

# AstroChemical Newsletter #67

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## Abstracts

### Chemical Kinetics Simulations of Ice Chemistry on Porous Versus Non-Porous Dust Grains

**Drew A. Christianson, Robin T. Garrod**

The degree of porosity in interstellar dust-grain material is poorly defined, although recent work has suggested that the grains could be highly porous. Aside from influencing the optical properties of the dust, porosity has the potential to affect the chemistry occurring on dust-grain surfaces, via increased surface area, enhanced local binding energies, and the possibility of trapping of molecules within the pores as ice mantles build up on the grains. Through computational kinetics simulations, we investigate how interstellar grain-surface chemistry and ice composition are affected by the porosity of the underlying dust-grain material. Using a simple routine, idealized three-dimensional dust-grains are constructed, atom by atom, with varying degrees of porosity. Diffusive chemistry is then simulated on these surfaces using the off-lattice microscopic Monte Carlo chemical kinetics model, MIMICK, assuming physical conditions appropriate to dark interstellar clouds. On the porous grain surface, the build-up of ice mantles, mostly composed of water, leads to the covering over of the pores, leaving empty pockets. Once the pores are completely covered, the chemical and structural behavior is similar to non-porous grains of the same size. The most prominent chemical effect of the presence of grain porosity is the trapping of molecular hydrogen, formed on the grain surfaces, within the ices and voids inside the grain pores. Trapping of H<sub>2</sub> in this way may indicate that other volatiles, such as inert gases not included in these models, could be trapped within dust-grain porous structures when ices begin to form.

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### Multi-frequency high spectral resolution observations of HCN toward the circumstellar envelope of Y CVn

**J. P. Fonfría, E. J. Montiel, J. Cernicharo, C. N. DeWitt, M. J. Richter, J. H. Lacy, T. K. Greathouse, M. Santander-García, M. Agúndez, S. Massalkhi**

High spectral resolution observations toward the low mass-loss rate C-rich, J-type AGB star Y CVn have been carried out at 7.5, 13.1 and 14.0  $\mu\text{m}$  with SOFIA/EXES and IRTF/TEXES. Around 130 HCN and H<sup>13</sup>CN lines of bands  $\nu_2$ ,  $2\nu_2$ ,  $2\nu_2-\nu_2$ ,  $3\nu_2-2\nu_2$ ,  $3\nu_2-\nu_2$ , and  $4\nu_2-2\nu_2$  have been identified involving lower levels with energies up to  $\sim 3900$  K. These lines have been complemented with the pure rotational lines  $J=1-0$  and  $3-2$  of the vibrational states up to  $2\nu_2$  acquired with the IRAM 30 m telescope, and with the continuum taken with ISO. We have analyzed the data with a ro-vibrational diagram

and a code which models the absorption and emission of the circumstellar envelope of an AGB star. The continuum is produced by the star with a small contribution from dust grains comprising warm to hot SiC and cold amorphous carbon. The HCN abundance distribution seems to be anisotropic. The ejected gas is accelerated up to the terminal velocity ( $\sim 8$  km/s) from the photosphere to  $\sim 3R^*$  but there is evidence of higher velocities ( $>9-10$  km/s) beyond this region. In the vicinity of Y CVn, the line widths are as high as  $\sim 10$  km/s, which implies a maximum turbulent velocity of 6 km/s or the existence of other physical mechanisms probably related to matter ejection that involve higher gas expansion velocities than expected. HCN is rotationally and vibrationally out of LTE throughout the whole envelope. A difference of about 1500 K in the rotational temperature at the photosphere is needed to explain the observations at 7.5 and 13-14  $\mu\text{m}$ . Our analysis finds a total HCN column density that ranges from  $\sim 2.1 \times 10^{18}$  to  $3.5 \times 10^{18}$   $\text{cm}^{-2}$ , an abundance with respect to  $\text{H}_2$  of  $3.5 \times 10^{-5}$  to  $1.3 \times 10^{-4}$ , and a  $^{12}\text{C}/^{13}\text{C}$  isotopic ratio of  $\sim 2.5$  throughout the whole envelope.

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## Linking ice and gas in the Lambda Orionis Barnard 35A cloud

**G. Perotti, J. K. Jørgensen, H. J. Fraser, A.N. Suutarinen, L. E. Kristensen, W. R. M. Rocha, P. Bjerke, K. M. Pontoppidan**

Dust grains play an important role in the synthesis of molecules in the interstellar medium, from the simplest species to complex organic molecules. How some of these solid-state molecules are converted into gas-phase species is still a matter of debate. Our aim is to directly compare ice and gas abundances of methanol ( $\text{CH}_3\text{OH}$ ) and CO, and to investigate the relationship between ice and gas in low-mass protostellar envelopes. We present Submillimeter Array and Atacama Pathfinder Experiment observations of gas-phase  $\text{CH}_3\text{OH}$  and CO towards the multiple protostellar system IRAS05417+0907 located in the B35A cloud. We use archival AKARI ice data toward the same target to calculate  $\text{CH}_3\text{OH}$  and CO gas-to-ice ratios. The CO isotopologues emissions are extended, whereas the  $\text{CH}_3\text{OH}$  emission is compact and traces the giant outflow emanating from IRAS05417+0907. A discrepancy between submillimeter dust emission and  $\text{H}_2\text{O}$  ice column density is found for B35A-4 and B35A-5, similar to what has previously been reported. B35A-2 and B35A-3 are located where the submillimeter dust emission peaks and show  $\text{H}_2\text{O}$  column densities lower than for B35A-4. The difference between the submillimeter continuum emission and the infrared  $\text{H}_2\text{O}$  ice observations suggests that the distributions of dust and  $\text{H}_2\text{O}$  ice differ around the young stellar objects in this dense cloud. The reason for this may be that the sources are located in different environments resolved by the interferometric observations: B35A-2, B35A-3 and in particular B35A-5 are situated in a shocked region plausibly affected by sputtering and heating impacting the submillimeter dust emission pattern, while B35A-4 is situated in a more quiescent part of the cloud. Gas and ice maps are essential to connect small-scale variations in the ice composition with large-scale astrophysical phenomena probed by gas observations.

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## Physics and Chemistry on the Surface of Cosmic Dust Grains: A Laboratory View

**Alexey Potapov and Martin McCoustra**

Dust grains play a central role in the physics and chemistry of cosmic environments. They influence the optical and thermal properties of the medium due to their interaction with stellar radiation; provide surfaces for the chemical reactions that are responsible for the synthesis of a significant fraction of key astronomical molecules; and they are building blocks of pebbles, comets, asteroids, planetesimals, and planets. In this paper, we review experimental studies of physical and chemical processes, such as adsorption, desorption, diffusion, and reactions forming molecules, on the surface of reliable cosmic dust grain analogues as related to processes in diffuse, translucent, and dense interstellar clouds, protostellar envelopes, planet-forming disks, and planetary atmospheres. The information that such experiments reveal should be flexible enough to be used in many different environments. In addition, we provide a forward look discussing new ideas, experimental approaches, and research directions.

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## **Chemical post-processing of magneto-hydrodynamical simulations of star-forming regions: robustness and pitfalls**

**Simón Ferrada-Chamorro, Alessandro Lupi, Stefano Bovino**

A common approach to model complex chemistry in numerical simulations is via post-processing of existing magneto-hydrodynamic simulations, relying on computing the evolution of chemistry over the dynamic history of a subset of particles from within the raw simulation. Here, we validate such a technique, assessing its ability to recover the abundances of chemical species, using the chemistry package KROME. We also assess, for the first time, the importance of the main free input parameters, by means of a direct comparison with a self-consistent state-of-the-art simulation in which chemistry was directly coupled to hydrodynamics. We have found that the post-processing is highly reliable, with an accuracy at the percent level, even when the most relaxed input parameters are employed. In particular, our results show that the number of particles used does not affect significantly the average properties, although it suppresses the appearance of possibly important spatial features. On the other hand, the choice of the integration time-step plays a crucial role. Longer integration time-steps can produce large errors, as the post-processing solution will be forced towards chemical equilibrium, a condition that does not always necessarily apply. When the interpolation-based reconstruction of chemical properties is performed, the errors further increase up to a factor of  $\sim 2$ . Concluding, our results suggest that this technique is extremely useful when exploring the relative quantitative effect of different chemical parameters and/or networks, without the need of re-running simulations multiple times, but some care should be taken in the choice of particles sub-sample and integration time-step.

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## **Detection of Interstellar H<sub>2</sub>CCCHC<sub>3</sub>N: A Link Between Chains and Rings in Cold Cores?**

**C. N. Shingledecker, K. L. K. Lee, J. T. Wandishin, N. Balucani, A. M. Burkhardt, S. B. Charnley, R. Loomis, M. Schreffler, M. Siebert, M. C. McCarthy, B. A. McGuire**

The chemical pathways linking the small organic molecules commonly observed in molecular clouds to the large, complex, polycyclic species long-suspected to be carriers of the ubiquitous unidentified infrared emission bands remain unclear. To investigate whether the formation of mono- and poly-cyclic molecules observed in cold cores could form via the bottom-up reaction of ubiquitous carbon-chain species with, e.g. atomic hydrogen, a search is made for possible intermediates in data taken as part of the GOTHAM (GBT Observations of TMC-1 Hunting for Aromatic Molecules) project. Markov-Chain Monte Carlo (MCMC) Source Models were run to obtain column densities and excitation temperatures. Astrochemical models were run to examine possible formation routes, including a novel grain-surface pathway involving the hydrogenation of C<sub>6</sub>N and HC<sub>6</sub>N, as well as purely gas-phase reactions between C<sub>3</sub>N and both propyne (CH<sub>3</sub>CCH) and allene (CH<sub>2</sub>CCH<sub>2</sub>), as well as via the reaction CN + H<sub>2</sub>CCCHCCH. We report the first detection of cyanoacetyleneallene (H<sub>2</sub>CCCHC<sub>3</sub>N) in space toward the TMC-1 cold cloud using the Robert C. Byrd 100 m Green Bank Telescope (GBT).

Cyanoacetyleneallene may represent an intermediate between less-saturated carbon-chains, such as the cyanopolyynes, that are characteristic of cold cores and the more recently-discovered cyclic species like cyanocyclopentadiene. Results from our models show that the gas-phase allene-based formation route in particular produces abundances of H<sub>2</sub>CCCHC<sub>3</sub>N that match the column density of  $2 \times 10^{11} \text{ cm}^{-2}$  obtained from the MCMC Source Model, and that the grain-surface route yields large abundances on ices that could potentially be important as precursors for cyclic molecules.

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## Millimeter-wave spectroscopy of the <sup>13</sup>CH<sub>3</sub>OD isotopic species of methyl alcohol

**L.-H. Xu, R. M. Lees, O. Zakharenko, H. S. P. Müller, F. Lewen, S. Schlemmer, K. M. Menten**

The dramatic increase in sensitivity, spectral coverage and resolution of radio astronomical facilities in recent years has opened new possibilities for observation of chemical differentiation and isotopic fractionation in protostellar sources to shed light on their spatial and temporal evolution. In warm interstellar environments, methanol is an abundant species, hence spectral data for its isotopic forms are of special interest. In the present work, the millimeter-wave spectrum of the <sup>13</sup>CH<sub>3</sub>OD isotopologue has been investigated over the region from 150–510 GHz to provide a set of transition frequencies for potential astronomical application. The focus is on two types of prominent <sup>13</sup>CH<sub>3</sub>OD spectral groupings, namely the a-type qR-branch multiplets and the b-type Q-branches. Line positions are reported for the qR(J) clusters for J=3 to 10 for the vt=0 and 1 torsional states, and for a number of vt=0 and 1 rQ(J) or pQ(J) line series up to J=25. The frequencies have been fitted to a multi-parameter torsion-rotation Hamiltonian, and upper level excitation energies have been calculated from the resulting molecular constants.

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## H<sub>2</sub> formation on interstellar grains and the fate of reaction energy

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

Molecular hydrogen is the most abundant molecular species in the Universe. While no doubts exist that it is mainly formed on the interstellar dust grain surfaces, many details of this process remain poorly known. In this work, we focus on the fate of the energy released by the H<sub>2</sub> formation on the dust icy mantles, how it is partitioned between the substrate and the newly formed H<sub>2</sub>, a process that has a profound impact on the interstellar medium. We carried out state-of-art ab-initio molecular dynamics simulations of H<sub>2</sub> formation on periodic crystalline and amorphous ice surface models. Our calculations show that up to two thirds of the energy liberated in the reaction (~300 kJ/mol ~3.1eV) is absorbed by the ice in less than 1 ps. The remaining energy (~140 kJ/mol ~1.5 eV) is kept by the newly born H<sub>2</sub>. Since it is ten times larger than the H<sub>2</sub> binding energy on the ice, the new H<sub>2</sub> molecule will eventually be released into the gas-phase. The ice water molecules within ~4 angstrom from the reaction site acquire enough energy, between 3 and 14 kJ/mol (360–1560 K), to potentially liberate other frozen H<sub>2</sub> and, perhaps, frozen CO molecules. If confirmed, the latter process would solve the long standing conundrum of the presence of gaseous CO in molecular clouds. Finally, the vibrational state of the newly formed H<sub>2</sub> drops from highly excited states ( $\nu = 6$ ) to low ( $\nu \leq 2$ ) vibrational levels in a timescale of the order of ps.

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## The vertical and adiabatic ionization energies of silicon carbide clusters, (SiC)<sub>n</sub>, with n=1-12

**D. Gobrecht**

Silicon carbide (SiC) is one of the major cosmic dust components in carbon-rich environments. However, the formation of SiC dust is not well understood. In particular, the initial stages of the SiC condensation (i.e. the SiC nucleation) remain unclear, as the basic building blocks (i.e. molecular clusters) exhibit atomic segregation at the (sub-)nanoscale. We report vertical and adiabatic ionization energies of small silicon carbide clusters, (SiC)<sub>n</sub>, n=2-12, ranging from 6.6-10.0 eV, which are lower than for the SiC molecule (~ 10.6 eV). The most favorable structures of the singly ionized (SiC)<sub>n</sub><sup>+</sup>, n=5-12, cations resemble their neutral counterparts. However, for sizes n=2-4, these structural analogues are metastable and different cation geometries are favored. Moreover, we find that the (SiC)<sub>5</sub><sup>+</sup> cation is likely to be a transition state. Therefore, we place constraints on the stability limit for small, neutral (SiC)<sub>n</sub> clusters to persist ionization through (inter)-stellar radiation fields or high temperatures.

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## Millimeter- and submillimeter-wave spectrum of trans-formaldoxime (CH<sub>2</sub>NOH)

**Luyao Zou, Jean-Claude Guillemin, Roman A. Motiyenko and Laurent Margulès**

Context. Among the six atoms of N-containing molecules with the formula of CH<sub>3</sub>NO, only formamide (H<sub>2</sub>NCHO), the most stable structural isomer, has been detected in the interstellar medium (ISM). The formaldoxime isomer may be formed, for example, by the reaction of formaldehyde (H<sub>2</sub>CO) or methanimine (H<sub>2</sub>CNH) and hydroxylamine (H<sub>2</sub>NOH), which are all detected in the ISM. The lack of high accuracy millimeter- and

submillimeter-wave measurements hinders the astronomical search for formaldoxime. Aims. The aim of this work is to provide the direct laboratory measurement of the millimeter- and submillimeter-wave spectrum of trans-formaldoxime. Methods. Formaldoxime was synthesized and its rotational spectrum was recorded at room temperature in a glass flow cell using the millimeter- and submillimeter-wave spectrometer in Lille. The SPFIT program in the CALPGM suite was used to fit the spectrum. Results. Rotational lines of trans-formaldoxime from both the ground state and  $v_{12} = 1$  vibrational excited states have been measured and assigned from 150 to 660 GHz. Spectroscopic constants were derived to the tenth order using both Watson's A and S reduction Hamiltonian.

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## The CH radical at radio wavelengths: Revisiting emission in the 3.3 GHz ground-state lines

**A. M. Jacob, K. M. Menten, H. Wiesemeyer, G. N. Ortiz-Leon**

The intensities of the three widely observed radio-wavelength hyperfine structure (HFS) lines between the  $\{\Lambda\}$ -doublet components of the rotational ground state of CH are inconsistent with LTE and indicate ubiquitous population inversion. While this can be qualitatively understood assuming a pumping cycle that involves collisional excitation processes, the relative intensities of the lines and in particular the dominance of the lowest frequency satellite line has not been well understood. This has limited the use of CH radio emission as a tracer of the molecular interstellar medium. We present the first interferometric observations, with the Karl G. Jansky Very Large Array, of the CH 9 cm ground state HFS transitions at 3.264 GHz, 3.335 GHz, and 3.349 GHz toward four high mass star-forming regions (SFRs) Sgr B2 (M), G34.26+0.15, W49 (N), and W51. We investigate the nature of the (generally) weak CH ground state masers by employing synergies between the ground state HFS transitions themselves and with the far-infrared lines, near 149  $\mu\text{m}$  (2 THz), that connect these levels to an also HFS split rotationally excited level. Employing recently calculated collisional rate coefficients, we perform statistical equilibrium calculations with the non-LTE radiative transfer code MOLPOP-CEP in order to model the excitation conditions traced by the ground state HFS lines of CH and to infer the physical conditions in the emitting regions while also accounting for the effects of far-infrared line overlap.

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## Ethynyl around the HII regions S255 and S257

**Buslaeva Anna I., Kirsanova Maria. S., Punanova Anna F.**

We present the results of the ethynyl (C<sub>2</sub>H) emission line observations towards the HII regions S255 and S257 and the molecular cloud between them. Radial profiles of line brightness, column density, and abundance of C<sub>2</sub>H are obtained. We show that the radial profile of the ethynyl abundance is almost flat towards the HII regions and drops by a factor of two towards the molecular cloud. At the same time, we find that the abundance of ethynyl is at maximum towards the point sources in the molecular cloud - the stars with emission lines or emitting in X-ray. The line profiles are consistent with the assumption that both HII regions have front and back neutral walls that move

relative to each other.

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## The complex organic molecular content in the L1498 starless core

**I. Jimenez-Serra , A. I. Vasyunin , S. Spezzano , P. Caselli , G. Cosentino , and S. Viti**

Observations carried out toward starless and pre-stellar cores have revealed that complex organic molecules are prevalent in these objects, but it is unclear what chemical processes are involved in their formation. Recently, it has been shown that complex organics are preferentially produced at an intermediate-density shell within the L1544 pre-stellar core at radial distances of  $\sim 4000$  au with respect to the core center. However, the spatial distribution of complex organics has only been inferred toward this core and it remains unknown whether these species present a similar behaviour in other cores. We report high-sensitivity observations carried out toward two positions in the L1498 pre-stellar core, the dust peak and a position located at a distance of  $\sim 11000$  au from the center of the core where the emission of CH<sub>3</sub>OH peaks. Similarly to L1544, our observations reveal that small O-bearing molecules and N-bearing species are enhanced by factors  $\sim 4$ -14 toward the outer shell of L1498. However, unlike L1544, large O-bearing organics such as CH<sub>3</sub>CHO, CH<sub>3</sub>OCH<sub>3</sub> or CH<sub>3</sub>OCHO are not detected within our sensitivity limits. For N-bearing organics, these species are more abundant toward the outer shell of the L1498 pre-stellar core than toward the one in L1544. We propose that the differences observed between O-bearing and N-bearing species in L1498 and L1544 are due to the different physical structure of these cores, which in turn is a consequence of their evolutionary stage, with L1498 being younger than L1544.

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## Dynamics of HeHHe<sup>+</sup> Rotational State Changes Induced by Collision with He: A Possible New Path in Early Universe Chemistry

**L. González-Sánchez, E. Yurtsever, R. Wester, and F. A. Gianturco**

Ab initio calculations are employed to generate the rigid rotor (RR) potential energy surface (PES) describing the interaction of the linear molecular cation HeHHe<sup>+</sup>, at its equilibrium geometry, with the neutral He atom. The resulting interaction is employed to investigate the efficiency of rotational state-changing collisions at the temperatures relevant to the early universe conditions, where the latter molecule has been postulated to exist, albeit not yet observed. The inelastic rate coefficients are found to be fairly large and are compared with those found for another important cation just recently observed in the interstellar medium: the HeH<sup>+</sup> polar molecule. The possibility for this cation to provide new options to energy dissipation routes under early universe conditions after the recombination era is briefly discussed

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## Discovery in space of ethanolamine, the simplest phospholipid head group

**Víctor M. Rivilla, Izaskun Jiménez-Serra, Jesús Martín-Pintado, Carlos Briones, Lucas F. Rodríguez-Almeida, Fernando Rico-Villas, Belén Tercero, Shaoshan Zeng, Laura Colzi, Pablo de Vicente, Sergio Martín, Miguel A. Requena-Torres**

Cell membranes are a key element of life because they keep the genetic material and metabolic machinery together. All present cell membranes are made of phospholipids, yet the nature of the first membranes and the origin of phospholipids are still under debate. We report here the first detection in space of ethanolamine,  $\text{NH}_2\text{CH}_2\text{CH}_2\text{OH}$ , which forms the hydrophilic head of the simplest and second most abundant phospholipid in membranes. The molecular column density of ethanolamine in interstellar space is  $N=(1.51\pm 0.07)\times 10^{13}\text{ cm}^{-2}$ , implying a molecular abundance with respect to  $\text{H}_2$  of  $(0.9\text{--}1.4)\times 10^{-10}$ . Previous studies reported its presence in meteoritic material but they suggested that it is synthesized in the meteorite itself by decomposition of amino acids. However, we find that the proportion of the molecule with respect to water in the interstellar medium is similar to the one found in the meteorite ( $10^{-6}$ ). These results indicate that ethanolamine forms efficiently in space and, if delivered onto early Earth, it could have contributed to the assembling and early evolution of primitive membranes.

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## First survey of $\text{HCNH}^+$ in high-mass star-forming cloud cores

**Fontani F., Colzi L., Redaelli E., Sipilä O., Caselli P.**

Most stars in the Galaxy, including the Sun, were born in high-mass star-forming regions. It is hence important to study the chemical processes in these regions to better understand the chemical heritage of both the Solar System and most stellar systems in the Galaxy. The molecular ion  $\text{HCNH}^+$  is thought to be a crucial species in ion-neutral astrochemical reactions, but so far it has been detected only in a handful of star-forming regions, and hence its chemistry is poorly known. We have observed with the IRAM-30m Telescope 26 high-mass star-forming cores in different evolutionary stages in the  $J=3\text{--}2$  rotational transition of  $\text{HCNH}^+$ . We report the detection of  $\text{HCNH}^+$  in 16 out of 26 targets. This represents the largest sample of sources detected in this molecular ion so far. The highest fractional abundances of  $\text{HCNH}^+$  w.r.t.  $\text{H}_2$  are found towards cold starless cores. We run two chemical models, a "cold" one and a "warm" one, which attempt to match as much as possible the average physical properties of the cold(er) starless cores and of the warm(er) targets. The reactions occurring in the latter case are investigated in this work for the first time. Our predictions indicate that in the warm model  $\text{HCNH}^+$  is mainly produced by reactions with  $\text{HCN}$  and  $\text{HCO}^+$ , while in the cold one the main progenitor species of  $\text{HCNH}^+$  are  $\text{HCN}^+$  and  $\text{HNC}^+$ . The results indicate that the chemistry of  $\text{HCNH}^+$  is different in cold/early and warm/evolved cores, and the abundance ratios  $[\text{HCNH}^+]/[\text{HCN}]$  and  $[\text{HCNH}^+]/[\text{HCO}^+]$  are useful astrochemical tools to discriminate between different evolutionary phases in the process of star formation.

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## Catalytic Role of Refractory Interstellar Grain Analogs on H<sub>2</sub> Formation

Tushar Suhasaria and Vito Mennella

Refractory dust grains have an important role to play in the chemistry of star and planet-forming regions. Their surfaces interact with interstellar gas and act as a catalyst for the formation of simple and complex molecules in space. Several mechanisms have been invoked to explain how molecular hydrogen is formed in reactions on dust grain surfaces in different regions of space. In this article, we give an overview of our understanding of the laboratory experiments, conducted over the last 20 years, that deal with H<sub>2</sub> formation on interstellar grain analogs in space simulated conditions.

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## The reactivity of methanimine radical cation (H<sub>2</sub>CNH<sup>•+</sup>) and its isomer aminomethylene (HCNH<sub>2</sub><sup>•+</sup>) with methane

V. Richardson, C. Alcaraz, W.D. Geppert, M. Polasek, C. Romanzin, D. Sundelin, R. Thissen, P. Tosi, J. Zabka, D. Ascenzi

Experimental and theoretical studies are presented on the reactions of the isomeric radical cations H<sub>2</sub>CNH<sup>•+</sup> and HCNH<sub>2</sub><sup>•+</sup> with CH<sub>4</sub>. Ionic isomers were generated selectively by VUV dissociative photoionization of azetidine and cyclopropylamine precursors respectively. Both exclusively give H<sub>2</sub>CNH<sub>2</sub><sup>+</sup> plus CH<sub>3</sub><sup>•</sup> as products, but differences are observed related to a competition between stripping and complex-mediated H-transfer. Astrochemical implications for Titan's atmosphere are briefly discussed, where the presence of methanimine (H<sub>2</sub>CNH), a key prebiotic molecule and a potential precursor for tholins, is proposed on the basis of atmospheric models and the observation of CH<sub>2</sub>NH<sub>2</sub><sup>+</sup> ions in Cassini mass spectrometric data.

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## The reactivity of methanimine radical cation (H<sub>2</sub>CNH<sup>•+</sup>) and its isomer aminomethylene (HCNH<sub>2</sub><sup>•+</sup>) with C<sub>2</sub>H<sub>4</sub>

D. Sundelin, D. Ascenzi, V. Richardson, C. Alcaraz, M. Polasek, C. Romanzin, R. Thissen, P. Tosi, J. Zabka, W. Geppert

Experimental and theoretical studies are presented on the reactivity of H<sub>2</sub>CNH<sup>•+</sup> (methanimine) and HCNH<sub>2</sub><sup>•+</sup> (aminomethylene) with ethene (C<sub>2</sub>H<sub>4</sub>). Selective isomer generation is performed via dissociative photoionization of suitable neutral precursors and reactive cross sections and branching ratios are measured as a function of photon and collision energies. Differences between isomers' reactivity are discussed in light of ab-initio calculations on reaction mechanisms. The main products, for both isomers, are H-elimination, most likely occurring from covalently bound adducts (giving c-CH<sub>2</sub>CH<sub>2</sub>CHNH<sup>+</sup>/CH<sub>2</sub>NHCHCH<sub>2</sub><sup>+</sup>) and H<sup>•</sup> atom transfer to yield H<sub>2</sub>CNH<sub>2</sub><sup>+</sup>. The astrochemical implications of the results are briefly addressed.

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## Infrared predissociation spectroscopy of protonated methyl cyanide, CH<sub>3</sub>CNH<sup>+</sup>

Aravindh N. Marimuthu, Frank Huis in't Veld, Sven Thorwirth, Britta Redlich, Sandra Brünken

The gas phase vibrational spectrum of CH<sub>3</sub>CNH<sup>+</sup> is investigated using a messenger infrared predissociation (IRPD) action spectroscopic method. Vibrational bands were recorded in the 300-1700 cm<sup>-1</sup> and 2200-3000 cm<sup>-1</sup> regions making use of the widely tunable free electron laser for infrared experiments, FELIX, coupled to a cryogenic ion trap instrument. Band assignments were aided by high-level quantum-chemical calculations, which showed excellent agreement with the experimental data. Effects of the neon atom used as messenger in the IRPD method are investigated in detail. The data presented here will support astronomical searches for the CH<sub>3</sub>CNH<sup>+</sup> ion in space, and provides a basis for high-resolution ro-vibrational and pure rotational studies in vibrationally excited states.

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## Announcements

### Astrochemistry in the JWST era

The Astrochemistry Group invites you to the 2021 annual meeting, to be held virtually and hosted by the University of Leeds, from 16th to 18th June 2021. The meeting, on the topic of "Astrochemistry in the JWST era" will also include the annual general meeting (AGM) of the Astrochemistry Group on 17th June 2021. We welcome all contributions on the theme of astrochemistry including observations, modelling, experiments, and instrumentation. There are 12 contributed talk slots available over the course of the meeting and abstract submission is due by 1st June 2021. The meeting sessions are scheduled daily from 1pm to 4pm BST (UTC+1) to facilitate international participation.

In this joint RSC/RAS meeting, and as a look forward to the launch of JWST, we have invited speakers with expertise in JWST observations and instrumentation (TBC), laboratory experiments on solid-state infrared spectroscopy (Professor Harold Linnartz, Leiden Observatory), and computational models of molecular spectra at infrared wavelengths (Professor Jonathan Tennyson, UCL). We also invite contributions from all areas of astrochemistry, and in particular would like to encourage emerging (post-graduate and post-doctoral) researchers in astrochemistry to attend the meeting and present their work to the community.

Further details on the meeting can be found here:

<https://www.rsc.org/events/detail/47252/astrochemistry-in-the-jwst-era>

Registration and abstract submission can be done via this link:

<https://forms.gle/d6MNFoR7XWZijvA9>

For further information please contact the meeting organiser: Catherine Walsh (c.walsh1@leeds.ac.uk).

### MOlecular Sciences for Earth and Space (MOSES): PhD positions

MOlecular Sciences for Earth and Space (MOSES): 6 PhD positions available at the

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Deadline: July 1, 2021 - 6:00 pm (CET)

For info on the MOSES doctoral school: <http://www.ssm.unina.it/en/doctoral-programmes/>