

# AstroChemical Newsletter #22

August 2017

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## Abstracts

### Thermal and energetic processing of astrophysical ice analogues rich in SO<sub>2</sub>

Z. Kanuchova, Ph. Boduch, A. Domaracka, M.E. Palumbo, H. Rothard, G. Strazzulla

Sulfur is an abundant element in the cosmos and it is thus an important contributor to astrochemistry in the interstellar medium and in the Solar System. Astronomical observations of the gas and of the solid phases in the dense interstellar/circumstellar regions have evidenced that sulfur is underabundant. The hypothesis to explain such a circumstance is that it is incorporated in some species in the solid phase (i.e. as frozen gases and/or refractory solids) and/or in the gas phase, which for different reasons have not been observed so far. Here we wish to give a contribution to the field by studying the chemistry induced by thermal and energetic processing of frozen mixtures of sulfur dioxide (one of the most abundant sulfur-bearing molecules observed so far) and water. We present the results of a series of laboratory experiments concerning thermal processing of different H<sub>2</sub>O:SO<sub>2</sub> mixtures and ion bombardment 30 keV He<sup>+</sup> of the same mixtures. We used in situ FTIR spectroscopy to investigate the induced effects. The results indicate that ionic species such as HSO<sub>3</sub><sup>-</sup>, HSO<sub>4</sub><sup>-</sup>, and S<sub>2</sub>O<sub>5</sub><sup>(2-)</sup> are easily produced. Energetic processing also produces SO<sub>3</sub> polymers and a sulfurous refractory residue. The produced ionic species exhibit spectral features in a region that, in astronomical spectra of dense molecular clouds, is dominated by strong silicate absorption. However, such a dominant feature is associated with some spectral features, some of which have not yet been identified. We suggest adding the sulfur-bearing ionic species to the list of candidates to help explain some of those features.

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### Detection of Buckminsterfullerene emission in the diffuse interstellar medium

O. Berné, N. L. J. Cox, G. Mulas, C. Joblin

Emission of fullerenes in their infrared vibrational bands has been detected in space near hot stars. The proposed attribution of the diffuse interstellar bands at 9577 and 9632 Å to electronic transitions of the buckminsterfullerene cation (i.e. C<sub>60</sub><sup>+</sup>) was recently supported by new laboratory data, confirming the presence of this species in the diffuse interstellar medium (ISM). In this letter, we present the detection, also in the diffuse ISM, of the 17.4 and 18.9 μm emission bands commonly attributed to vibrational bands of neutral C<sub>60</sub>. According to classical models that compute the charge state of large molecules in space, C<sub>60</sub> is expected to be mostly neutral in the diffuse ISM. This is in agreement with the abundances of diffuse C<sub>60</sub> we derive here from observations. We also find that C<sub>60</sub> is less abundant in the diffuse ISM than in star-forming regions, supporting the theory that C<sub>60</sub> can be formed in these regions.

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### A new study of the chemical structure of the Horsehead nebula: the influence of grain-surface chemistry

R. Le Gal, E. Herbst, G. Dufour, P. Gratier, M. Ruaud, T. Vidal, V. Wakelam

A wide variety of molecules have recently been detected in the Horsehead nebula photodissociation region (PDR) suggesting that: (i) gas-phase and grain chemistries should both contribute to the formation of organic molecules, and (ii) far-ultraviolet (FUV) photodesorption may explain the release into the gas phase of grain surface species. In order to tackle these specific problems and more generally in order to better constrain the chemical structure of these types of environments we present a study of the Horsehead nebula gas-grain chemistry. To do so we used the 1D astrochemical gas-grain code Nautilus with an appropriate physical structure computed with the Meudon PDR Code and compared our modeled outcomes with published observations and with previously modeled results when available. The use of a large set of chemical reactions coupled with the time-dependent code Nautilus allows us to reproduce most of the observations well, including those of the first detections in a PDR of the organic molecules HCOOH, CH<sub>2</sub>CO, CH<sub>3</sub>CHO and CH<sub>3</sub>CCH, which are mostly associated with hot cores. We also provide some abundance predictions for other molecules of interest. Understanding the chemistry behind the detection of these organic molecules is crucial to better constrain the environments these molecules can probe.

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### The complexity of Orion: an ALMA view. II. gGg'-Ethylene Glycol and Acetic Acid

C. Favre, L. Paganì, P. Goldsmith, E. Bergin, M. Carvajal, I. Kleiner, G. Melnick and R. Snell

We report the first detection and high angular resolution (1.8"x1.1") imaging of acetic acid (CH<sub>3</sub>COOH) and gGg'-ethylene glycol (gGg'(CH<sub>2</sub>OH)<sub>2</sub>) towards the Orion Kleinmann-Low nebula. The observations were carried out at ~1.3mm with ALMA during the Cycle 2. A notable result is that the spatial distribution of the acetic acid and ethylene glycol emission differs from that of the other O-bearing molecules within Orion-KL. Indeed, while the typical emission of O-bearing species harbors a morphology associated with a "V-shape" linking the Hot Core region to the Compact Ridge (with an extension towards the BN object), that of acetic acid and ethylene glycol mainly peaks at about 2" southwest from the hot core region (near sources l and n). We find that the measured CH<sub>3</sub>COOH:gGg'(CH<sub>2</sub>OH)<sub>2</sub> and CH<sub>3</sub>COOH:gGg'(CH<sub>2</sub>OH)<sub>2</sub> ratios differ from the ones measured towards the low-mass protostar IRAS 16293-2422 by more than one order of magnitude. Our best hypothesis to explain these findings is that CH<sub>3</sub>COOH, aGg'(CH<sub>2</sub>OH)<sub>2</sub> and gGg'(CH<sub>2</sub>OH)<sub>2</sub> are formed on the icy-surface of grains and then released into the gas-phase, via co-desorption with water, due to a bullet of matter ejected during the explosive event that occurred in the heart of the Nebula about 500-700 years ago.

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### Methanol Formation via Oxygen Insertion Chemistry in Ices

J. Bergner, K. Oberg, M. Rajappan

We present experimental constraints on the insertion of oxygen atoms into methane to form methanol in astrophysical ice analogs. In gas-phase and theoretical studies this process has previously been demonstrated to have a very low or non-existent energy barrier, but the energetics and mechanisms have not yet been characterized in the solid state. We use a deuterium UV lamp filtered by a sapphire window to selectively dissociate O<sub>2</sub> within a mixture of O<sub>2</sub>:CH<sub>4</sub> and observe efficient production of CH<sub>3</sub>OH via O(1D) insertion. CH<sub>3</sub>OH growth curves are fit with a kinetic model, and we observe no temperature dependence of the reaction rate constant at temperatures below the oxygen desorption temperature of 25K. Through an analysis of side products we determine the branching ratio of ice-phase oxygen insertion into CH<sub>4</sub>: ~65% of insertions lead to CH<sub>3</sub>OH with the remainder leading instead to H<sub>2</sub>CO formation. There is no evidence for CH<sub>3</sub> or OH radical formation, indicating that the fragmentation is not an important channel and that insertions typically lead to increased chemical complexity. CH<sub>3</sub>OH formation from O<sub>2</sub> and CH<sub>4</sub> diluted in a CO-dominated ice similarly shows no temperature dependence, consistent with expectations that insertion proceeds with a small or non-existent barrier. Oxygen insertion chemistry in ices should therefore be efficient under low-temperature ISM-like conditions, and could provide an important channel to complex organic molecule formation on grain surfaces in cold interstellar regions such as cloud cores and protoplanetary disk midplanes.

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### Detection of Interstellar HC<sub>5</sub>O in TMC-1 with the Green Bank Telescope

B. McGuire, A. Burkhardt, C. Shingledecker, S. Kalenskii, E. Herbst, A. Remijan, and M. McCarthy

We report the detection of the carbon-chain radical HC<sub>5</sub>O for the first time in the interstellar medium toward the cold core TMC-1 using the 100 m Green Bank Telescope. We observe four hyperfine components of this radical in the J = 17/2 - 15/2 rotational transition that originates from the <sup>2</sup>P fine structure level of its ground state and calculate an abundance of 1.7 x 10<sup>-10</sup>/H<sub>2</sub>, assuming an excitation temperature of T = 7 K. No indication of HC<sub>3</sub>O, HC<sub>4</sub>O, or HC<sub>6</sub>O, is found in these or archival observations of the source, while we report tentative evidence for HC<sub>7</sub>O. We compare calculated upper limits and the abundance of HC<sub>5</sub>O to predictions based on (1) the abundance trend of the analogous HcN family in TMC-1 and (2) a gas-grain chemical model. We find that the gas-grain chemical model well reproduces the observed abundance of HC<sub>5</sub>O, as well as the upper limits of HC<sub>3</sub>O, HC<sub>6</sub>O, and HC<sub>7</sub>O, but HC<sub>4</sub>O is overproduced. The prospects for astronomical detection of both shorter and longer HCnO chains are discussed.

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### Complex organics in IRAS 4A revisited with ALMA and PdBI: Striking contrast between two neighbouring protostellar cores

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We used the Atacama Large (sub-)Millimeter Array (ALMA) and the IRAM Plateau de Bure Interferometer (PdBI) to image, with an angular resolution of 0.5" (120 au) and 1" (235 au), respectively, the emission from 11 different organic molecules in the protostellar binary NGC1333 IRAS 4A. We clearly disentangled A1 and A2, the two protostellar cores present. For the first time, we were able to derive the column densities and fractional abundances simultaneously for the two objects, allowing us to analyse the chemical differences between them. Molecular emission from organic molecules is concentrated exclusively in A2 even though A1 is the strongest continuum emitter. The protostellar core A2 displays typical hot corino abundances and its deconvolved size is 70 au. In contrast, the upper limits we placed on molecular abundances for A1 are extremely low, lying about one order of magnitude below prestellar values. The difference in the amount of organic molecules present in A1

and A2 ranges between one and two orders of magnitude. Our results suggest that the optical depth of dust emission at these wavelengths is unlikely to be sufficiently high to completely hide a hot corino in A1 similar in size to that in A2. Thus, the significant contrast in molecular richness found between the two sources is most probably real. We estimate that the size of a hypothetical hot corino in A1 should be less than 12 au. Our results favour a scenario in which the protostar in A2 is either more massive and/or subject to a higher accretion rate than A1, as a result of inhomogeneous fragmentation of the parental molecular clump. This naturally explains the smaller current envelope mass in A2 with respect to A1 along with its molecular richness.

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## On the spectroscopic constants, first electronic state, vibrational frequencies, and isomerization of hydroxymethylene (HCOH<sup>+</sup>)

Riley A. Theis, Ryan C. Fortenberry

The hydroxymethylene cation (HCOH<sup>+</sup>) is believed to be chemically independent of the more stable formaldehyde cation isomer in interstellar chemistry and may likely be a precursor to methanol in chemical reaction networks. Previous work is corroborated here showing that the trans conformer of HCOH<sup>+</sup> is 3.48 kcal/mol lower than the cis on the potential energy surface. The small energy difference between the conformers and the much larger dipole moment of cis-HCOH<sup>+</sup> (2.73 D) make this conformer more likely to be observed than trans-HCOH<sup>+</sup> via telescopic rotational spectroscopy. A strong adiabatic shift is also predicted in the first electronic excitation into the 1 2A''/2 2A state out of either conformer into a C1 structure reducing the excitation wavelength from the near-ultraviolet all the way into the near-infrared. The full set of fundamental vibrational frequencies are also computed here at high-level. The 3306.0 cm<sup>-1</sup> and 3225.3 cm<sup>-1</sup> hydroxide stretches, respective of bare trans- and cis-HCOH<sup>+</sup>, are in agreement with previous theory but are significantly higher than the frequencies determined from previous experiment utilizing argon tagging techniques. This shift is likely because the proton-bound complex created with the argon tag reduces the experimental frequencies. Lower-level computations including the argon tag bring the hydroxide stretches much closer to the experimental frequencies indicating that the predicted frequencies for bare HCOH<sup>+</sup> are likely well-described.

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## SiS in the Circumstellar Envelope of IRC +10216: Maser and Quasi-thermal Emission

Y. Gong, Y., C. Henkel, J. Ott, K. M. Menten, M. R. Morris, D. Keller, M. J. Claussen, M. Grasshoff, R. Q. Mao

We present new Effelsberg 100-m, Australia Telescope Compact Array (ATCA), and Very Large Array observations of rotational SiS transitions in the circumstellar envelope (CSE) of IRC +10216. Thanks to the high angular resolution achieved by the ATCA observations, we unambiguously confirm that the molecule's J=1-0 transition exhibits maser action in this CSE, as first suggested more than 30 years ago. The maser emission's radial velocity, peaking at a local standard of rest velocity of -39.862±0.065 km/s, indicates that it arises from an almost fully accelerated shell. Monitoring observations show time variability of the SiS (1-0) maser. The two lowest-J SiS quasi-thermal emission lines trace a much more extended emitting region than previous high-J SiS observations. Their distributions show that the SiS quasi-thermal emission consists of two components: one is very compact (radius < 1.5", corresponding to < 3e15 cm), and the other extends out to a radius >11". An incomplete shell-like structure is found in the northeast, which is indicative of existing SiS shells. Clumpy structures are also revealed in this CSE. The gain of the SiS (1-0) maser (optical depths of about -5 at the blueshifted side and, assuming inversion throughout the entire line's velocity range, about -2 at the redshifted side) suggests that it is unsaturated. The SiS (1-0) maser can be explained in terms of ro-vibrational excitation caused by infrared pumping, and we propose that infrared continuum emission is the main pumping source.

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## On dust irradiation in planetary nebulae in the context of survivability of ices

Ararat Yeghikyan

A large number of molecules are observed in planetary nebulae, including simple and - the most common (H<sub>2</sub>, CO and OH), more complex (H<sub>2</sub>O, SiO, HCN, HNC, HCO<sup>+</sup>), and even the polycyclic aromatic hydrocarbons and fullerenes containing a few dozen and more atoms. Water molecules are observed, as a rule, in the young objects, in the gas phase (water "fountains" and related water masers) and solid phase (emission of crystalline ice particles). On the other hand, the results of calculations by the Cloudy computer program, given in this paper, show that the abundance of water ice in planetary nebulae, other conditions being equal, depends on the ionization rate of hydrogen, which depends in turn on the flux of energetic particles (protons and alpha particles) in the range of MeV energies and higher. Calculated water ice column densities reach values of up to 1e19-1e20 cm<sup>-2</sup> at the usual average ISM H<sub>2</sub> ionisation rate of 1e-16 s<sup>-1</sup> and sharply decrease at rates that are a thousand times larger. The possibility of an increased flux of energetic particles in planetary nebulae under conditions of the standard interacting stellar winds scenario is discussed, and it is concluded that the flux may locally exceed by 1-3 orders of magnitude that of galactic cosmic rays. This may have important implications for the chemistry of complex compounds under conditions of planetary nebulae, in particular, for models of the origin of fullerenes.

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## Helium broadened propane absorption cross sections in the far-IR

A. Wong, B. Billinghamurst, P.F. Bernath

Infrared absorption spectra for pure and He broadened propane have been recorded in the far-IR region (650-1300 cm<sup>-1</sup>) at the Canadian Light Source (CLS) facility using either the synchrotron or internal glowbar source depending on the required resolution. The measurements were made for 4 temperatures in the range 202-292 K and for 3 pressures of He broadening gas up to 100 Torr. Infrared absorption cross sections are derived from the spectra and the integrated cross sections are within 10 % of the corresponding values from the Pacific Northwest National Laboratory (PNNL) for all temperatures and pressures.

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## On the Energetics of the HCO<sup>+</sup> + C → CH<sup>+</sup> + CO Reaction and Some Astrochemical Implications

Daniel W. Savin, Roshan G. Bhaskar, Shreyas Vissapragada, and Xavier Urbain

We explore the energetics of the titular reaction, which current astrochemical databases consider open at typical dense molecular (i.e., dark) cloud conditions. As is common for reactions involving the transfer of light particles, we assume that there are no intersystem crossings of the potential energy surfaces involved. In the absence of any such crossings, we find that this reaction is endoergic and will be suppressed at dark cloud temperatures. Updating accordingly a generic astrochemical model for dark clouds changes the predicted gas-phase abundances of 224 species by greater than a factor of 2. Of these species, 43 have been observed in the interstellar medium. Our findings demonstrate the astrochemical importance of determining the role of intersystem crossings, if any, in the titular reaction.

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## The gaseous phase as a probe of the astrophysical solid phase chemistry

N. Abou Mrad, F. Duvernay, R. Isnard, T. Chiavassa and G. Danger.

In support to space missions and spectroscopic observations, laboratory experiments on ice analogs enable a better understanding of organic matter formation and evolution in astrophysical environments. Herein, we report the monitoring of the gaseous phase of processed astrophysical ice analogs to determine if the gaseous phase can elucidate chemical mechanisms and dominant reaction pathways occurring in the solid ice submitted to VUV irradiation at low temperature and subsequently warmed. Simple (CH<sub>3</sub>OH), binary (H<sub>2</sub>O:CH<sub>3</sub>OH, CH<sub>3</sub>OH:NH<sub>3</sub>) and ternary ice analogs (H<sub>2</sub>O:CH<sub>3</sub>OH:NH<sub>3</sub>) were VUV-processed and warmed. The evolution of volatile organic compounds in the gaseous phase shows a direct link between their relative abundances in the gaseous phase and the radical and thermal chemistries modifying the initial ice composition. The correlation between the gaseous and solid phases may have a crucial importance to decipher the organic composition of astrophysical objects. As an example, possible solid compositions of comet Lovejoy are suggested using abundances of organics in its comae.

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## Adsorption of Water, Methanol, and Formic Acid on Fe<sub>2</sub>NiP, a Meteoritic Mineral Analogue

Danna Qasim, Logan Vlasak, Aaron Pital, Thomas Beckman, Nsamba Mutanda, and Heather Abbott-Lyon

The surface of an analogue to the meteoritic mineral schreibersite or (Fe,Ni)3P was investigated to provide insight into the interaction of the mineral surface with prebiotic molecules such as water, methanol, and formic acid. A protocol for creating synthetic metal-phosphide samples with a surface reflectivity suitable for reflection-absorption infrared spectroscopy (RAIRS) was developed and is outlined in this paper. Scanning electron microscopy coupled with energy dispersive spectroscopy revealed an average defect size less than 1 μm and evidence of subsurface phosphorus segregation. At surface temperatures between 120 and 140 K, RAIRS spectra indicate that water and formic acid interact molecularly with surface atoms, while methanol appears to dissociate into methoxy and protons upon adsorption. The observed infrared spectra provide insight into the adsorption geometries of these prebiotic molecules on synthetic schreibersite. This data suggests the importance of the schreibersite mineral surface in aqueous-phase schreibersite-mediated phosphorylation experiments that have been performed by others and strengthens the argument that schreibersite-induced chemistry could occur in astrochemical environments.

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## Cometary materials originating from interstellar ices : clues from laboratory experiments

A. Fresneau, N. Abou Mrad, L. LS d'Hendecourt, F. Duvernay, L. Flandinet, F-R Orthous-Daunay, V. Vuitton, R. Thissen, T. Chiavassa, G. Danger

We use laboratory experiments to derive information on the chemistry occurring during the evolution of astrophysical ices from dense molecular clouds to interplanetary objects. Through a new strategy that consists of coupling very high resolution mass spectrometry and infrared spectroscopy (FT-IR), we investigate the molecular content of the organic residues synthesized from different initial ice compositions. We also obtain information on the evolution of the soluble part of the residues after their over-irradiation. The results give insight into the role of water ice as a trapping and diluting agent during the chemical evolution. They also give information about the importance of the amount of ammonia in such ices, particularly regarding its competition with the carbon chemistry. All of these results allow us to build a first mapping of the evolution of soluble organic matter based on its chemical and physical history. Furthermore, our results suggest that interstellar ices should lead to organic materials enriched in heteroatoms that present similarities with cometary materials but strongly differ from meteoritic organic material, especially in their C/N ratios.

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## Uniform Supersonic Chemical Reactors: 30 Years of Astrochemical History and Future Challenges

A. Potapov, A. Canosa, E. Jiménez, and B.R. Rowe

The interstellar medium is of great interest to us as the place where stars and planets are born and from where, probably, the molecular precursors of life came to Earth. Astronomical observations, astrochemical modeling, and laboratory astrochemistry should go hand in hand to understand the chemical pathways to the formation of stars, planets, and biological molecules. We review here laboratory experiments devoted to investigations on the reaction dynamics of species of astrochemical interest at the temperatures of the interstellar medium and which were performed by using one of the most popular techniques in the field, CRESU. We discuss new technical developments and scientific ideas for CRESU, which, if realized, will bring us one step closer to understanding of the astrochemical history and the future of our universe.

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## Solid CO<sub>2</sub> in quiescent dense molecular clouds, Comparison between Spitzer and laboratory spectra

T. Suhasaria, G. A. Baratta, S. Ioppolo, H. Zacharias, and M. E. Palumbo

Carbon dioxide (CO<sub>2</sub>) is among the most abundant species detected in icy grain mantles in star forming regions. Laboratory experiments showed that CO<sub>2</sub> molecules are efficiently formed in the solid state under interstellar conditions. Solid CO<sub>2</sub> can be formed through energetic (e.g., UV photolysis, electron and ion bombardment) and non-energetic mechanisms (atom-addition reactions). We have investigated the role of low-energy cosmic-ray bombardment in the formation of solid CO<sub>2</sub> in quiescent dense molecular clouds. We performed laboratory experiments to study the formation of CO<sub>2</sub> after ion irradiation with 200 keV H<sup>+</sup> of astrophysically relevant ice mixtures. Laboratory spectra are then used to fit the profile of the CO<sub>2</sub> bending mode band observed at about 15.2 μm (660 cm<sup>-1</sup>) by the Spitzer Space Telescope in the line of sight to background sources. From a qualitative point of view, good fits to observations are obtained by considering either three or four laboratory components. However, from a quantitative point of view, a better result is obtained with four components that is when a spectrum of CO<sub>2</sub> formed after ion irradiation of CH<sub>3</sub>OH ice is added to the fitting procedure. Our results support the hypothesis that energetic processing of icy grain mantles is an efficient formation mechanism of CO<sub>2</sub> ice also in quiescent dark cloud regions and indirectly suggest the presence of CH<sub>3</sub>OH in icy grain mantles in interstellar cold regions.

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## Rate constants for the formation of SiO by radiative association

M. Cairnie, R. C. Forrey, J. F. Babb, P. C. Stancil and B. M. McLaughlin

Accurate molecular data for the low-lying states of SiO are computed and used to calculate rate constants for radiative association of Si and O. Einstein A-coefficients are also calculated for transitions between all of the bound and quasi-bound levels for each molecular state. The radiative widths are used together with elastic tunneling widths to define effective radiative association rate constants which include both direct and indirect (inverse predissociation) formation processes. The indirect process is evaluated for two kinetic models which represent limiting cases for astrophysical environments. The first case scenario assumes an equilibrium distribution of quasi-bound states and would be applicable whenever collisional and/or radiative excitation mechanisms are able to maintain the population. The second case scenario assumes that no excitation mechanisms are available which corresponds to the limit of zero radiation temperature and zero atomic density. Rate constants for SiO formation in realistic astrophysical environments would presumably lie between these two limiting cases.

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## Sulphur-bearing molecules in AGB stars I: The occurrence of hydrogen sulfide

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Through a survey of (sub-)millimetre emission lines of various sulphur-bearing molecules, we aim to determine which molecules are the primary carriers of sulphur in different types of AGB stars. In this paper, the first in a series, we investigate the occurrence of H<sub>2</sub>S in AGB circumstellar envelopes and determine its abundance, where possible. We have surveyed 20 AGB stars with a range of mass-loss rates and of different chemical types using the APEX telescope to search for rotational transition lines of five key sulphur-bearing molecules: CS, SiS, SO, SO<sub>2</sub> and H<sub>2</sub>S. Here we present our results for H<sub>2</sub>S, including detections, non-detections and detailed radiative transfer modelling of the detected lines. We compare results based on different descriptions of the molecular excitation of H<sub>2</sub>S and different abundance distributions, including those derived from chemical modelling results. We detected H<sub>2</sub>S towards five AGB stars, all of which have high mass-loss rates of  $\dot{M} \geq 5 \times 10^{-6} M_{\odot} \text{ yr}^{-1}$  and are oxygen-rich. H<sub>2</sub>S was not detected towards the carbon or S-type stars that fall in a similar mass-loss range. For the stars in our sample with detections, we find peak o-H<sub>2</sub>S abundances relative to H<sub>2</sub> between 4e-7 and 2.5e-5. Overall, we conclude that H<sub>2</sub>S can play a significant role in oxygen-rich AGB stars with higher mass-loss rates, but is unlikely to play a key role in stars of other chemical types or the lower mass-loss rate oxygen-rich stars. For two sources, V1300 Aql and GX Mon, H<sub>2</sub>S is most likely the dominant sulphur-bearing molecule in the circumstellar envelope.

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## Species-to-species rate coefficients for the H<sub>3</sub><sup>+</sup> + H<sub>2</sub> reacting system

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We study the possible influence of rotational excitation on the abundances of the H<sub>3</sub><sup>+</sup> isotopologs in physical conditions corresponding to starless cores and protostellar envelopes. For this purpose we developed a new rate coefficient set for the chemistry of the H<sub>3</sub><sup>+</sup> isotopologs, allowing for rotational excitation, using state-to-state rate coefficients from Hugo et al (2009). We find that the new so-called species-to-species model produces different results to the previously-used ground-state-to-species model at high density and toward increasing temperatures (T > 10 K); the new rates clearly decrease the deuteration of H<sub>3</sub><sup>+</sup>. For D<sub>3</sub><sup>+</sup> the difference in abundance can be an order of magnitude depending on the model. The spin-state abundance ratios of the various H<sub>3</sub><sup>+</sup> isotopologs are also affected by the consideration of excited rotational states, the inclusion of which in chemical models is very important in studies of deuteration at higher temperatures, for example in protostellar envelopes.

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## CALYPSO view of SVS 13A with PdBI: Multiple jet sources

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Aims. We wish to clarify the origin of the multiple jet features emanating from the binary protostar SVS 13A (= VLA4A/VLA4B). Methods. We used the Plateau de Bure Interferometer to map at 0.3–0.8" (~70–190 au) dust emission at 1.4 mm, CO(2–1), SiO(5–4), SO(6–5). Revised proper motions for VLA4A/4B and jet wiggling models are computed to clarify their respective contribution. Results. VLA4A shows compact dust emission suggestive of a disk < 50 au, and is the hot corino source, while CO/SiO/SO counter-parts to the small-scale H<sub>2</sub> jet originate from VLA4B and reveal the jet variable velocity structure. This jet exhibits ≈ 3" wiggling consistent with orbital motion around a yet undetected ≈ 20–30 au companion to VLA4B, or jet precession. Jet wiggling combined with velocity variability can explain the large apparent angular momentum in CO bullets. We also uncover a synchronicity between CO jet bullets and knots in the HH7–11 chain demonstrating that they trace two distinct jets. Their ≈ 300 yr twin outburst period may be triggered by close perihelion approach of VLA4A in an eccentric orbit around VLA4B. A third jet is tentatively seen at PA ≈ 0°. Conclusions. SVS13 A harbors at least 2 and possibly 3 distinct jet sources. The CO and HH7–11 jets are launched from quasi-coplanar disks, separated by 20–70 au. Their synchronous major events every 300 yr favor external triggering by close binary interactions, a scenario also invoked for FU Or outbursts.

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## Prebiotic Molecules formation through the gas-phase reaction between HNO and CH<sub>2</sub>CHOH<sub>2</sub><sup>+</sup>

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Context. Knowing how the molecules that are present in the ISM can evolve to more complex ones is an interesting topic in interstellar chemistry. The study of possible reactions between detected

species can help to understand the evolution in complexity of the interstellar matter and also allows knowing the formation of new molecules which could be candidates to be detected. We focus our attention on two molecules detected in space, vinyl alcohol (CH<sub>2</sub>CHOH) and azanone (HNO). Aims. We aim to carry out a theoretical study of the ion-molecule reaction between protonated vinyl alcohol and azanone. The viability of formation of complex organic molecules (COMs) from these reactants is expected to provide some insight into the formation of prebiotic species through gas phase reactions. Methods. The reaction of protonated vinyl alcohol with azanone has been theoretically studied by using ab initio methods. Stationary points on the potential energy surface (PES) were characterized at the second-order Moller-Plesset level in conjunction with the augcc-pVTZ (correlation-consistent polarized valence triple-zeta) basis set. In addition, the electronic energies were refined by means of single-point calculations at the CCSD(T) level (coupled cluster single and double excitation model augmented with a non-iterative treatment of triple excitations) with the same basis set. Results. From a thermodynamic point of view, twelve products, composed of carbon, oxygen, nitrogen, and hydrogen which could be precursors in the formation of more complex biological molecules, can be obtained from this reaction. Among these, we focus especially on ionized glycine and two of its isomers. The analysis of the PES shows that only formation of cis- and trans-O-protonated imine acetaldehyde, CH<sub>2</sub>NHCOH<sup>+</sup> and, CHNHCHOH<sup>+</sup>, are viable under interstellar conditions. Conclusions. The reaction of protonated vinyl alcohol with azanone can evolve in the interstellar medium to more complex organic molecules of prebiotic interest. Our results suggest that imine acetaldehyde could be a feasible candidate molecule to be searched for in space.

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## Announcements

### PhD and Post-doc positions in computational astrochemistry at the University of Stuttgart, Germany

Subject: PhD and Post-doc positions in computational astrochemistry at the University of Stuttgart, Germany. PhD and Post-Doc positions are available, funded by an ERC Consolidator grant in the group of Johannes Kaestner at the University of Stuttgart, Germany. We simulate the tunnel effect in chemistry by developing new techniques and applying them to challenging reactions in astrochemistry, but also in biochemistry and catalysis. Quantum mechanical tunneling of atoms is accurately treated by instanton theory. Simulations can monitor tunneling directly and can complement experimental approaches which detect the consequences. In cold environments, any reaction with a barrier is facilitated through tunneling, e.g. in the water formation network of the formation of complex organic molecules from CO and hydrogen. For the Postdoc position we are seeking an outstanding individual with a strong research track record, as evidenced by publications in peer-reviewed journals and presentations at workshops and conferences. Experience in the simulation of astrochemical reaction networks or the theoretical prediction of rate constants is required, additional experience with quantum chemistry is helpful. For the PhD student position, you should have a background in chemistry, physics, astronomy or a related discipline and should have a strong interest in astrochemistry and computer simulations. To fit into the team, you should be willing to collaborate with experimentalists as well as modelers and astronomers. Excellent English skills are a prerequisite. We offer the successful candidates an intellectually challenging position in the inspiring atmosphere of an interdisciplinary team connected to the SimTech cluster of excellence at the University of Stuttgart. Ample computer time is available. Advanced training in different fields and participation at international conferences are highly encouraged. If you are interested in PhD or Post-Doc positions, please send your application (CV, list of publications, certificates of relevant university degrees, contact details for references) via email to Johannes Kästner, Institute for Theoretical Chemistry, University of Stuttgart, or contact him in an informal manner. More information can be obtained from <http://www.uni-stuttgart.de/theochem/TUNNELCHEM>