# AstroChemical Newsletter #8

## June 2016

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# Abstracts

### Sticking of molecules on non-porous amorphous water ice

**J. He, K. Acharyya, G. Vidali**

Accurate modeling of physical and chemical processes in the interstellar medium requires detailed knowledge of how atoms and molecule adsorb on dust grains. However, the sticking coefficient, a number between 0 and 1 that measures the first step in the interaction of a particle with a surface, is usually assumed in simulations of ISM environments to be either 0.5 or 1. Here we report on the determination of the sticking coefficient of H2, D2, N2, O2, CO, CH4, and CO2 on non-porous amorphous solid water (np-ASW). The sticking coefficient was measured over a wide range of surface temperatures using a highly collimated molecular beam. We showed that the standard way of measuring the sticking coefficient---the King-Wells method---leads to the underestimation of trapping events in which there is incomplete energy accommodation of the molecule on the surface. Surface scattering experiments with the use of a pulsed molecular beam are used instead to measure the sticking coefficient. Based on the values of the measured sticking coefficient we suggest a useful general formula of the sticking coefficient as a function of grain temperature and molecule-surface binding energy. We use this formula in a simulation of ISM gas-grain chemistry to find the effect of sticking on the abundance of key molecules both on grains and in the gas-phase.

ApJ, 823, 1
DOI: 10.3847/0004-637X/823/1/56
Full-text URL: http://arxiv.org/abs/1602.06341

### Effect of multilayer ice chemistry on gas-phase deuteration in starless cores

**O. Sipilä, P. Caselli, V. Taquet**

Aims. We aim to investigate whether a multilayer ice model can be as successful as a bulk ice model in reproducing the observed abundances of various deuterated gas-phase species toward starless cores. Methods. We calculate abundances for various deuterated species as functions of time adopting fixed physical conditions. We also estimate abundance gradients by adopting a modified Bonnor-Ebert sphere as a core model. In the multilayer ice scenario, we consider desorption from one or several monolayers on the surface. Results. We find that the multilayer model predicts abundances of DCO+ and N2D+ that are about an order of magnitude lower than observed, caused by the trapping of CO and N2 into the grain mantle. As a result of the mantle trapping, deuteration efficiency in the gas phase increases and we find stronger deuterium fractionation in ammonia than what has been observed. Another distinguishing feature of the multilayer model is that D3+ becomes the main deuterated ion at high density. The bulk ice model is generally easily reconciled with observations. Conclusions. Our results underline that more theoretical and experimental work is needed to understand the composition and morphology of interstellar ices, and the desorption processes that can act on them. With the current constraints, the bulk ice model appears to be better in reproducing observations than the multilayer ice model. According to our results, the H2D+ to N2D+ abundance ratio is higher than 100 in the multilayer model, while only a few × 10 in the bulk model, and so observations of this ratio could provide information on the ice morphology in starless cores. Observations of the abundance of D3+ compared to H2D+ and D2H+ would provide additional constraints for the models.

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### Reaction rates and kinetic isotope effects of H2 + OH → H2O + H

**J. Meisner, J. Kästner**

We calculated reaction rate constants including atom tunneling of the reaction of dihydrogen with the hydroxy radical down to a temperature of 50 K. Instanton theory and canonical variational theory with microcanonical optimized multidimensional tunneling were applied using a fitted potential energy surface [J. Chen et al., J. Chem. Phys. 138, 154301 (2013)]. All possible protium/deuterium isotopologues were considered. Atom tunneling increases at about 250 K (200 K for deuterium transfer). Even at 50 K the rate constants of all isotopologues remain in the interval 4 · 10^−20 to 4 · 10^−17 cm3 s^-1, demonstrating that even deuterated versions of the title reaction are possibly relevant to astrochemical processes in molecular clouds. The transferred hydrogen atom dominates the kinetic isotope effect at all temperatures.

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DOI: 10.1063/1.4948319

Full-text URL: http://scitation.aip.org/content/aip/journal/jcp/144/17/10.1063/1.4948319

## Statistical model for the abundance of deuterated ammonia in interstellar space

**Gunnar Nyman, University of Gothenburg**

The elemental abundance of deuterium to normal hydrogen in the universe is on the order of 1e−5. A random distribution would therefore give a ratio of triply deuterated ammonia, ND3, to NH3 of 1e−15. Observations indicate an ND3 to NH3 ratio of roughly 1e−3, implying enrichment of triply deuterated ammonia by about twelve orders of magnitude. A simple model, based on the elemental abundances of N, D and H, is developed and solved analytically. At zero temperature the expressions are particularly simple. Effects of finite temperature are included through the partition functions of the isotopologues. It is found that the effect of finite temperature is modest in the temperature range 10 – 100 K. The results of the model are in good agreement with the observed abundances so local thermal equilibrium may therefore be a reasonable approximation and thus also be an explanation for the apparent enrichment of deuterated isotopologues.

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## A note on cement in asteroids

**G. Bilalbegovic**

Cement mineral tobermorite was formed in hydrothermal experiments on alternation of calcium-aluminum-rich inclusions (CAIs) in carbonaceous chondrite meteorites. Unidentified bands at 14 microns were measured for CAIs and the matrix of the Allende meteorite sample, as well as for Hektor and Agamemnon asteroids. The presence of cement nanoparticles may explain the feature at 14 microns.

Icarus 275, 249 (2016)
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Full-text URL: http://www.sciencedirect.com/science/article/pii/S0019103516300975

## Synchrotron-based valence shell photoionization of CH radical

**B. Gans, F. Holzmeier, J. Krüger, C. Falvo, A. Röder, A. Lopes, G. A. Garcia, C. Fittschen, J.-C. Loison, and C. Alcaraz**

We report the first experimental observations of X+ 1Σ+ ← X 2Π and a+ 3Π ← X 2Π single-photon ionization transitions of the CH radical performed on the DESIRS beamline at the SOLEIL synchrotron facility. The radical was produced by successive hydrogen-atom abstractions on methane by Fluorine atoms in a continuous microwave discharge flow tube. Mass-selected ion yields and photo-electron spectra were recorded as a function of photon energy using a double imaging photoelectron/photoion coincidence spectrometer. The ion yield appears to be strongly a ected by vibrational and electronic autoionizations, which allow the observation of high Rydberg states of the neutral species. The photoelectron spectra enable the rst direct determinations of the adiabatic ionization potential and the energy of the first triplet state of the cation with respect to its singlet ground state. This work also brings valuable information on the complex electronic structure of the CH radical and its cation and adds new observations to complement our understanding of Rydberg states and autoionization processes.

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DOI: 10.1063/1.4950880
Full-text URL: http://scitation.aip.org/content/aip/journal/jcp/144/20/10.1063/1.4950880

## Survey Observations of a Possible Glycine Precursor, Methanimine (CH2NH)

**Taiki Suzuki, Masatoshi Ohishi, Tomoya Hirota, Masao Saito, Liton Majumdar, Valentine Wakelam**

We conducted survey observations of a glycine precursor, methanimine or methylenimine (CH2NH), with the NRO 45 m telescope and the SMT telescope towards 12 high-mass and two low-mass star-forming regions in order to increase number of CH2NH sources and to better understand the characteristics of CH2NH sources. As a result of our survey, CH2NH was detected in eight sources, including four new sources. The estimated fractional abundances were ~10^8 in Orion KL and G10.47+0.03, while they were ~10^9 towards the other sources. Our hydrogen recombination line and past studies suggest that CH2NH-rich sources have less evolved HII regions. The less destruction rates by UV flux from the central star would be contributed to the high CH2NH abundances towards CH2NH-rich sources. Our gas-grain chemical simulations suggest that CH2NH is mostly formed in the gas-phase by neutral-neutral reactions rather than the product of thermal evaporation from the dust surfaces.

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## Exoplanetary Atmospheres—Chemistry, Formation Conditions, and Habitability

**N. Madhusudhan, M. Agúndez, J. I. Moses, Y. Hu**

Characterizing the atmospheres of extrasolar planets is the new frontier in exoplanetary science. The last two decades of exoplanet discoveries have revealed that exoplanets are very common and extremely diverse in their orbital and bulk properties. We now enter a new era as we begin to investigate the chemical diversity of exoplanets, their atmospheric and interior processes, and their formation conditions. Recent developments in the field have led to unprecedented advancements in our understanding of atmospheric chemistry of exoplanets and the implications for their formation conditions. We review these developments in the present work. We review in detail the theory of atmospheric chemistry in all classes of exoplanets discovered to date, from highly irradiated gas giants, ice giants, and super-Earths, to directly imaged giant planets at large orbital separations. We then review the observational detections of chemical species in exoplanetary atmospheres of these various types using different methods, including transit spectroscopy, Doppler spectroscopy, and direct imaging. In addition to chemical detections, we discuss the advances in determining chemical abundances in these atmospheres and how such abundances are being used to constrain exoplanetary formation conditions and migration mechanisms. Finally, we review recent theoretical work on the atmospheres of habitable exoplanets, followed by a discussion of future outlook of the field.

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## The ALMA-PILS survey: First detections of deuterated formamide and deuterated isocyanic acid in the interstellar medium

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Formamide (NH2CHO) has previously been detected in several star-forming regions and is thought to be a precursor for different prebiotic molecules. Its formation mechanism is still debated, however. Observations of formamide, related species, and their isopotologues may provide useful clues to the chemical pathways leading to their formation. The Protostellar Interferometric Line Survey (PILS) represents an unbiased, high angular resolution and sensitivity spectral survey of the low-mass protostellar binary IRAS 16293–2422 with the Atacama Large Millimeter/submillimeter Array (ALMA). For the first time, we detect the three singly deuterated forms of NH2CHO (NH2CDO, cis- and trans- NHDCHO), as well as DNCO towards the component B of this binary source. The images reveal that the different isotopologues are all present in the same region. Based on observations of the 13C isotopologues of formamide and a standard 12C/13C ratio, the deuterium fractionation is found to be similar for the three different forms with a value of about 2%. The DNCO/HNCO ratio is also comparable to the D/H ratio of formamide (~1%). These results are in agreement with the hypothesis that NH2CHO and HNCO are chemically related through grain-surface formation.

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Full-text URL: http://arxiv.org/pdf/1605.02562.pdf

## Resolving the extended atmosphere and the inner wind of Mira (o Ceti) with long ALMA baselines

**K. T. Wong, T. Kamiński, K. M. Menten, F. Wyrowski**

The prototypical Mira variable, omi Cet (Mira), has been observed as a Science Verification target in the 2014 ALMA Long Baseline Campaign with a longest baseline of 15 km. ALMA clearly resolves the images of the continuum and molecular line emission/absorption at an angular resolution of ~30 mas at 220 GHz. We image the data of the 28SiO v=0, 2 J=5-4 and H2O nu_2=1 J(Ka,Kc)=5(5,0)-6(4,3) transitions and extract spectra from various lines-of-sight towards Mira's extended atmosphere. In the course of imaging, we encountered ambiguities in the resulting images and spectra that appear to be related to the performance of the CLEAN algorithm. We resolve Mira's millimetre continuum emission and our data are consistent with a radio photosphere with a brightness temperature of 2611 +/- 51 K, in agreement with recent results obtained with the VLA. We do not confirm the existence of a compact region (<5 mas) of enhanced brightness. We derive the gas density, kinetic temperature, molecular abundance and outflow/infall velocities in Mira's extended atmosphere by modelling the SiO and H2O lines. We find that SiO-bearing gas starts to deplete beyond 4 Rstar and at a kinetic temperature of ~< 600 K. The inner dust shells are probably composed of grain types other than pure silicates. During this observation, Mira's atmosphere generally exhibited infall motion, with a shock front of velocity ~< 12 km/s outside the radio photosphere. The structures predicted by the hydrodynamical model CODEX can reproduce the observed spectra in astonishing detail; while some other models fail when confronted with the new data. Combined with radiative transfer modelling, ALMA successfully demonstrates the ability to reveal the physical conditions of the extended atmospheres and inner winds of AGB stars in unprecedented detail.

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Full-text URL: http://arxiv.org/abs/1603.03371

## The role of SiO as a tracer of past star-formation events: The case of the high-mass protocluster NGC 2264-C

**Lopez-Sepulcre, Yoshimasa Watanabe, Nami Sakai, Ryuta Furuya, Osamu Saruwatari, Satoshi Yamamoto**

NGC 2264-C is a high-mass protocluster where several star-formation events are known to have occurred. To investigate whether past protostellar activity has left a chemical imprint in this region, we mapped it in SiO(J=2-1), a shock tracer, and several other molecular lines with the Nobeyama 45 m telescope. Our observations show the presence of a complex network of protostellar outflows. The strongest SiO emission lies beyond a radius of ~0.1 pc with respect to the center of the clump, and is characterized by broad (>10 km/s) lines and abundances of ~1.4×10^-8 with respect to H2. Interestingly, SiO appears relatively depleted (χ(SiO)~4×10^-9) within this radius, despite it being affected by molecular outflow activity. We attribute this to fast condensation of SiO back onto dust grains and/or rapid gas-phase destruction of SiO, favored by the high density present in this area (>10^6 cm^−3). Finally, we identify a peripheral, narrow-line (~2 km/s-1) component, where SiO has an abundance of a few times 10^-11. After considering different options, we conclude that this weak emission may be tracing protostellar shocks from the star formation episode that preceded the current one, which have decelerated over time and eventually resulted in SiO being largely depleted/destroyed. Alternatively, a population of unresolved low-mass protostars may be responsible for the narrow SiO emission. High-angular resolution observations are necessary to distinguish between these two possibilities and thus understand the role of SiO as a chemical tracer of past star-formation episodes in massive protoclusters.

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## First detections of the key prebiotic molecule PO in star-forming regions

**V. M. Rivilla, F. Fontani, M. T. Beltrán, A. Vasyunin, P. Caselli, J. Martín-Pintado, and R. Cesaroni.**

Phosphorus is a crucial element in biochemistry, especially the P-O bond, which is key for the formation of the backbone of the deoxyribonucleic acid. So far, PO has only been detected towards the envelope of evolved stars, and never towards star-forming regions. We report the first detection of PO towards two massive star-forming regions, W51 e1/e2 and W3(OH), using data from the IRAM 30m telescope. PN has also been detected towards the two regions. The abundance ratio PO/PN is 1.8 and 3 for W51 and W3(OH), respectively. Our chemical model indicates that the two molecules are chemically related and are formed via gas-phase ion-molecule and neutral-neutral reactions during the cold collapse. The molecules freeze out onto grains at the end of the collapse and desorb during the warm-up phase once the temperature reaches ~35 K. Similar abundances of the two species are expected during a period of 5e4 yr at the early stages of the warm-up phase, when the temperature is in the range 35-90 K. The observed molecular abundances of 1e-10 are predicted by the model if a relatively high initial abundance of 5e-9 of depleted phosphorus is assumed.

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## Detection of HF toward PKS 1830–211, search for interstellar H2F+, and laboratoty study of H2F+ and H2Cl+ dissociative recombination

**K. Kawaguchi, S. Muller, J. H. Black, T. Amano, F. Matsushima, R. Fujimori, Y. Okabayahsi, H. Nagahiro, Y. Miyamoto, and J. Tang**

We report extragalactic observations of two fluorine-bearing species, hydrogen fluoride (HF) and fluoronium (H2F+), in the z = 0.89 absorber in front of the lensed blazar PKS 1830−211 with the Atacama Large Millimeter/submillimeter Array. HF was detected toward both southwest and northeast images of the blazar, with column densities >3.4 × 1e14 cm−2 and 0.18 × 1e14 cm−2, respectively. H2F+ was not detected, down to an upper limit (3σ) of 8.8 × 1e11 cm−2 and an abundance ratio of [H2F+]/[HF] $\leqslant $ 1/386. We also searched for H2F+ toward the Galactic sources NGC 6334 I and W51C, and toward Galactic center clouds with the Herschel HIFI spectrometer.6 The upper limit on the column density was derived to be 2.5 × 1e11 cm−2 in NGC 6334 I, which is 1/68 of that for H2Cl+. In constrast, the ortho transition of H2Cl+ is detected toward PKS 1830–211. To understand the small abundance of interstellar H2F+, we carried out laboratory experiments to determine the rate constants for the ion–electron recombination reaction by infrared time-resolved spectroscopy. The constants determined are k e (209 K) = $(1.1\pm 0.3)\times {10}^{-7}$ cm3 s−1 and 0.46 ± 0.05 × 1e-7 cm3 s−1 for H2F+ and H2Cl+, respectively. The difference in the dissociative recombination rates between H2F+ and H2Cl+ by a factor ~2 and the cosmic abundance ratio [F]/[Cl] ≈ 1/6 are not enough to explain the much smaller abundance of H2F+. The difference in the formation mechanism of H2F+ and H2Cl+ in interstellar space would be a major factor in the small abundance of H2F+.

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## An observational study of dust nucleation in Mira (o Ceti): I. Variable features of AlO and other Al-bearing species

**Kamiński, T.; Wong, K. T.; Schmidt, M. R.; Müller, H. S. P.; Gottlieb, C. A.; Cherchneff, I.; Menten, K. M.; Keller, D.; Brünken, S.; Winters, J. M.; Patel, N. A.**

Context: Dust is efficiently produced by cool giant stars, but the condensation of inorganic dust is poorly understood. Aims:

Identify and characterize aluminum bearing species in the circumstellar gas of Mira (o Ceti) in order to elucidate their role in the production of Al2O3 dust. Methods: Multiepoch spectral line observations at (sub-)millimeter, far-infrared, and optical wavelengths including: maps with ALMA which probe the gas distribution in the immediate vicinity of the star at ~30 mas; observations with ALMA, APEX, and Herschel in 2013-2015 for studying cycle and inter-cycle variability of the rotational lines of Al bearing molecules; optical records as far back as 1965 to examine variations in electronic transitions over time spans of days to decades; and velocity measurements and excitation analysis of the spectral features which constrain the physical parameters of the gas. Results: Three diatomic molecules AlO, AlOH, and AlH, and atomic Al I are the main observable aluminum species in Mira, although a significant fraction of aluminum might reside in other species that have not yet been identified. Strong irregular variability in the (sub-)millimeter and optical features of AlO (possibly the direct precursor of Al2O3) indicates substantial changes in the excitation conditions, or varying abundance that is likely related to shocks in the star. The inhomogeneous distribution of AlO might influence the spatial and temporal characteristics of dust production. Conclusions: We are unable to quantitatively trace aluminum depletion from the gas, but the rich observational material constrains time dependent chemical networks. Future improvements should include spectroscopic characterization of higher aluminum oxides, coordinated observations of dust and gas species at different variability phases, and tools to derive abundances in shock excited gas.

accepted to A&A
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# Announcements

### Vacancy for a post-doctoral position at the Leuven University, Belgium, in the field of laboratory experiments for astrochemical research

At the Leuven University (Belgium), we seek an excellent candidate for a post-doctoral research position ready to play a key role in the interdisciplinary ERC Consolidator Grant AEROSOL (2016–2020, PI. Prof. Leen Decin). The aim of the project is to boost our under- standing of the physics and chemistry characterizing the stellar winds around evolved stars. The project builds upon novel observations (including ALMA, Herschel, etc.), detailed the- oretical wind models, and targeted laboratory experiments (see http://fys.kuleuven.be/ ster/Projects/aerosol/aerosol). The candidate will interact closely with a team con- sisting of astrophysicists, chemists, and computational mathematicians. Specifically, we seek a post-doctoral researcher with expertise in gas-phase reaction ki- netics. The experimental research concerns the determination of rate coefficients and prod- uct distributions of elementary gas-phase reactions involving key reactive species (Si- and S-bearing species and HCCO radicals) in stellar winds for which data is currently lack- ing. Specifically, several advanced laser-spectroscopic and chemiluminescence techniques will be employed to follow photolytically-generated reactive species in real time in a novel temperature-graded reaction vessel (200−900 K) coupled with cavity-ringdown/Fourier-trans- form infrared spectroscopy to elucidate reaction product channels. In addition, we will concentrate on the construction and exploitation of a novel low-temperature Laval-nozzle apparatus with the aim to obtain the rates of the same gas-phase reactions at temperatures below 200 K. Candidates should have an interest in physical chemistry, high-resolution laser spec- troscopy, and technical experimentation. The post-doctoral researcher will collaborate with Prof. S. Carl from the Department of Chemistry, division of Quantum and Physical chem- istry. The experimental work will be carried out in the modern and fully-equipped new research laboratories of the Department of Chemistry. The group currently enjoys and en- courages further close collaboration with researches in the department employing high-level quantum chemical calculations on species related to this project. The application material should be sent by e-mail to katrijn.clemer@ster.kuleuven.be at the latest by 15 July 2016. The full job description is available here:
https://fys.kuleuven.be/ster/vacancies/AEROSOL_vacancy_2016/at_download/file

### PHD position in LERMA - Cergy, France

Title : Laboratory studies of the formation of complex organic molecules on cold interstellar surfaces; Supervisor : Pr François Dulieu ; Starting 01/10/2016: More details : https://lerma.obspm.fr/spip.php?article327