2CN + CH3;α = 5.05 10-13 cm3 molec-1 s-1, β = 1.82, γ = 7.93 K for the channel leading to CH3NHCN + H.

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Determining the effects of clumping and porosity on the chemistry in a non-uniform AGB outflow

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(abridged) In the inner regions of AGB outflows, several molecules have been detected with abundances much higher than those predicted from thermodynamic equilibrium (TE) chemical models. The presence of the majority of these species can be explained by shock-induced non-TE chemical models, where shocks caused by the pulsating star take the chemistry out of TE in the inner region. Moreover, a non-uniform density structure has been detected in several AGB outflows. A detailed parameter study on the quantitative effects of a non-homogeneous outflow has so far not been performed. We implement a porosity formalism for treating the increased leakage of light associated with radiation transport through a clumpy, porous medium. The effects from the altered UV radiation field penetration on the chemistry, accounting also for the increased reaction rates of two-body processes in the overdense clumps, are examined. We present a parameter study of the effect of clumping and porosity on the chemistry throughout the outflow. Both the higher density within the clumps and the increased UV radiation field penetration have an important impact on the chemistry, as they both alter the chemical pathways. The increased amount of UV radiation in the inner region leads to photodissociation of parent species, releasing the otherwise deficient elements. We find an increased abundance in the inner region of all species not expected to be present assuming TE chemistry, such as HCN in O-rich outflows, H2O in C-rich outflows, and NH3 in both. Outflows whose clumps have a large overdensity and that are very porous to the interstellar UV radiation field yield abundances comparable to those observed in O- and C-rich outflows for most of the unexpected species investigated. The inner wind abundances of H2O in C-rich outflows and of NH3 in O- and C-rich outflows are however underpredicted.

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Detection of HOCO+ in the protostar IRAS 16293-2422

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The protonated form of CO2, HOCO+, is assumed to be an indirect tracer of CO2 in the millimeter/submillimeter regime since CO2 lacks a permanent dipole moment. Here, we report the detection of two rotational emission lines (4 0,4-3 0,3) and (5 0,5-4 0,4) of HOCO+ in IRAS 16293-2422. For our observations, we have used EMIR heterodyne 3 mm receiver of the IRAM 30m telescope. The observed abundance of HOCO+ is

compared with the simulations using the 3-phase NAUTILUS chemical model. Implications of the measured abundances of HOCO+ to study the chemistry of CO2 ices using JWST-MIRI and NIRSpec are discussed as well.

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Cosmic ray processing of N2-containing interstellar ice analogues at dark cloud conditions

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N2 is believed to lock considerable part of nitrogen elemental budget and, therefore, to be one of the most abundant ice constituent in cold dark clouds. This laboratory-based research utilizes high energetic processing of N2 containing interstellar ice analogues using 200 keV H+ and He+ ions that mimics cosmic ray processing of the interstellar icy grains. It aims to investigate the formation of (iso)cyanates and cyanides in the ice mantles at the conditions typical for cold dark clouds and prestellar cores. Investigation of cosmic ray processing as a chemical trigger mechanism is explained by the high stability of N2 molecules that are chemically inert in most of the atom- and radical-addition reactions and cannot be efficiently dissociated by cosmic ray induced UV-field. Two sets of experiments are performed to closer address solid-state chemistry occurring in two distinct layers of the ice formed at different stages of dark cloud evolution, i.e. `H2O-rich' and `CO-rich' ice layers. Formation of HNCO and OCN- is discussed in all of the performed experiments. Corresponding kinetic curves for HNCO and OCN- are obtained. Furthermore, a feature around 2092 cm-1 assigned to the contributions of 13CO, CN-, and HCN is analysed. The kinetic curves for the combined HCN/CN- abundance are derived. In turn, normalized formation yields are evaluated by interpolation of the obtained results to the low irradiation doses relevant to dark cloud stage. The obtained values can be used to interpret future observations towards cold dark clouds using James Webb Space Telescope.

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Hydrogenated Benzene in Circumstellar Environments: Insights into the Photostability of Super-hydrogenated PAHs

Quitián-Lara, Heidy M.; Fantuzzi, Felipe; Nascimento, Marco A. C.; Wolff, Wania; Boechat-Roberty, Heloisa M.

Polycyclic aromatic hydrocarbons (PAHs), comprised of fused benzene (C6H6) rings, emit infrared radiation (3–12 μm) due to the vibrational transitions of the C–H bonds of the aromatic rings. The 3.3 μm aromatic band is generally accompanied by the band at 3.4 μm assigned to the vibration of aliphatic C–H bonds of compounds such as PAHs with an excess of peripheral H atoms (H n –PAHs). Herein we study the stability of fully hydrogenated benzene (or cyclohexane, C6H12) under the impact of stellar radiation in the photodissociation region (PDR) of NGC 7027. Using synchrotron radiation and time-of-flight mass spectrometry, we investigated the ionization and dissociation processes at energy ranges of UV (10–200 eV) and soft X-rays (280–310 eV). Density Functional Theory (DFT) calculations were used to determine the most stable structures and the relevant low-lying isomers of singly charged C6H12 ions. Partial Ion Yield (PIY) analysis gives evidence of the higher tendency toward dissociation of cyclohexane in comparison to benzene. However, because of the high photoabsorption cross-section of benzene at the C1s resonance edge, its photodissociation and photoionization cross-sections are enhanced, leading to a higher efficiency of dissociation of benzene in the PDR of NGC 7027. We suggest that a similar effect is experienced by PAHs in X-ray photon-rich environments, which ultimately acts as an auxiliary protection mechanism of super-hydrogenated polycyclic hydrocarbons. Finally, we propose that the single photoionization of cyclohexane could enhance the abundance of branched molecules in interstellar and circumstellar media.

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Interstellar bromine abundance is consistent with cometary ices from Rosetta

N.F.W. Ligterink, M. Kama

Cometary ices are formed during star and planet formation, and their molecular and elemental makeup can be related to the early solar system via the study of inter- and protostellar material. The first cometary abundance of the halogen element bromine (Br) was recently made available by the Rosetta mission. Its abundance in protostellar gas is thus far unconstrained, however. We set out to place the first observational constraints on the interstellar gas-phase abundance of bromine (Br). We further aim to compare the protostellar Br abundance with that measured by Rosetta in the ices of comet 67P/Churyumov-Gerasimenko. Archival Herschel data of Orion KL, Sgr B2(N), and NGC 6334I are examined for the presence of HBr and HBr+ emission or absorption lines. A chemical network for modelling HBr in protostellar molecular gas is compiled to aid in the interpretation. HBr and HBr+ were not detected towards any of our targets. However, in the Orion KL Hot Core, our upper limit on HBr/H2O is a factor of ten below the ratio measured in comet 67P. This result is consistent with the chemical network prediction that HBr is not a dominant gas-phase Br carrier. Cometary HBr is likely predominantly formed in icy grain mantles which lock up nearly all elemental Br.

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Discovery of the Ubiquitous Cation NS+ in Space Confirmed by Laboratory Spectroscopy

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We report the detection in space of a new molecular species that has been characterized spectroscopically and fully identified from astrophysical data. The observations were carried out with the IRAM 30 m telescope. The molecule is ubiquitous as its J=2-1 transition has been found in cold molecular clouds, prestellar cores, and shocks. However, it is not found in the hot cores of Orion-KL and in the carbon-rich evolved star IRC+10216. Three rotational transitions in perfect harmonic relation J=2/3/5 have been identified in the prestellar core B1b. The molecule has a 1Σ electronic ground state and its J=2-1 transition presents the hyperfine structure characteristic of a molecule containing a nucleus with spin 1. A careful analysis of possible carriers shows that the best candidate is NS+. The derived rotational constant agrees within 0.3%–0.7% with ab initio calculations. NS+ was also produced in the laboratory to unambiguously validate the astrophysical assignment. The observed rotational frequencies and determined molecular constants confirm the discovery of the nitrogen sulfide cation in space. The chemistry of NS+ and related nitrogen-bearing species has been analyzed by means of a time-dependent gas-phase model. The model reproduces well the observed NS/NS+ abundance ratio, in the range 30–50, and indicates that NS+ is formed by reactions of the neutral atoms N and S with the cations SH+ and NH+, respectively.

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ALMA Astrochemical Observations of the Infrared-luminous Merger NGC 3256

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In external galaxies, molecular composition may be influenced by extreme environments such as starbursts and galaxy mergers. To study such molecular chemistry, we observed the luminous infrared galaxy and merger NGC 3256 using the Atacama Large Millimeter/submillimeter Array. We covered most of the 3 and 1.3 mm bands for a multispecies, multitransition analysis. We first analyzed intensity ratio maps of selected lines such as HCN/HCO+, which shows no enhancement at an active galactic nucleus. We then compared the chemical compositions within NGC 3256 at the two nuclei, tidal arms, and positions with influence from galactic outflows. We found the largest variation in SiO and CH3OH, species that are likely to be enhanced by shocks. Next, we compared the chemical compositions in the nuclei of NGC 3256, NGC 253, and Arp 220; these galactic nuclei have varying star formation efficiencies. Arp 220 shows higher abundances of SiO and HC3N than NGC 3256 and NGC 253. Abundances of most species do not show a strong correlation with star formation efficiencies, although the CH3CCH abundance seems to have a weak positive correlation with the star formation efficiency. Lastly, the chemistry of spiral arm positions in NGC 3256 is compared with that of W51, a Galactic molecular cloud complex in a spiral arm. We

found higher fractional abundances of shock tracers, and possibly also a higher dense gas fraction in NGC 3256 compared with W51.

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Multiple Paths of Deuterium Fractionation in Protoplanetary Disks

Aikawa, Y., Furuya, K., Hincelin, U., and Herbst, E.

We investigate deuterium chemistry coupled with the nuclear spin-state chemistry of H2 and H3+ in protoplanetary disks. Multiple paths of deuterium fractionation are found; exchange reactions with D atoms, such as HCO+ + D, are effective in addition to those with HD. In a disk model with grain sizes appropriate for dark clouds, the freeze-out of molecules is severe in the outer midplane, while the disk surface is shielded from UV radiation. Gaseous molecules, including DCO+, thus become abundant at the disk surface, which tends to make their column density distribution relatively flat. If the dust grains have grown to millimeter size, the freeze- out rate of neutral species is reduced and the abundances of gaseous molecules, including DCO+ and N2D+, are enhanced in the cold midplane. Turbulent diffusion transports D atoms and radicals at the disk surface to the midplane, and stable ice species in the midplane to the disk surface. The effects of turbulence on chemistry are thus multifold; while DCO+ and N2D+ abundances increase or decrease depending on the regions, HCN and DCN in the gas and ice are greatly reduced at the innermost radii, compared to the model without turbulence. When cosmic rays penetrate the disk, the ortho-topara ratio (OPR) of H2 is found to be thermal in the disk, except in the cold (<=10 K) midplane. We also analyze the OPR of H3+ and H2D+, as well as the main reactions of H2D+, DCO+, and N2D+, in order to analytically derive their abundances in the cold midplane.

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Tetrahedral hydrocarbon nanoparticles in space: X-ray spectra

G Bilalbegović, A Maksimović, L A Valencic

It has been proposed, or confirmed, that diamond nanoparticles exist in various environments in space: close to active galactic nuclei, in the vicinity of supernovae and pulsars, in the interior of several planets in the Solar system, in carbon planets and other exoplanets, carbon-rich stars, meteorites, in X-ray active Herbig Ae/Be stars, and in the interstellar medium. Using density functional theory methods we calculate the carbon K-edge X-ray absorption spectrum of two large tetrahedral nanodiamonds: C26H32 and C51H52. We also study and test our methods on the astrophysical molecule CH4, the smallest C-H tetrahedral structure. A possible detection of nanodiamonds from X-ray spectra by future telescopes, such as the project Arcus, is proposed. Simulated spectra of the diffuse interstellar medium using Cyg X-2 as a source show that nanodiamonds studied in this work can be detected by Arcus, a high resolution X-ray spectrometer mission selected by NASA for a Phase A concept study.

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High Spectral Resolution SOFIA/EXES Observations of C2H2 toward Orion-IRc2

Naseem Rangwala, Sean W. J. Colgan, Romane Le Gal, Kinsuk Acharyya, Xinchuan Huang, Timothy J. Lee, Eric Herbst, Curtis deWitt, Matt Richter, Adwin Boogert and Mark McKelvey

We present high spectral resolution observations from 12.96 to 13.33 microns toward Orion IRc2 using the mid-infrared spectrograph, Echelon-Cross-Echelle Spectrograph (EXES), at Stratospheric Observatory for Infrared Astronomy (SOFIA). These observations probe the physical and chemical conditions of the Orion hot core, which is sampled by a bright, compact, mid-infrared background continuum source in the region, IRc2. All 10 of the rovibrational C2H2 transitions expected in our spectral coverage are detected with high signal-to-noise ratios (S/Ns), yielding continuous coverage of the R-branch lines from J = 9–8 to J = 18–17, including both ortho and para species. Eight of these rovibrational transitions are newly reported detections. The isotopologue, 13CCH2, is clearly detected with a high S/N. This enabled a direct

measurement of the 12C/13C isotopic ratio for the Orion hot core of 14 ± 1 and an estimated maximum value of 21. We also detected several HCN rovibrational lines. The ortho and para C2H2 ladders are clearly separate, and tracing two different temperatures, 226 K and 164 K, respectively, with a non-equilibrium ortho to para ratio (OPR) of 1.7 ± 0.1. Additionally, the ortho and para V LSR values differ by about 1.8 ± 0.2 km s−1, while the mean line widths differ by 0.7 ± 0.2 km s−1, suggesting that these species are not uniformly mixed along the line of sight to IRc2. We propose that the abnormally low C2H2 OPR could be a remnant from an earlier, colder phase, before the density enhancement (now the hot core) was impacted by shocks generated from an explosive event 500 years ago.

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Chemistry of a newly detected circumbinary disk in Ophiuchus

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(Abridged) Astronomers recently started discovering exoplanets around binary systems. Therefore, understanding the formation and evolution of circumbinary disks is crucial for a complete scenario of planet formation. The aim of this paper is to present the detection of a circumbinary disk around Oph-IRS67 and analyse its structure. We present high-angular-resolution (0.4", 60 AU) observations of C17O, H13CO+, C34S, SO2, C2H and c-C3H2 molecular transitions with ALMA at 0.8 mm. The spectrally and spatially resolved maps reveal the kinematics of the circumbinary disk as well as its chemistry. Molecular abundances are estimated using RADEX. The continuum emission reveals the presence of a circumbinary disk around the two sources. This disk has a diameter of ~620 AU and is well traced by C17O and H13CO+ emission. C2H and c-C3H2 trace a higher-density region which is spatially offset from the sources (~430 AU). Finally, SO2 shows compact emission around one of the sources, Oph-IRS67 B. The molecular transitions which trace the circumbinary disk are consistent with a Keplerian profile on disk scales (< 200 AU) and an infalling profile for envelope scales (> 200 AU). The Keplerian fit leads to a mass of 2.2 Msun. Inferred CO abundances w.r.t. H2 are comparable to the canonical ISM value of 2.7e-4. This study proves the first detection of the circumbinary disk associated with Oph-IRS67. The disk is chemically differentiated from the nearby high-density region. The lack of methanol emission suggests the extended disk dominates the mass budget in the inner- most regions of the protostellar envelope, generating a flat density profile where less material is exposed to high temperatures. Thus, complex organic molecules would be associated with lower column densities. Finally, Oph-IRS67 is a promising candidate for the detection of both circumstellar disks with higher-angular-resolution observations.

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A Possible Progenitor of the Interstellar Sulfide Bond: Rovibrational Characterization of the Hydrogen Disulfide Cation HSSH+

Ryan C. Fortenberry & Joseph S. Francisco

S2H (HSS) has been observed very recently in the interstellar medium, specifically in the Horsehead nebula. The protonated form, S2H2 +, is believed to be a necessary intermediate in its creation in the gas phase in UV-irradiated regions. However, little is known about this radical cation. This work showcases that the trans-HSSH+ isomer is 0.12 eV lower in energy than the cis with a 1.05 eV upper limit to the torsional rotation barrier. Additionally, the vibrational frequencies and rotational constants for both structures are provided in full here for the first time. The cis isomer is likely the more detectable since it possesses a permanent dipole moment and has a high-intensity vibrational frequency for the antisymmetric H−S−S bend at 926 cm−1 (10.8 μm), in the heart of the mid-IR spectral range. A third isomer, H2S−S+ is also reported herein lying ~0.9 eV in energy above trans-HSSH+. This isomer could play a role in the formation of S2H since it would be kinetically favored in the reaction of sulfur cations with hydrogen sulfide. Further assessment of this third, higher-energy isomer is left for future work.

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Tracing the atomic nitrogen abundance in star-forming regions with ammonia deuteration

K. Furuya, M. V. Persson

Partitioning of elemental nitrogen in star-forming regions is not well constrained. Most nitrogen is expected to be partitioned among atomic nitrogen, molecular nitrogen (N2), and icy N-bearing molecules, such as NH3 and N2. Atomic nitrogen is not directly observable in the cold gas. In this paper, we propose an indirect way to constrain the amount of atomic nitrogen in the cold gas of star-forming clouds, via deuteration in ammonia ice, the [ND2H/NH2D]/[NH2D/NH3] ratio. Using gas-ice astrochemical simulations, we show that if atomic nitrogen remains as the primary reservoir of nitrogen during cold ice formation stages, the [ND2H/NH2D]/[NH2D/NH3] ratio is close to the statistical value of 1/3 and lower than unity, whereas if atomic nitrogen is largely converted into N-bearing molecules, the ratio should be larger than unity. Observability of ammonia isotopologues in the inner hot regions around low-mass protostars, where ammonia ice has sublimated, is also discussed. We conclude that the [ND2H/NH2D]/[NH2D/NH3] ratio can be quantified using a combination of VLA and ALMA observations with reasonable integration times, at least toward IRAS 16293-2422 where high molecular column densities are expected.

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Detection of interstellar HCS and its metastable isomer HSC: new pieces in the puzzle of sulfur chemistry

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We present the first identification in interstellar space of the thioformyl radical (HCS) and its metastable isomer HSC. These species were detected toward the molecular cloud L483 through observations carried out with the IRAM 30 m telescope in the λ3 mm band. We derive beam-averaged column densities of 7e12 cm-2 for HCS and 1.8e11 cm-2 for HSC, which translate into fractional abundances relative to H2 of 2e-10 and 6e-12, respectively. Although the amount of sulfur locked by these radicals is low, their detection allows placing interesting constraints on the chemistry of sulfur in dark clouds. Interestingly, the H2CS/HCS abundance ratio is found to be quite low, 1, in contrast with the oxygen analog case, in which the H2CO/HCO abundance ratio is around 10 in dark clouds. Moreover, the radical HCS is found to be more abundant than its oxygen analog, HCO. The metastable species HOC, the oxygen analog of HSC, has not yet been observed in space. These observational constraints are compared with the outcome of a recent model of the chemistry of sulfur in dark clouds. The model underestimates the fractional abundance of HCS by at least one order of magnitude, overestimates the H2CS/HCS abundance ratio, and does not provide an abundance prediction for the metastable isomer HSC. These observations should prompt a revision of the chemistry of sulfur in interstellar clouds.

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Announcements

Post-doctoral position in Laboratory Astrophysics at the Institut de Planétologie et d'Astrophysique de Grenoble, France

The Institut de Planétologie et d'Astrophysique de Grenoble (IPAG) in Univ. Grenoble Alpes, France invites applications for a postdoctoral research position in Laboratory Astrophysics. The appointment is initially for one year and may be extended to two more years, is funded by the French Scientific Research Center (CNRS) and is paid according to the French public service scale. 15 k€/year will be allocated to the successful candidate to carry his/her research project. IPAG is located in Grenoble (France), a lively and scenic university town. The postdoc will carry out original research related to the formation and evolution of complex organic matter in the solar system (and beyond) through the analysis by very high-resolution mass spectrometry of laboratory analogues and/or extraterrestrial samples. The postdoc will be joining the mass spectrometry group of the "planeto" team (~20 faculties, technicians, postdocs and students) and will closely work with Dr. Véronique Vuitton (PI of the research project) and with other colleagues at IPAG (F.-R. Orthous-Daunay, L. Bonal, E. Quirico),

as well as in the Paris area and the United States. The mass spectrometry group has a solid experience in Titan's atmospheric chemistry as well as in the evolution of the organic matter present in small bodies (comets, meteorites) and is currently expanding its interests to Pluto and extrasolar planets. It has also significantly contributed to several space missions (e.g. Cassini-Huygens and Rosetta). Applicants must hold a Ph.D. with a solid background in analytical chemistry and/or laboratory astrophysics and have strong interest in planetary sciences and/or geochemistry and/or astrobiology. Experience in mass spectrometry and/or liquid chromatography and/or scientific programming is an asset. Applicants should send a curriculum vitae, a list of publications, a summary of previous research (2 pages max.), research interests (1 page max.), and the names of at least two persons who can be contacted for letters of references. Applications can be sent in electronic form or regular post (documents will not be returned) to the address below by April 15, 2018. Applications will be considered until the position is filled. The preferred starting date is June 1, 2018. Applications should be sent to: Dr. Véronique Vuitton Institut de Planétologie et d'Astrophysique de Grenoble Université Grenoble Alpes - Bât OSUG A CS 40700 38058 Grenoble Cedex 9 France

II Italian Workshop on Astrochemistry: "Chemical Evolution in our Galaxy: Spectroscopy, Observations and Reactivity"

Website: http://smart.sns.it/astrochem2/ As a continuation of the first Italian Workshop on Astrochemistry, held in March 2016 at Palazzo Strozzi (Firenze), the focus of this 2 nd edition is still the synergy between astronomers and chemists to comprehend the chemical complexity and evolution in our Galaxy. The unprecedented performances offered by new observational facilities, from cm-wavelengths to the THz window, are indeed revolutionizing the census of the chemical complexity in space. Specifically, interstellar Complex Organic Molecules (iCOMs) have been observed in all the evolutionary stages leading to the formation of stars (from cold starless cores to proto-stars and proto-planetary disks). Thanks to the great advances in the modeling of gas-phase and surface chemistry through laboratory works as well as quantum chemistry calculations, we now have new tools to investigate the formation routes of iCOMs in space, building blocks of pre-biotic molecules such as amino-acids and sugars. The workshop will be focused on the topics: * Observations of interstellar complex molecules * Kinetics and molecular spectroscopy * Computational and Laboratory Reactivity * Prebiotic Chemistry It will take place in Follonica in the unique environment of a former Ilva Foundry in Follonica (a maritime town in the province of Grosseto), recently restored and with spaces destined to the Scuola Normale Superiore. The list of invited speakers list features international scientists and the language of the workshop will be English.

NASA Laboratory Astrophysics Workshop Community Input

https://docs.google.com/forms/d/e/1FAIpQLSeHSWCLgiCJRoE2VTwbM1D3gWgjJhqVKpltrQVs3GohJpKuWg/viewform?c=0&w=1 As you know, there will be a NASA Laboratory Astrophysics Workshop (LAW) in Athens, GA on April 8-11. The purpose of NASA LAW 2018 is to identify and prioritize, in a report, the critical laboratory astrophysics data needs to meet the demands of NASA's current and near-term astrophysics missions. The LAW meeting will provide a forum within which the community can present and review the current state of knowledge in laboratory astrophysics and identify challenges and opportunities for the field. For that purpose, in addition to talks and posters, there will also be break-out sessions during which participants will be able to give their inputs on the following topics: FIR/Submm, UV/Optical/Mid-IR, X-ray/EUV, Gamma-ray/Nuclear/Plasmas, Databases/Codes/Archives, and Decadal Survey Planning. We would like to get some input from you, the Lab Astro Community, to make sure what you think the science needs and priorities should be are taken into account. We would appreciate if you could please take a look at the following questions and answer as many as you can. There is also a spot to fill in other topics that you feel may be relevant.