

# AstroChemical Newsletter #89

April 2023

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## Abstracts

### The kinematics of the magnetized protostellar core IRAS15398-3359

F. S. Tabatabaei, E. Redaelli, P. Caselli, F. O. Alves

Observations of protostellar envelopes are essential to understand better the process of gravitational collapse toward star and planet formation. From a theoretical perspective, magnetic fields are considered an important factor during the early stages of star formation, especially during the main accretion phase. We aim to study the relation between kinematics and magnetic fields at a very early stage of the star formation process by using data from the Atacama Pathfinder EXperiment (APEX) single dish antenna with the angular resolution of 28". We observed the two molecular lines C18O(2-1) and DCO+(3-2), toward the Class 0 young stellar object IRAS15398-3359. We implement a multi-component Gaussian fitting on the molecular data to study the kinematics. Also, we use previous polarization observations on this source to predict the influence of the magnetic field on the core. The velocity gradient along the central object can be explained as an ongoing outflow motion. We report flowing of material from the filament toward the central object, and of the merging of two velocity components in the C18O (2-1) emission around the protostar position, probably due to the merging of filamentary clouds. Our analysis shows that the large-scale magnetic field line observed previously is preferentially aligned to the rotation axis of the core.

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### Reaction dynamics on amorphous solid water surfaces using interatomic machine learned potentials. Microscopic energy partition revealed from the P + H -> PH reaction

G. Molpeceres, V. Zaverkin, K. Furuya, Y. Aikawa, J. Kästner

Energy redistribution after a chemical reaction is one of the few mechanisms to explain the diffusion and desorption of molecules which require more energy than the thermal energy available in quiescent molecular clouds (10 K). This energy distribution can be important in phosphorous hydrides, elusive yet fundamental molecules for interstellar prebiotic chemistry. We studied the reaction dynamics of the P + H -> PH reaction on amorphous solid water, a reaction of astrophysical interest, using ab-initio molecular dynamics with atomic forces evaluated by a neural network interatomic potential. We found that the exact nature of the initial phosphorous binding sites is less relevant for the energy dissipation process because the nascent PH molecule rapidly migrates to sites with higher binding energy after the reaction. Non-thermal diffusion and

desorption-after-reaction were observed and occurred early in the dynamics, essentially decoupled from the dissipation of the chemical reaction energy. From an extensive sampling of reactions on sites, we constrained the average dissipated reaction energy within the simulation time (50 ps) to be between 50 and 70 %. Most importantly, the fraction of translational energy acquired by the formed molecule was found to be mostly between 1 and 5 %. Including these values, specifically for the test cases of 2% and 5% of translational energy conversion, in astrochemical models, reveals very low gas-phase abundances of PH<sub>x</sub> molecules and reflects that considering binding energy distributions is paramount for correctly merging microscopic and macroscopic modelling of non-thermal surface astrochemical processes. Finally, we found that PD molecules dissipate more of the reaction energy. This effect can be relevant for the deuterium fractionation and preferential distillation of molecules in the interstellar medium.

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## Where does the energy go during the interstellar NH<sub>3</sub> formation on water ice? A computational study

**Stefano Ferrero, Stefano Pantaleone, Cecilia Ceccarelli, Piero Ugliengo, Mariona Sodupe, Albert Rimola**

In the coldest (10–20 K) regions of the interstellar medium, the icy surfaces of interstellar grains serve as solid-state supports for chemical reactions. Among their plausible roles, that of third body is advocated, in which the reaction energies of surface reactions dissipate throughout the grain, stabilizing the product. This energy dissipation process is poorly understood at the atomic scale, although it can have a high impact on Astrochemistry. Here, we study, by means of quantum mechanical simulations, the formation of NH<sub>3</sub> via successive H-additions to atomic N on water ice surfaces, paying special attention to the third body role. We first characterize the hydrogenation reactions and the possible competitive processes (i.e., H-abstractions), in which the H-additions are more favourable than the H-abstractions. Subsequently, we study the fate of the hydrogenation reaction energies by means of ab initio molecular dynamics simulations. Results show that around 58–90% of the released energy is quickly absorbed by the ice surface, inducing a temporary increase of the ice temperature. Different energy dissipation mechanisms are distinguished. One mechanism, more general, is based on the coupling of the highly excited vibrational modes of the newly formed species and the libration modes of the icy water molecules. A second mechanism, exclusive during the NH<sub>3</sub> formation, is based on the formation of a transient H<sub>3</sub>O<sup>+</sup>/NH<sub>2</sub><sup>-</sup> ion pair, which significantly accelerates the energy transfer to the surface. Finally, the astrophysical implications of our findings relative to the interstellar synthesis of NH<sub>3</sub> and its chemical desorption into the gas are discussed.

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## Enhanced star formation through the high-temperature formation of H<sub>2</sub> on carbonaceous dust grains

**Francesco Grieco, Patrice Theulé, Ilse De Looze, François Dulieu**

The microphysics of molecular hydrogen formation has implications on galactic-scale star formation rates over cosmic times. It is the cooling agent needed to initiate the

cloud collapse regulating the star formation efficiency. H<sub>2</sub> formation is inefficient in the gas phase under typical interstellar conditions, needing dust grains as catalysts. Small carbonaceous grains with sizes from ~4 to ~100-200 Angstrom, including Polycyclic Aromatic Hydrocarbons (PAHs), have been shown to increase the H<sub>2</sub> formation rates due to their large surface-to-volume ratios. H<sub>2</sub> formation on PAHs was previously thought to reduce above temperatures of 50K and H atom recombination was believed to be highly efficient only below 20K. Until now, both laboratory experiments and theoretical modeling have suggested that H<sub>2</sub> cannot form on grains with temperatures above 100K. Here we report evidence, through direct laboratory measurements, of the high efficiency formation of H<sub>2</sub> at temperatures up to 250K on a carbonaceous surface mimicking interstellar dust. By pushing their formation towards warmer temperatures, the H<sub>2</sub> molecules could start contributing significantly to the cooling of warmer gas (T~50-250K). This will have a huge impact on our understanding of H<sub>2</sub> formation in nearby galaxies and its efficiency in high-redshift galaxies where the CMB (Cosmic Microwave Background) already pushes dust temperatures to >20K.

Nat Astron (2023)

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Full-text URL: <https://hal-amu.archives-ouvertes.fr/OSU-INSTITUT-PYTHEAS/hal-04031936v1>

## **A vibrational action spectroscopic study of the Renner-Teller- and spin-orbit-affected cyanoacetylene radical cation HC<sub>3</sub>N<sup>+</sup>**

**K. Steenbakkers, A. N. Marimuthu, B. Redlich, G. C. Groenenboom, S. Brünken**

The linear radical cation of cyanoacetylene, HC<sub>3</sub>N<sup>+</sup>(2Π), is not only of astrophysical interest, being the, so far undetected, cationic counterpart of the abundant cyanoacetylene, but also of fundamental spectroscopic interest due to its strong spin-orbit and Renner-Teller interactions. Here, we present the first broadband vibrational action spectroscopic investigation of this ion through the infrared predissociation (IRPD) method using a Ne tag. Experiments have been performed using the FELion cryogenic ion-trap instrument in combination with the FELIX free-electron lasers and a Laservision optical parametric oscillator/optical parametric amplifier system. The vibronic splitting patterns of the three interacting bending modes (ν<sub>5</sub>, ν<sub>6</sub>, ν<sub>7</sub>), ranging from 180 to 1600 cm<sup>-1</sup>, could be fully resolved revealing several bands that were previously unobserved. The associated Renner-Teller and intermode coupling constants have been determined by fitting an effective Hamiltonian to the experimental data, and the obtained spectroscopic constants are in reasonable agreement with previous photoelectron spectroscopy (PES) studies and ab initio calculations on the HC<sub>3</sub>N<sup>+</sup> ion. The influence of the attached Ne atom on the infrared spectrum has been investigated by ab initio calculations at the RCCSD(T)-F12a level of theory, which strongly indicates that the discrepancies between the IRPD and PES data are a result of the effects of the Ne attachment.

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## **Mechanisms of SiO oxidation: Implications for dust formation**

**Stefan Andersson, David Gobrecht, Rosendo Valero**

Reactions of SiO molecules have been postulated to initiate efficient formation of silicate

dust particles in outflows around dying (AGB) stars. Both OH radicals and H<sub>2</sub>O molecules can be present in these environments and their reactions with SiO and the smallest SiO cluster, Si<sub>2</sub>O<sub>2</sub>, affect the efficiency of eventual dust formation. Rate coefficients of gas-phase oxidation and clustering reactions of SiO, Si<sub>2</sub>O<sub>2</sub> and Si<sub>2</sub>O<sub>3</sub> have been calculated using master equation calculations based on density functional theory calculations. The calculations show that the reactions involving OH are fast. Reactions involving H<sub>2</sub>O are not efficient routes to oxidation but may under the right conditions lead to hydroxylated species. The reaction of Si<sub>2</sub>O<sub>2</sub> with H<sub>2</sub>O, which has been suggested as efficient producing Si<sub>2</sub>O<sub>3</sub>, is therefore not as efficient as previously thought. If H<sub>2</sub>O molecules dissociate to form OH radicals, oxidation of SiO and dust formation could be accelerated. Kinetics simulations of oxygen-rich circumstellar environments using our proposed reaction scheme suggest that under typical conditions only small amounts of SiO<sub>2</sub> and Si<sub>2</sub>O<sub>2</sub> are formed and that most of the silicon remains as molecular SiO.

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## **A major asymmetric ice trap in a planet-forming disk: IV. Nitric oxide gas and a lack of CN tracing sublimating ices and a C/O ratio < 1**

**M. Leemker, A. S. Booth, E. F. van Dishoeck, N. van der Marel, B. Tabone, N. F. W. Ligterink, N. G. C. Brunken, and M. R. Hogerheijde**

Most well-resolved disks observed with ALMA show signs of dust traps. These dust traps set the chemical composition of the planet forming material in these disks, as the dust grains with their icy mantles are trapped at specific radii and could deplete the gas and dust of volatiles at smaller radii. In this work we analyse the first detection of nitric oxide (NO) in a protoplanetary disk. We aim to constrain the nitrogen chemistry and the gas-phase C/O ratio in the highly asymmetric dust trap in the Oph-IRS 48 disk. We use ALMA observations of NO, CN, C<sub>2</sub>H, and related molecules and model the effect of the dust trap on the physical and chemical structure using the thermochemical code DALI. Furthermore, we explore how ice sublimation contributes to the observed emission lines. NO is only observed at the location of the dust trap but CN and C<sub>2</sub>H are not detected in the Oph-IRS 48 disk. This results in an CN/NO column density ratio of <0.05 and thus a low C/O ratio at the location of the dust trap. The main gas-phase formation pathways to NO through OH and NH in the fiducial model predict NO emission that is an order of magnitude lower than is observed. The gaseous NO column density can be increased by factors ranging from 2.8 to 10 when the H<sub>2</sub>O and NH<sub>3</sub> gas abundances are significantly boosted by ice sublimation. However, these models are inconsistent with the upper limits on the H<sub>2</sub>O and OH column densities derived from observations. We propose that the NO emission in the Oph-IRS 48 disk is closely related to the nitrogen containing ices sublimating in the dust trap. The non-detection of CN constrains the C/O ratio both inside and outside the dust trap to be <1 if all nitrogen initially starts as N<sub>2</sub> and  $\leq 0.6$ , consistent with the Solar value, if (part of) the nitrogen initially starts as N or NH<sub>3</sub>.

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## Millimeter-wave spectrum of 2-propanimine

Luyao Zou, Jean-Claude Guillemin, Arnaud Belloche, Jes K Jørgensen, Laurent Margulès, Roman A Motiyenko, Peter Groner

Up to date, only six imines have been detected in the interstellar medium. The 3-carbon imine, 2-propanimine ((CH<sub>3</sub>)<sub>2</sub>C = NH), is predicted to be the structural isomer with the lowest energy in the C<sub>3</sub>H<sub>7</sub>N group, and appears to be a good candidate for astronomical searches. Unexpectedly, no microwave or millimeter wave spectrum is available for 2-propanimine. In this work, we provide the first high-resolution millimeter wave spectrum of 2-propanimine and its analysis. With the guide of this laboratory measurement, we aim to search for 2-propanimine in two molecule-rich sources Sgr B2(N) and IRAS 16293–2422 using observations from the Atacama Large Millimeter/submillimeter Array (ALMA). Starting from a synthesized sample, we measured the spectrum of 2-propanimine from 50 to 500 GHz, and the ground state lines are successfully assigned and fitted using XIAM and ERHAM programs with the aid of theoretical calculations. The barriers to internal rotation of the two CH<sub>3</sub> tops are determined to be 531.956(64) cm<sup>-1</sup> and 465.013(26) cm<sup>-1</sup> by XIAM. These data are able to provide reliable prediction of transition frequencies for astronomical search. Although a few line matches exist, no confirmed detection of 2-propanimine has been found in the hot molecular core Sgr B2(N1S) and the Class 0 protostar IRAS 16293B. Upper-limits of its column density have been derived, and indicate that 2-propanimine is at least 18 times less abundant than methanimine in Sgr B2(N1S), and is at most 50 – 83 per cent of methanimine in IRAS 16293B.

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## Gas-phase formation and spectroscopic characterization of the disubstituted cyclopropenylidenes c-C<sub>3</sub>(C<sub>2</sub>H)<sub>2</sub>, c-C<sub>3</sub>(CN)<sub>2</sub>, and c-C<sub>3</sub>(C<sub>2</sub>H)(CN)

Athena R. Flint, Alexandria G. Watrous, Brent R. Westbrook, Dev J. Patel, and Ryan C. Fortenberry

**Aims.** The detection of c-C<sub>3</sub>HC<sub>2</sub>H and possible future detection of c-C<sub>3</sub>H<sub>2</sub>CN provide new molecules for reaction chemistry in the dense interstellar medium (ISM) where R-C<sub>2</sub>H and R-CN species are prevalent. Determination of chemically viable c-C<sub>3</sub>HC<sub>2</sub>H and c-C<sub>3</sub>H<sub>2</sub>CN derivatives and their prominent spectral features can accelerate potential astrophysical detection of this chemical family. This work characterizes three such derivatives: c-C<sub>3</sub>(C<sub>2</sub>H)<sub>2</sub>, c-C<sub>3</sub>(CN)<sub>2</sub>, and c-C<sub>3</sub>(C<sub>2</sub>H)(CN). **Methods.** Interstellar reaction pathways of small carbonaceous species are well replicated through quantum chemical means. Highly accurate cc-pVXZ-F12/CCSD(T)-F12 (X = D,T) calculations generate the energetics of chemical formation pathways as well as the basis for quartic force field and second-order vibrational perturbation theory rovibrational analysis of the vibrational frequencies and rotational constants of the molecules under study. **Results.** The formation of c-C<sub>3</sub>(C<sub>2</sub>H)<sub>2</sub> is as thermodynamically and, likely, as stepwise favorable as the formation of c-C<sub>3</sub>HC<sub>2</sub>H, rendering its detectability to be mostly dependent on the concentrations of the reactants. Both c-C<sub>3</sub>(C<sub>2</sub>H)<sub>2</sub> and c-C<sub>3</sub>(C<sub>2</sub>H)(CN) will be detectable through radioastronomical observation with large dipole moments of 2.84 D and 4.26 D, respectively, while c-C<sub>3</sub>(CN)<sub>2</sub> has an exceedingly small and likely unobservable dipole moment of 0.08 D. The most intense frequency for c-C<sub>3</sub>(C<sub>2</sub>H)<sub>2</sub> is ν<sub>2</sub> at 3316.9 cm<sup>-1</sup> (3.01 μm), with an intensity of 140 km mol<sup>-1</sup>. The mixed-substituent molecule c-

C<sub>3</sub>(C<sub>2</sub>H)(CN) has one frequency with a large intensity,  $\nu_1$ , at 3321.0 cm<sup>-1</sup> (3.01  $\mu$ m), with an intensity of 82 km mol<sup>-1</sup>. The molecule c-C<sub>3</sub>(CN)<sub>2</sub> lacks intense vibrational frequencies within the range that current instrumentation can readily observe. Conclusions. Both c-C<sub>3</sub>(C<sub>2</sub>H)<sub>2</sub> and c-C<sub>3</sub>(C<sub>2</sub>H)(CN) are viable candidates for astrophysical observation, with favorable reaction profiles and spectral data produced herein, but c-C<sub>3</sub>(CN)<sub>2</sub> will not be directly observable through any currently available remote sensing means, even if it forms in large abundances.

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## Circumplanetary disk ices II. Composition

**N. Oberg, S. Cazaux, I. Kamp, T.M. Bründl, W.F. Thai, C. Immerzeel**

The subsurface oceans of icy satellites are among the most compelling among the potentially habitable environments in our Solar System. The question of whether a liquid subsurface layer can be maintained over geological timescales depends on its chemical composition. The composition of icy satellites is linked to that of the circumplanetary disk (CPD) in which they form. The CPD accretes material from the surrounding circumstellar disk in the vicinity of the planet, however, the degree of chemical inheritance is unclear. We aim to investigate the composition of ices in chemically reset or inherited circumplanetary disks to inform interior modeling and the interpretation of in situ measurements of icy solar system satellites, with an emphasis on the Galilean moon system. We used a radiation-thermochemical code to produce circumplanetary disk models and extract the ice composition from time-dependent chemistry, incorporating gas-phase and grain-surface reactions. The initial sublimation of ices during accretion may result in a CO<sub>2</sub>-rich ice composition. Sublimated ammonia ice is destroyed by background radiation while drifting towards the CPD midplane. Liberated nitrogen becomes locked in N<sub>2</sub> due to efficient self-shielding, leaving ices depleted of ammonia. A significant ammonia ice component remains only when ices are inherited from the circumstellar disk. The observed composition of the Galilean moons is consistent with the sublimation of ices during accretion onto the CPD. In this scenario, the Galilean moon ices are nitrogen-poor and CO<sub>2</sub> on Callisto is endogenous and primordial. The ice composition is significantly altered after an initial reset of accreted circumstellar ice. The chemical history of the Galilean moons stands in contrast to the Saturnian system, where the composition of the moons corresponds more closely with the directly inherited circumstellar disk material.

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# Announcements

## **Mini-Symposium “Surface Astrochemistry” at 36th European Conference on Surface Science (ECOSS36)**

Lodz, Poland, August 28 - September 1, 2023.

Call for abstracts for a talk in a mini-symposium (MS) “Surface Astrochemistry” at 36th European Conference on Surface Science (ECOSS36)

The aim of this mini-symposium is to inform the community on the recent work (theoretical, experimental and observational) that has been done in the field of surface science in astrochemistry. This is important in order to update the community on the recent discoveries, which will lead to understanding the big picture of complex and/or prebiotic molecular formation catalyzed by carbonaceous, silicate or ice surfaces in space. This MS will be 2 hour session that opens the floor for discussion of new future research directions.

The abstract submission opens on March 13, 2023, and closes on May 14, 2023.

More information about the MS can be found on <https://www.ecoss36.uni.lodz.pl/mini-symposia>