

# AstroChemical Newsletter #5

March 2016

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

### Laboratory astrochemistry: catalytic conversion of acetylene to polycyclic aromatic hydrocarbons over SiC grains

T. Q. Zhao, Q. Li, B. S. Liu, R. K. E. Gover, P. J. Sarre and A. S.C. Cheung

Catalytic conversion reactions of acetylene on a solid SiC grain surface lead to the formation of polycyclic aromatic hydrocarbons (PAHs) and are expected to mimic chemical processes in certain astrophysical environments. Gas-phase PAHs and intermediates were detected in situ using time-of-flight mass spectrometry, and their formation was confirmed using GC-MS in a separate experiment by flowing acetylene gas through a fixed-bed reactor. Activation of acetylene correlated closely with the dangling bonds on the SiC surface which interact with and break the C–C  $\pi$  bond. The addition of acetylene to the resulting radical site forms a surface ring structure which desorbs from the surface. The results of HRTEM and TG indicate that soot and graphene formation on the SiC surface depends strongly on reaction temperature. We propose that PAHs as seen through the 'UIR' emission bands can be formed through decomposition of a graphene-like material, formed on the surface of SiC grains in carbon-rich circumstellar envelopes.

Phys. Chem. Chem. Phys., 2016, 18, 3489-3496

DOI: [10.1039/C5CP06425B](https://doi.org/10.1039/C5CP06425B)

Full-text URL: [http://www.chemistry.hku.hk/download/Chem\(201602\)share/SiCpaperAR.pdf](http://www.chemistry.hku.hk/download/Chem(201602)share/SiCpaperAR.pdf)

### Measuring the Distribution and Excitation of Cometary CH<sub>3</sub>OH Using ALMA

M. A. Cordiner, S. B. Charnley, M. J. Mumma, D. Bockelée-Morvan, N. Biver, G. Villanueva, L. Paganini, S. N. Milam, A. J. Remijan, D. C. Lis, J. Crovisier, J. Boissier, Y.-J. Kuan, I. M. Coulson

The Atacama Large Millimeter/submillimeter Array (ALMA) was used to obtain measurements of spatially and spectrally resolved CH<sub>3</sub>OH emission from comet C/2012 K1 (PanSTARRS) on 28-29 June 2014. Detection of 12-14 emission lines of CH<sub>3</sub>OH on each day permitted the derivation of spatially-resolved rotational temperature profiles (averaged along the line of sight), for the innermost 5000 km of the coma. On each day, the CH<sub>3</sub>OH distribution was centrally peaked and approximately consistent with spherically symmetric, uniform outflow. The azimuthally-averaged CH<sub>3</sub>OH rotational temperature ( $T_{rot}$ ) as a function of sky-projected nucleocentric distance ( $\rho$ ), fell by about 40 K between  $\rho=0$  and 2500 km on 28 June, whereas on 29 June,  $T_{rot}$  fell by about 50 K between  $\rho=0$  km and 1500 km. A remarkable ( $\sim 50$  K) rise in  $T_{rot}$  at  $\rho=1500$ -2500 km on 29 June was not present on 28 June. The observed variations in CH<sub>3</sub>OH rotational temperature are

interpreted primarily as a result of variations in the coma kinetic temperature due to adiabatic cooling, and heating through Solar irradiation, but collisional and radiative non-LTE excitation processes also play a role.

Accepted in *Astronomy in Focus*, Volume 1. (2016)

Full-text URL: <http://arxiv.org/pdf/1602.03488v2.pdf>

## Sulphur molecules in the circumstellar envelopes of M-type AGB stars

**T. Danilovich, E. De Beck, J. H. Black, H. Olofsson, K. Justtanont**

The sulphur compounds SO and SO<sub>2</sub> have not been widely studied in the circumstellar envelopes of asymptotic giant branch (AGB) stars. By presenting and modelling a large number of SO and SO<sub>2</sub> lines in the low mass-loss rate M-type AGB star R Dor, and modelling the available lines of those molecules in a further four M-type AGB stars, we aim to determine their circumstellar abundances and distributions. We use a detailed radiative transfer analysis based on the accelerated lambda iteration method to model circumstellar SO and SO<sub>2</sub> line emission and molecular data files for both SO and SO<sub>2</sub> that are more extensive than those previously available. Using 17 SO lines and 98 SO<sub>2</sub> lines to constrain our models for R Dor, we find an SO abundance of  $6.7 \times 10^{-6}$  and an SO<sub>2</sub> abundance of  $5 \times 10^{-6}$  with both species having high abundances close to the star. We also modelled <sup>34</sup>SO and found an abundance of  $3.1 \times 10^{-7}$ , giving an <sup>32</sup>SO/<sup>34</sup>SO ratio of 21.6. We derive similar results for the circumstellar SO and SO<sub>2</sub> abundances and their distributions for the low mass-loss rate object W Hya. For these stars, the circumstellar SO and SO<sub>2</sub> abundances are much higher than predicted by chemical models and these two species may account for all available sulphur. For the higher mass-loss rate stars, we find shell-like SO distributions with peak abundances that decrease and peak abundance radii that increase with increasing mass-loss rate. The positions of the peak SO abundance agree very well with the photodissociation radii of H<sub>2</sub>O. We find evidence that SO is most likely through the photodissociation of H<sub>2</sub>O and the subsequent reaction between S and OH. The S-bearing parent molecule appears not to be H<sub>2</sub>S. The SO<sub>2</sub> models suggest an origin close to the star for this species, also disagreeing with current chemical models.

Accepted in *Astronomy & Astrophysics*

DOI: [10.1051/0004-6361/201527943](https://doi.org/10.1051/0004-6361/201527943)

Full-text URL: <http://arxiv.org/abs/1602.00517>

## Constraints on the H<sub>2</sub>O formation mechanism in the wind of carbon-rich AGB stars

**R. Lombaert, L. Decin, P. Royer, A. de Koter, N.L.J. Cox, E. González-Alfonso, D. Neufeld, J. De Ridder, M. Agúndez, J.A.D.L. Blommaert, T. Khouri, M.A.T. Groenewegen, F. Kerschbaum, J. Cernicharo, B. Vandenbussche and C. Waelkens**

Two mechanisms have been invoked to explain warm H<sub>2</sub>O vapor formation in carbon-rich AGB stars. In the first, periodic shocks passing through the medium immediately above the stellar surface lead to H<sub>2</sub>O formation. In the second, penetration of ultraviolet interstellar radiation through a clumpy circumstellar medium leads to the formation of H<sub>2</sub>O molecules in the intermediate wind. We aim to determine the properties of H<sub>2</sub>O emission for a sample of 18 carbon-rich AGB stars and subsequently constrain which of the above mechanisms provides the most likely warm H<sub>2</sub>O formation pathway. Using far-infrared spectra taken with the PACS instrument onboard the Herschel telescope, we combined two methods to identify H<sub>2</sub>O emission trends and interpreted these in terms of theoretically expected patterns in the H<sub>2</sub>O abundance.

Through the use of line-strength ratios, we analyzed the correlation between the strength of H<sub>2</sub>O emission and the mass-loss rate of the objects, as well as the radial dependence of the H<sub>2</sub>O abundance in the circumstellar outflow per individual source. We computed a model grid to account for radiative-transfer effects in the line strengths. We detect warm H<sub>2</sub>O emission close to or inside the wind acceleration zone of all sample stars, irrespective of their stellar or circumstellar properties. The predicted H<sub>2</sub>O abundances in carbon-rich environments are in the range of 10<sup>-6</sup> up to 10<sup>-4</sup> for Miras and semiregular-a objects, and cluster around 10<sup>-6</sup> for semiregular-b objects. These predictions are up to three orders of magnitude greater than what is predicted by state-of-the-art chemical models. We find a negative correlation between the H<sub>2</sub>O/CO line-strength ratio and gas mass-loss rate for rates larger than 5 × 10<sup>-7</sup> solar mass per year, regardless of the upper-level energy of the relevant transitions. This implies that the H<sub>2</sub>O formation mechanism becomes less efficient with increasing wind density. The negative correlation breaks down for the sources of lowest mass-loss rate, the semiregular-b objects. Observational constraints suggest that pulsationally induced shocks play an important role in warm H<sub>2</sub>O formation in carbon-rich AGB stars, although photodissociation by interstellar UV photons may still contribute. Both mechanisms fail in predicting the high H<sub>2</sub>O abundances we infer in Miras and semiregular-a sources, while our results for the semiregular-b objects are inconclusive.

A&A, 2016, accepted

DOI: [10.1051/0004-6361/201527049](https://doi.org/10.1051/0004-6361/201527049)

Full-text URL: <http://arxiv.org/pdf/1601.07017v1.pdf>

## A chemical model for the interstellar medium in galaxies

**S. Bovino, T. Grassi, P. R. Capelo, D. R. G. Schleicher, R. Banerjee**

We present and test chemical models for three-dimensional hydrodynamical simulations of galaxies. We explore the effect of changing key parameters such as metallicity, radiation and non-equilibrium versus equilibrium metal cooling approximations on the transition between the gas phases in the interstellar medium. The microphysics is modelled by employing the public chemistry package KROME and the chemical networks have been tested to work in a wide range of densities and temperatures. We describe a simple H/He network following the formation of H<sub>2</sub>, and a more sophisticated network which includes metals. Photochemistry, thermal processes, and different prescriptions for the H<sub>2</sub> catalysis on dust are presented and tested within a one-zone framework. The resulting network is made publicly available on the KROME webpage. We find that employing an accurate treatment of the dust-related processes induces a faster H<sub>1</sub>-H<sub>2</sub> transition. In addition, we show when the equilibrium assumption for metal cooling holds, and how a non-equilibrium approach affects the thermal evolution of the gas and the H<sub>1</sub>-H<sub>2</sub> transition. These models can be employed in any hydrodynamical code via an interface to KROME and can be applied to different problems including isolated galaxies, cosmological simulations of galaxy formation and evolution, supernova explosions in molecular clouds, and the modelling of star-forming regions. The metal network can be used for a comparison with observational data of CII 158 μm emission both for high-redshift as well as for local galaxies.

accepted in A&A

Full-text URL: <http://arxiv.org/abs/1510.07016>

## Far-infrared study of tracers of oxygen chemistry in diffuse clouds

**H. Wiesemeyer, R. Güsten, S. Heyminck, H.W. Hübers, K.M. Menten, D.A. Neufeld, H. Richter, R. Simon, J. Stutzki, B. Winkel, F. Wyrowski**

Context. The chemistry of the diffuse interstellar medium rests upon three pillars: exothermic ion-neutral reactions ("cold chemistry"), endothermic neutral-neutral reactions with significant activation barriers ("warm chemistry"), and reactions on the surfaces of dust grains. While warm chemistry becomes important in the shocks associated with turbulent dissipation regions, the main path for the formation of interstellar OH and H<sub>2</sub>O is that of cold chemistry. Aims. The aim of this study is to observationally confirm the association of atomic oxygen with both atomic and molecular gas phases, and to understand the measured abundances of OH and OH<sup>+</sup> as a function of the available reservoir of H<sub>2</sub>. Methods. We obtained absorption spectra of the ground states of OH, OH<sup>+</sup> and OI with high-velocity resolution, with GREAT on-board SOFIA, and with the THz receiver at the APEX. We analyzed them along with ancillary spectra of HF and CH from HIFI. To deconvolve them from the hyperfine structure and to separate the blend that is due to various velocity components on the sightline, we fit model spectra consisting of an appropriate number of Gaussian profiles using a method combining simulated annealing with downhill simplex minimization. Together with HF and/or CH as a surrogate for H<sub>2</sub>, and HI λ21 cm data, the molecular hydrogen fraction  $f_{\text{NH}_2} = N(\text{H}_2)/(N(\text{H}) + 2N(\text{H}_2))$  can be determined. We then investigated abundance ratios as a function of  $f_{\text{NH}_2}$ . Results. The column density of OI is correlated at a high significance with the amount of available molecular and atomic hydrogen, with an atomic oxygen abundance of  $3e-4$  relative to H nuclei. While the velocities of the absorption features of OH and OH<sup>+</sup> are loosely correlated and reflect the spiral arm crossings on the sightline, upon closer inspection they display an anticorrespondence. The arm-to-interarm density contrast is found to be higher in OH than in OH<sup>+</sup>. While both species can coexist, with a higher abundance in OH than in OH<sup>+</sup>, the latter is found less frequently in absence of OH than the other way around, which is a direct consequence of the rapid destruction of OH<sup>+</sup> by dissociative recombination when not enough H<sub>2</sub> is available. This conjecture has been substantiated by a comparison between the OH/OH<sup>+</sup> ratio with  $f_{\text{NH}_2}$ , showing a clear correlation. The hydrogen abstraction reaction chain OH<sup>+</sup> (H<sub>2</sub>,H) H<sub>2</sub>O<sup>+</sup> (H<sub>2</sub>,H)H<sub>3</sub>O<sup>+</sup> is confirmed as the pathway for the production of OH and H<sub>2</sub>O. Our estimate of the branching ratio of the dissociative recombination of H<sub>3</sub>O<sup>+</sup> to OH and H<sub>2</sub>O is confined within the interval of 84 to 91%, which matches laboratory measurements (74 to 83%). -- A correlation between the linewidths and column densities of OH<sup>+</sup> features is found to be significant with a false-alarm probability below 5%. Such a correlation is predicted by models of interstellar MHD turbulence. For OH the same correlation is found to be insignificant because there are more narrow absorption features. Conclusions. While it is difficult to assess the contributions of warm neutral-neutral chemistry to the observed abundances, it seems fair to conclude that the predictions of cold ion-neutral chemistry match the abundance patterns we observed.

A&A, Volume 585, January 2016

DOI: [10.1051/0004-6361/201526473](https://doi.org/10.1051/0004-6361/201526473)

Full-text URL: <http://arxiv.org/pdf/1602.03472v1.pdf>

## Chemistry as a diagnostic of prestellar core geometry

A. Tritsis, K. Tassis, K. Willacy

We present a new method for assessing the intrinsic 3D shape of prestellar cores from molecular column densities. We have employed hydrodynamic simulations of contracting, isothermal cores considering three intrinsic geometries: spherical, cylindrical/filamentary and disk-like. We have coupled our hydrodynamic simulations with non-equilibrium chemistry. We find that a) when cores are observed very elongated (i.e. for aspect ratios  $\leq 0.15$ ) the intrinsic 3D geometry can be probed by their 2D molecular emission maps, since these exhibit significant qualitative

morphological differences between cylindrical and disk-like cores. Specifically, if a disk-like core is observed as a filamentary object in dust emission, then it will be observed as two parallel filaments in N<sub>2</sub>H<sup>+</sup>; b) for cores with higher aspect ratios (i.e. 0.15 ~ 0.9) we define a metric  $\Delta$  that quantifies whether a molecular column density profile is centrally peaked, depressed or flat. We have identified one molecule (CN) for which  $\Delta$  as a function of the aspect ratio probes the 3D geometry of the core; and c) for cores with almost circular projections (i.e. for aspect ratios ~ 1), we have identified three molecules (OH, CO and H<sub>2</sub>CO) that can be used to probe the intrinsic 3D shape by close inspection of their molecular column density radial profiles. We alter the temperature and the cosmic-ray ionization rate and demonstrate that our method is robust against the choice of parameters.

Accepted for publication by MNRAS

DOI: [10.1093/mnras/stw329](https://doi.org/10.1093/mnras/stw329)

Full-text URL: <http://arxiv.org/pdf/1602.03187.pdf>

## Statistical ortho-to-para ratio of water desorbed from ice at 10 kelvin

**Tetsuya Hama, Akira Kouchi, Naoki Watanabe**

The anomalously low ortho-to-para ratios (OPRs) exhibited by gaseous water in space have been used to determine the formation temperature (<50 kelvin) of ice on cold interstellar dust. This approach assumes that the OPR of water desorbed from ice is related to the ice formation temperature on the dust. However, we report that water desorbed from ice at 10 kelvin shows a statistical high-temperature OPR of 3, even when the ice is produced in situ by hydrogenation of O<sub>2</sub>, a known formation process of interstellar water. This invalidates the assumed relation between OPR and temperature. The necessary reinterpretation of the low OPRs will help elucidate the chemical history of interstellar water from molecular clouds and processes in the early solar system, including comet formation.

Science 01 Jan 2016: Vol. 351, Issue 6268, pp. 65-67

DOI: [10.1126/science.aad4026](https://doi.org/10.1126/science.aad4026)

Full-text URL: <http://science.sciencemag.org/content/351/6268/65.full>

## How chemistry influences cloud structure, star formation, and the IMF

**S. Hocuk, S. Cazaux, M. Spaans, P. Caselli**

In the earliest phases of star-forming clouds, stable molecular species, such as CO, are important coolants in the gas phase. Depletion of these molecules on dust surfaces affects the thermal balance of molecular clouds and with that their whole evolution. For the first time, we study the effect of grain surface chemistry (GSC) on star formation and its impact on the initial mass function (IMF). We follow a contracting translucent cloud in which we treat the gas-grain chemical interplay in detail, including the process of freeze-out. We perform 3d hydrodynamical simulations under three different conditions, a pure gas-phase model, a freeze-out model, and a complete chemistry model. The models display different thermal evolution during cloud collapse. The equation of state (EOS) of the gas becomes softer with CO freeze-out and the results show that at the onset of star formation, the cloud retains its evolution history such that the number of formed stars differ (by 7%) between the three models. While the stellar mass distribution results in a different IMF when we consider pure freeze-out, with the complete treatment of the GSC, the divergence from a pure gas-phase model is minimal. We find that the impact of freeze-out is balanced by the non-thermal processes; chemical and photodesorption. We also find an average filament width of 0.12 pc ( $\pm 0.03$  pc), and speculate that this may be a result from the changes in



the EOS caused by the gas-dust thermal coupling. We conclude that GSC plays a big role in the chemical composition of molecular clouds and that surface processes are needed to accurately interpret observations, however, that GSC does not have a significant impact as far as star formation and the IMF is concerned.

Accepted for publication in MNRAS

DOI: [10.1093/mnras/stv2817](https://doi.org/10.1093/mnras/stv2817)

Full-text URL: <http://arxiv.org/pdf/1511.06696v2.pdf>

## Partition functions and equilibrium constants for diatomic molecules and atoms of astrophysical interest

**Barklem, P. S. and Collet, R**

Partition functions and dissociation equilibrium constants are presented for 291 diatomic molecules for temperatures in the range from near absolute zero to 10 000 K, thus providing data for many diatomic molecules of astrophysical interest at low temperature. The calculations are based on molecular spectroscopic data from the book of Huber and Herzberg with significant improvements from the literature, especially updated data for ground states of many of the most important molecules by Irikura. Dissociation energies are collated from compilations of experimental and theoretical values. Partition functions for 284 species of atoms for all elements from H to U are also presented based on data collected at NIST. The calculated data are expected to be useful for modelling a range of low density astrophysical environments, especially star-forming regions, protoplanetary disks, the interstellar medium, and planetary and cool stellar atmospheres. The input data, which will be made available electronically, also provides a possible foundation for future improvement by the community.

Accepted in A&A

DOI: [10.1051/0004-6361/201526961](https://doi.org/10.1051/0004-6361/201526961)

Full-text URL: <http://www.aanda.org/articles/aa/pdf/forth/aa26961-15.pdf>

## Formation and recondensation of complex organic molecules during protostellar luminosity outbursts

**V. Taquet, E. Wirström, S. B. Charnley**

During the formation of stars, the accretion of the surrounding material toward the central object is thought to undergo strong luminosity outbursts, followed by long periods of relative quiescence, even at the early stages of star formation when the protostar is still embedded in a large envelope. We investigated the gas phase formation and the recondensation of the complex organic molecules (COMs) di-methyl ether and methyl formate, induced by sudden ice evaporation processes occurring during luminosity outbursts of different amplitudes in protostellar envelopes. For this purpose, we updated a gas phase chemical network forming complex organic molecules in which ammonia plays a key role. The model calculations presented here demonstrate that ion-molecule reactions alone could account for the observed presence of di-methyl ether and methyl formate in a large fraction of protostellar cores, without recourse to grain-surface chemistry, although they depend on uncertain ice abundances and gas phase reaction branching ratios. In spite of the short outburst timescales of about one hundred years, abundance ratios of the considered species with respect to methanol higher than 10 % are predicted during outbursts due to their low binding energies relative to water and methanol that delay their recondensation during the cooling. Although the current luminosity of most embedded protostars would be too low to produce these complex species in hot core regions that can be

observable with current sub-millimetric interferometers, previous luminosity outburst events would induce a formation of COMs in extended regions of protostellar envelopes with sizes increasing by up to one order of magnitude.

Accepted for publication in The Astrophysical Journal

Full-text URL: <http://arxiv.org/abs/1602.05364>

## VUV photo-processing of PAH cations: quantitative study on the ionization versus fragmentation processes

**Junfeng Zhen, Sarah Rodriguez Castillo, Christine Joblin, Giacomo Mulas, Hassan Sabbah, Alexandre Giuliani, Laurent Nahon, Serge Martin, Jean-Philippe Champeaux, Paul M. Mayer**

Interstellar polycyclic aromatic hydrocarbons (PAHs) are strongly affected by the absorption of vacuum ultraviolet (VUV) photons in the interstellar medium (ISM), yet the branching ratio between ionization and fragmentation is poorly studied. This is crucial for the stability and charge state of PAHs in the ISM in different environments, affecting in turn the chemistry, the energy balance, and the contribution of PAHs to the extinction and emission curves. We studied the interaction of PAH cations with VUV photons in the 7-20 eV range from the synchrotron SOLEIL beamline, DESIRS. We recorded by action spectroscopy the relative intensities of photo-fragmentation and photo-ionization for a set of eight PAH cations ranging in size from 14 to 24 carbon atoms, with different structures. At photon energies below  $\sim 13.6$  eV fragmentation dominates for the smaller species, while for larger species ionization is immediately competitive after the second ionization potential (IP). At higher photon energies, all species behave similarly, the ionization yield gradually increases, leveling off between 0.8 and 0.9 at  $\sim 18$  eV. Among isomers, PAH structure appears to mainly affect the fragmentation cross section, but not the ionization cross section. We also measured the second IP for all species and the third IP for two of them, all are in good agreement with theoretical ones confirming that PAH cations can be further ionized in the diffuse ISM. Determining actual PAH dication abundances in the ISM will require detailed modeling. Our measured photo-ionization yields for several PAH cations provide a necessary ingredient for such models.

Accepted for publication in The Astrophysical Journal

Full-text URL: <http://arxiv.org/pdf/1602.05015v1.pdf>

## Methanol ice VUV photo-processing: GC-MS analysis of volatile organic compounds

**N. Abou Mrad, F. Duvernay, T. Chiavassa, G. Danger**

Next to water, methanol is one of the most abundant molecules in astrophysical ices. A new experimental approach is presented here for the direct monitoring via gas chromatography coupled to mass spectrometry GC-MS of a sublimating photo-processed pure methanol ice. Unprecedentedly, in a same analysis, compelling evidences for the formation of 33 volatile organic compounds are provided. These latter are C1 to C6 products including alcohols, aldehydes, ketones, esters, ethers and carboxylic acids. Few C3 and all C4 detected compounds have been identified for the first time. Tentative detection of few C5 and C6 compounds are also presented. GC-MS allows for the first time the direct quantification of C2 to C4 photoproducts and shows that their abundances decrease with the increase of their carbon chain length. These qualitative and quantitative measurements provide important complementary results to previous experiments, and present interesting similarities with observations of sources rich in methanol.

## Rovibrationally-Resolved Photodissociation of SH<sup>+</sup>

E. C. McMillan, G. Shen, J. F. McCann, B. M. McLaughlin, P. C. Stancil

Photodissociation cross sections for the SH<sup>+</sup> radical are computed from all rovibrational (RV) levels of the ground electronic state X 3Σ<sup>-</sup> for wavelengths from threshold to 500 nm. The five electronic transitions, 2 3Σ<sup>-</sup> ← X 3Σ<sup>-</sup>, 3 3Σ<sup>-</sup> ← X 3Σ<sup>-</sup>, A 3Π ← X 3Σ<sup>-</sup>, 2 3Π ← X 3Σ<sup>-</sup>, and 3 3Π ← X 3Σ<sup>-</sup>, are treated with a fully quantum-mechanical two-state model, {i.e. no non-adiabatic coupling between excited states was included in our work.}. The photodissociation calculations incorporate adiabatic potentials and transition dipole moment functions computed in the multireference configuration interaction approach along with the Davidson correction (MRCI+Q), but adjusted to match available experimental molecular data and asymptotic atomic limits. Local thermodynamic equilibrium (LTE) photodissociation cross sections were computed which assume a Boltzmann distribution of RV levels in the X 3Σ<sup>-</sup> molecular state of the SH<sup>+</sup> cation. The LTE cross sections are presented for temperatures in the range 1000-10,000 K. Applications of the current photodissociation cross sections to interstellar gas, photon-dominated regions, and stellar atmospheres are briefly discussed.

Accepted in J Phys. B: At. Mol. Opt. Phys. for the special issue on Atomic and molecular data for astrophysics

Full-text URL: <http://arxiv.org/pdf/1602.05430v1.pdf>

## Elusive anion growth in Titan's atmosphere: Low temperature kinetics of the C<sub>3</sub>N<sup>-</sup> + HC<sub>3</sub>N reaction

J. Bourgalais, N. Jamal-Eddine, B. Joalland, M. Capron, M. Balaganesh, J.-C. Guillemin, S. D. Le Picard, A. Faure, S. Carles, L. Biennier

Ion chemistry appears to be deeply involved in the formation of heavy molecules in the upper atmosphere of Titan. These large species form the seeds of the organic aerosols responsible for the opaque haze surrounding the biggest satellite of Saturn. The chemical pathways involving individual anions remain however mostly unknown. The determination of the rates of the elementary reactions with ions and the identification of the products are essential to the progress in our understanding of Titan's upper atmosphere. We have taken steps in that direction through the investigation of the low temperature reactivity of C<sub>3</sub>N<sup>-</sup>, which was tentatively identified in the spectra measured by the CAPS-ELS instrument of the Cassini spacecraft during its high altitude flybys. The reaction of this anion with HC<sub>3</sub>N, one of the most abundant trace organics in the atmosphere, has been studied over the 49–294 K temperature range in uniform supersonic flows using the CRESU technique. The proton transfer is found to be the main exit channel (> 91%) of the C<sub>3</sub>N<sup>-</sup> + HC<sub>3</sub>N reaction. It remains however indistinguishable with the non-isotopically labeled C<sub>3</sub><sup>15</sup>N<sup>-</sup> reactant. The T<sup>-1/2</sup> temperature dependence of this proton transfer reaction and its global rate are reasonably well reproduced theoretically using an average dipole orientation model. A minor exit channel, reactive detachment (< 9%), has also been uncovered, although the nature of the neutral products has not been determined. It is concluded that the C<sub>3</sub><sup>14</sup>N<sup>-</sup> + HC<sub>3</sub>N reaction cannot contribute to the growth of molecular anions in the upper atmosphere of Titan. Due to the low branching into the neutral exit channel, it cannot contribute



either to the growth of neutrals even assuming a complete mass transfer.

Icarus 271 (2016) 194–201

DOI: [10.1016/j.icarus.2016.02.003](https://doi.org/10.1016/j.icarus.2016.02.003)

Full-text URL: <http://www.sciencedirect.com/science/article/pii/S0019103516000622>

## Exploiting single photon vacuum ultraviolet photoionization to unravel the synthesis of complex organic molecules in interstellar ices

Matthew J. Abplanalp , Marko Förstel , Ralf I. Kaiser

Complex organic molecules (COM) such as aldehydes, ketones, carboxylic acids, esters, and amides are ubiquitous in the interstellar medium, but traditional gas phase astrochemical models cannot explain their formation routes. By systematically exploiting on line and in situ vacuum ultraviolet photoionization coupled with reflectron time of flight mass spectrometry (PI-ReTOF-MS) and combining these data with infrared spectroscopy (FTIR), we reveal that complex organic molecules can be synthesized within interstellar ices that are condensed on interstellar grains via non-equilibrium reactions involving suprathermal hydrogen atoms at temperatures as low as 5 K. By probing for the first time specific structural isomers without their degradation (fragment-free), the incorporation of tunable vacuum ultraviolet photoionization allows for a much greater understanding of reaction mechanisms that exist in interstellar ices compared to traditional methods, thus eliminating the significant gap between observational and laboratory data that existed for the last decades. With the commission of the Atacama Large Millimeter/Submillimeter Array (ALMA), the number of detections of more complex organic molecules in space will continue to grow – including biorelevant molecules connected to the Origins of Life theme – and an understanding of these data will rely on future advances in sophisticated physical chemistry laboratory experiments.

Chemical Physics Letters, Volume 644, 16 January 2016, Pages 79–98

DOI: [10.1016/j.cplett.2015.11.029](https://doi.org/10.1016/j.cplett.2015.11.029)

Full-text URL: <http://www.sciencedirect.com/science/article/pii/S0009261415008805>

## Ultra-low-temperature Reactions of Carbon Atoms With Hydrogen Molecules

S. A. Krasnokutski, M. Kuhn, M. Renzler, C. Jäger, Th. Henning, and P. Scheier

The reactions of carbon atoms with dihydrogen have been investigated in liquid helium droplets at  $T = 0.37$  K. A calorimetric technique was applied to monitor the energy released in the reaction. The barrierless reaction between a single carbon atom and a single dihydrogen molecule was detected. Reactions between dihydrogen clusters and carbon atoms have been studied by high-resolution mass spectrometry. The formation of hydrocarbon cations of the type  $C_mH_n^+$  with  $m = 1-4$  and  $n = 1-15$  was observed. With enhanced concentration of dihydrogen, the mass spectra demonstrated the main "magic" peak assigned to the  $CH_5^+$  cation. A simple formation pathway and the high stability of this cation suggest its high abundance in the interstellar medium.

2016 ApJL, 818, L31

DOI: [10.3847/2041-8205/818/2/L31](https://doi.org/10.3847/2041-8205/818/2/L31)

Full-text URL: <http://iopscience.iop.org/article/10.3847/2041-8205/818/2/L31/pdf>

# Announcements

## 2016 Annual Laboratory Astrophysics Division of the AAS Meeting

2016 Annual Laboratory Astrophysics Division of the AAS Meeting San Diego, CA June 13-16, 2016 <http://lad.aas.org/meetings/lad2016> Key dates: Last day for Early Registration: February 22nd, 2016 (Today!) Regular Registration: March 3, 2016 Abstracts: March 3, 2016 The 2016 LAD meeting will be devoted to the interplay between laboratory astrophysics and other fields in astronomy, planetary science and related sciences. The meeting will be held jointly with the 228th Meeting of the AAS, and feature the inaugural 2015 Laboratory Astrophysics Prize talk by Lou Allamandola, a talk by the 2016 Laboratory Astrophysics Prize winner Peter Beiersdorfer, and a talk by the inaugural LAD Early Career Prize Winner Francois Lique. The sessions will cover the full range of LAD topics, with special focus on interplay with observatories such as ALMA, Hitomi (nee' Astro-H — now launched!), and NuSTAR. The session titles and invited speakers are listed below; each session has room for contributed talks. A parallel 4-day long poster session, with all posters up the entire time, is also planned. We encourage you to submit.

Sessions: Bridging Laboratory & Astrophysics: Dust & Ices with ALMA & Hitomi Monday, 13 June 2014: 10:00 am-11:30 am Laboratory astrophysics is the Rosetta Stone that enables astronomers to understand and interpret the cosmos. This session will focus on the interplay between astrophysics with theoretical and experimental studies into the underlying dust and ice processes, which drive our Universe, focusing on connections to ALMA or Hitomi observations. Confirmed Speakers: • Lou Allamandola, NASA/Ames Research Center [Inaugural Laboratory Astrophysics Prize Talk] • Lia Corrales, MIT

Bridging Laboratory and Astrophysics: Molecules seen with ALMA I Monday, 13 June 2014: 2:00 pm-3:30 pm Laboratory astrophysics is the Rosetta Stone that enables astronomers to understand and interpret the cosmos. This session will focus on the interplay between astrophysics with theoretical and experimental studies into the underlying molecular processes, which drive our Universe, with special attention to connections with ALMA observations. Confirmed Speakers: • Viviana Guzman, Harvard • Paola Caseli, MPE

Bridging Laboratory and Astrophysics: Molecules seen with ALMA II Tuesday, 14 June 2014: 10:00 am-11:30 am Laboratory astrophysics is the Rosetta Stone that enables astronomers to understand and interpret the cosmos. This session will focus on the interplay between astrophysics with theoretical and experimental studies into the underlying molecular processes, which drive our Universe, with special attention to connections with ALMA observations. Confirmed Speakers: • Francois Lique, University Le Havre [Inaugural LAD Early Career Prize Talk] • Lucy Ziurys, University of Arizona

Bridging Laboratory and Astrophysics: Planetary Physics seen with ALMA and Hitomi Tuesday, 14 June 2014: 2:00pm-3:30 pm Laboratory astrophysics is the Rosetta Stone that enables astronomers to understand and interpret the cosmos. This session will focus on the interplay between astrophysics with theoretical and experimental studies into the underlying planetary science processes, which drive our Universe, with special attention to observations done with ALMA and Hitomi. Confirmed Speakers: • Martin Cordiner, NASA/Goddard Space Flight Center • Geoff Blake, CalTech

Bridging Laboratory and Astrophysics: Atomic Physics seen with Hitomi Wednesday, 15 June 2014: 10:00 am-11:30 am Laboratory astrophysics is the Rosetta Stone that enables astronomers to understand and interpret the cosmos. This session will focus on the interplay between astrophysics with theoretical and experimental studies into the underlying atomic processes, which drive our Universe, with special attention to observations done with Hitomi. Confirmed Speakers: • Peter Beiersdorfer, Lawrence Livermore National Lab [2016 Laboratory Astrophysics Prize Talk] • Renata Cumbee, University of Georgia

Bridging Laboratory and Astrophysics: Atomic, Nuclear, & Particles Physics with Hitomi and NuSTAR Wednesday, 15 June 2014: 2:00pm-3:30 pm Laboratory astrophysics is the Rosetta Stone that enables astronomers to

understand and interpret the cosmos. This session will focus on the interplay between astrophysics with theoretical and experimental studies into the underlying nuclear processes, which drive our Universe, with special attention to observations done with Hitomi and NuSTAR. Confirmed Speakers: • Javier Garcia, Harvard-Smithsonian Center for Astrophysics • Steven Boggs, UC-Berkeley Science Organizing Committee: Farid Salama, Randall Smith, Steven Federman, Paul Drake, Daniel Wolf Savin, John Black, Nancy Janet Chanover, Gianfranco Vidali, Karin Oberg, Edward Brown, Jan Cami, Oswald Siegmund --