

# AstroChemical Newsletter #59

October 2020

You can access the full abstracts by clicking the paper titles. Submit your abstracts before the 25th of each month for inclusion in the following newsletter.

## Abstracts

### ALMA chemical survey of disk-outflow sources in Taurus (ALMA-DOT) II: Vertical stratification of CO, CS, CN, H<sub>2</sub>CO, and CH<sub>3</sub>OH in a Class I disk

L. Podio, A. Garufi, C. Codella, D. Fedele, E. Bianchi, F. Bacciotti, C. Ceccarelli, C. Favre, S. Mercimek, K. Rygl, and L. Testi

The chemical composition of planets is inherited from that of the natal protoplanetary disk at the time of planet formation. Increasing observational evidence suggests that planet formation occurs in less than 1–2 Myr. This motivates the need for spatially resolved spectral observations of young Class I disks, as carried out by the ALMA chemical survey of Disk-Outflow sources in Taurus (ALMA-DOT). In the context of ALMA-DOT, we observe the edge-on disk around the Class I source IRAS 04302+2247 (the butterfly star) in the 1.3 mm continuum and five molecular lines. We report the first tentative detection of methanol (CH<sub>3</sub>OH) in a Class I disk and resolve, for the first time, the vertical structure of a disk with multiple molecular tracers. The bulk of the emission in the CO 2 – 1, CS 5 – 4, and o-H<sub>2</sub>CO 3(1,2) – 2(1,1) lines originates from the warm molecular layer, with the line intensity peaking at increasing disk heights,  $z$ , for increasing radial distances,  $r$ . Molecular emission is vertically stratified, with CO observed at larger disk heights (aperture  $z/r \sim 0.41 - 0.45$ ) compared to both CS and H<sub>2</sub>CO, which are nearly coplanar ( $z/r \sim 0.21 - 0.28$ ). In the outer midplane, the line emission decreases due to molecular freeze-out onto dust grains (freeze-out layer) by a factor of  $> 100$  (CO) and 15 (CS). The H<sub>2</sub>CO emission decreases by a factor of only about 2, which is possibly due to H<sub>2</sub>CO formation on icy grains, followed by a nonthermal release into the gas phase. The inferred [CH<sub>3</sub>OH]/[H<sub>2</sub>CO] abundance ratio is 0.5 – 0.6, which is 1 – 2 orders of magnitude lower than for Class 0 hot corinos, and a factor  $\sim 2.5$  lower than the only other value inferred for a protoplanetary disk (in TW Hya, 1.3 – 1.7). Additionally, it is at the lower edge but still consistent with the values in comets. This may indicate that some chemical reprocessing occurs in disks before the formation of planets and comets.

accepted by A&A Letters

DOI: [10.1051/0004-6361/202038952](https://doi.org/10.1051/0004-6361/202038952)

Full-text URL: <https://arxiv.org/abs/2008.12648>

### The effect of the slit configuration on the H<sub>2</sub> 1-0 S(1) to Br gamma line ratio of spatially resolved planetary nebulae

I. Aleman

The H<sub>2</sub> 1-0 S(1)/Br gamma ratio (R(Br gamma)) is used in many studies of the molecular content in planetary nebulae (PNe). As these lines are produced in different regions, the slit configuration used in spectroscopic observations may have an important effect on their ratio. In this work, observations and numerical simulations are used to demonstrate and quantify such effect in PNe. The study aims to assist the interpretation of observations and their comparison to models. The analysis shows that observed R(Br gamma) ratios reach only values up to 0.3 when the slit encompasses the entire nebula. Values higher than that are only obtained when the slit covers a limited region around the H<sub>2</sub> peak emission and the Br gamma emission is then minimized. The numerical simulations presented show that, when the effect of the slit configuration is taken into account, photoionization models can reproduce the whole range of observed R(Br gamma) in PNe, as well as the behaviour described above. The argument that shocks are needed to explain the higher values of R(Br gamma) is thus not valid. Therefore, this ratio is not a good indicator of the H<sub>2</sub> excitation mechanism as suggested in the literature.

(2020) MNRAS 497, 3180

DOI: [10.1093/mnras/staa2174](https://doi.org/10.1093/mnras/staa2174)

Full-text URL: <https://arxiv.org/abs/2007.12310>

### Computational studies into urea formation in the interstellar medium

Eren C S Slate, Rory Barker, Ryan T Euesden, Max R Revels, Anthony J H M Meijer

Formation routes, involving closed shell, radical, and charged species for urea, have been studied using computational methods to probe their feasibility in the interstellar medium. All reactions involving closed shell species were found to have prohibitive barriers. The radical–radical reaction possesses a barrier of only 4 kJ mol<sup>-1</sup>, which could be surmountable. A charged species based route was also investigated. A barrier of only 8 kJ mol<sup>-1</sup> was found in that case, when a partial water ice shell was included.

Monthly Notices of the Royal Astronomical Society, Volume 497, Issue 4, October 2020, Pages 5413–5420,

DOI: [10.1093/mnras/staa2436](https://doi.org/10.1093/mnras/staa2436)

Full-text URL: <https://doi.org/10.1093/mnras/staa2436>

## Structural investigation of doubly-dehydrogenated pyrene cations

S. Panchagnula, J. Bouwman, D. B. Rap, P. Castellanos, A. Candian, C. Mackie, S. Banhatti, S. Brunken, H. Linnartz, A. G. G. M. Tielens

The vibrationally resolved spectra of the pyrene cation and doubly-dehydrogenated pyrene cation ( $C_{16}H_{10}^+$ ;  $Py^+$  and  $C_{16}H_8^+$ ;  $ddPy^+$ ) are presented. Infrared predissociation spectroscopy is employed to measure the vibrational spectrum of both species using a cryogenically cooled 22-pole ion trap. The spectrum of  $Py^+$  allows a detailed comparison with harmonic and anharmonic density functional theory (DFT) calculated normal mode frequencies. The spectrum of  $ddPy^+$  is dominated by absorption features from two isomers ( $4,5-ddPy^+$  and  $1,2-ddPy^+$ ) with, at most, minor contributions from other isomers. These findings can be extended to explore the release of hydrogen from interstellar PAH species. Our results suggest that this process favours the loss of adjacent hydrogen atoms.

Phys. Chem. Chem. Phys., 2020, Advance Article

DOI: [10.1039/D0CP02272A](https://doi.org/10.1039/D0CP02272A)

Full-text URL: <https://arxiv.org/abs/2007.16156>

## Destruction route of solid-state formamide by thermal H atoms

T. Suhasaria and V. Mennella

Formamide ( $NH_2CHO$ ) is one of the simplest “CHON” molecules that has been observed in different environments in space. In star-forming regions, its abundance in the gas phase is correlated to isocyanic acid (HNCO), indicating a chemical relation between the two species. Many studies have investigated the different routes for the transformation of the two species from one to the other. We carry out an experimental analysis on the interaction of atomic H at 300 K with solid  $NH_2CHO$  to probe whether HNCO can form. The effects of H atom irradiation on  $NH_2CHO$  have been analyzed by Fourier-transform infrared spectroscopy. During irradiation, a decrease in the band intensity of the C–H, C=O, and N–H modes of  $NH_2CHO$  with a simultaneous increase in the N=C=O band intensity of HNCO is observed, indicating a transformation of  $NH_2CHO$  to HNCO. The corresponding destruction and formation cross-sections have been estimated from the trend of the normalized column densities as a function of the H atom fluence. The transformation follows a three-step reaction sequence driven by H atom exothermic abstractions that also induce sputtering of the products. No bands of aminomethanol were detected. The interaction of H atoms with  $NH_2CHO$  in space can be one of the promising mechanisms to explain the chemical relation between  $NH_2CHO$  and HNCO. In addition, the comparison of our results with those of other energetic processing agents suggests that H atoms play a crucial role in the destruction of  $NH_2CHO$  ice in dense regions of the interstellar medium.

2020, Astronomy & Astrophysics, 641, A88

DOI: [10.1051/0004-6361/202038004](https://doi.org/10.1051/0004-6361/202038004)

Full-text URL: <http://doi.org/10.1051/0004-6361/202038004>

## High-resolution Infrared Spectroscopy of Hot Molecular Gas in AFGL 2591 and AFGL 2136: Accretion in the Inner Regions of Disks around Massive Young Stellar Objects

Andrew G. Barr, Adwin Boogert, Curtis N. DeWitt, Edward Montiel, Matthew J. Richter, John H. Lacy, David A. Neufeld, Nick Indriolo, Yvonne Pendleton, Jean Chiar

We have performed a high-resolution 4–13  $\mu m$  spectral survey of the hot molecular gas associated with the massive protostars AFGL 2591 and AFGL 2136, utilizing the Echelon Cross Echelle Spectrograph (EXES) on board the Stratospheric Observatory for Infrared Astronomy, and the iSHELL instrument and Texas EchelonCross Echelle Spectrograph (TEXES) on the NASA Infrared Telescope Facility (IRTF). Here we present the results of this survey with analysis of CO, HCN,  $C_2H_2$ ,  $NH_3$ , and CS, deriving the physical conditions for each species. Also from the IRTF, iSHELL data at 3  $\mu m$  for AFGL 2591 are presented that show HCN and  $C_2H_2$  in emission. In the EXES and TEXES data, all species are detected in absorption, and temperatures and abundances are found to be high (600 K and  $1e-6$ , respectively). Differences of up to an order of magnitude in the abundances of transitions that trace the same ground-state level are measured for HCN and  $C_2H_2$ . The mid-infrared continuum is known to originate in a disk, hence we attribute the infrared absorption to arise in the photosphere of the disk. As absorption lines require an outwardly decreasing temperature gradient, we conclude that the disk is heated in the midplane by viscous heating due to accretion. We attribute the near-IR emission lines to scattering by molecules in the upper layers of the disk photosphere. The absorption lines trace the disk properties at 50 au where high-temperature gas-phase chemistry is taking place. Abundances are consistent with chemical models of the inner disk of Herbig disks.

2020, ApJ, 900, 2

DOI: [10.3847/1538-4357/abab05](https://doi.org/10.3847/1538-4357/abab05)

Full-text URL: <https://arxiv.org/abs/2007.11266>

## UV-ray irradiation never causes amorphization of crystalline CO<sub>2</sub>: A transmission electron microscopy study

Masashi Tsuge, Thanh Nguyen, Yasuhiro Oba, Tetsuya Hama, Akira Kouchi, Naoki Watanabe

The Crystallinity of ices, amorphous and crystalline, can be altered not only by heat but also by irradiation of UV-rays or

charged particles. In this work, the effect of UV-irradiation on the crystallinity of CO<sub>2</sub> ice was investigated by using a transmission electron microscope. A crystalline CO<sub>2</sub> ice was produced by annealing amorphous CO<sub>2</sub> ice. We found that UV-ray irradiation of CO<sub>2</sub> crystals at approximately 10 K does not cause amorphization in contrast to the reported amorphization of crystalline water ice below 70 K. We discuss the difference based on the expected UV photochemistry of CO<sub>2</sub> ice.

2020 Chem. Phys. Lett. in press

DOI: [10.1016/j.cplett.2020.137999](https://doi.org/10.1016/j.cplett.2020.137999)

Full-text URL: <https://www.sciencedirect.com/science/article/pii/S0009261420309143>

## Infrared Resonant Vibrationally Induced Restructuring of Amorphous Solid Water

J. A. Noble, H. M. Cuppen, S. Coussan, B. Redlich, S. Ioppolo

Amorphous solid water (ASW) is abundantly present in the interstellar medium where it forms a mantle on interstellar dust particles and it is the precursor for cometary ices. In space, ASW acts as a substrate for interstellar surface chemistry leading to complex molecules and it is postulated to play a critical role in proton-transfer reactions. Although ASW is widely studied and is generally well characterized by different techniques, energetically induced structural changes, such as ion, electron, and photon irradiation, in these materials are less well understood. Selective pumping of specific infrared (IR) vibrational modes can aid in understanding the role of vibrations in restructuring of hydrogen-bonding networks. Here, we present the first experimental results on hydrogen-bonding changes in ASW induced by the intense, nearly monochromatic mid-IR free-electron laser (FEL) radiation of the FELIX-2 beamline at the FELIX Laboratory at the Radboud University in Nijmegen, The Netherlands. The changes are monitored by reflection-absorption infrared spectroscopy. Upon resonant irradiation, a modification in the IR absorption band profile of ASW is observed in agreement with a growing crystalline-like contribution and a decreasing amorphous contribution. This phenomenon saturates within a few minutes of FEL irradiation, modifying upward of 94% of the irradiated ice. The effect is further analyzed in terms of hydrogen-bonding donors and acceptors, and the experiments are complemented with molecular dynamics simulations to constrain the effect at the molecular level.

2020 J. Phys. Chem. C, ASAP

DOI: [10.1021/acs.jpcc.0c04463](https://doi.org/10.1021/acs.jpcc.0c04463)

Full-text URL: <https://arxiv.org/abs/2009.01183>

## Neural-Network Assisted Study of Nitrogen Atom Dynamics on Amorphous Solid Water. I. Adsorption & Desorption

G. Molpeceres, Zaverkin, V. Kästner, J.

Dynamics of adsorption and desorption of atomic N on amorphous solid water are analyzed using molecular dynamics simulations. The underlying potential energy surface was provided by machine-learned interatomic potentials. Binding energies confirm the latest available theoretical and experimental results. The nitrogen sticking coefficient is close to unity at dust temperatures of 10 K but decreases at higher temperatures. We estimate a desorption time scale of 1 micro-s at 28 K. The estimated time scale allows chemical processes mediated by diffusion to happen before desorption, even at higher temperatures. We found that the energy dissipation process after a sticking event happens on the picosecond timescale at dust temperatures of 10 K, even for high energies of the incoming adsorbate. Our approach allows the simulation of large systems for reasonable time scales at an affordable computational cost and ab-initio accuracy. Moreover, it is generally applicable for the study of adsorption dynamics of interstellar radicals on dust surfaces.

Accepted in MNRAS

DOI: [10.1093/mnras/staa2891](https://doi.org/10.1093/mnras/staa2891)

Full-text URL: <https://arxiv.org/abs/2009.09994>

## Binding energies of interstellar molecules on crystalline and amorphous models of water ice by ab-initio calculations

S. Ferrero; L. Zamirri; C. Ceccarelli; A. Witzel; A. Rimola and P. Ugliengo

In the denser and colder ( $\leq 20$  K) regions of the interstellar medium (ISM), near-infrared observations have revealed the presence of sub-micron sized dust grains covered by several layers of H<sub>2</sub>O-dominated ices and “dirtied” by the presence of other volatile species. Whether a molecule is in the gas or solid-phase depends on its binding energy (BE) on ice surfaces. Thus, BEs are crucial parameters for the astrochemical models that aim to reproduce the observed evolution of the ISM chemistry. In general, BEs can be inferred either from experimental techniques or by theoretical computations. In this work, we present a reliable computational methodology to evaluate the BEs of a large set (21) of astrochemical relevant species. We considered different periodic surface models of both crystalline and amorphous nature to mimic the interstellar water ice mantles. Both models ensure that hydrogen bond cooperativity is fully taken into account at variance with the small ice cluster models. Density functional theory adopting both B3LYP-D3 and M06-2X functionals was used to predict the species/ice structure and their BE. As expected from the complexity of the ice surfaces, we found that each molecule can experience multiple BE values, which depend on its structure and position at the ice surface. A comparison of our computed data with literature data shows agreement in some cases and (large) differences in others. We discuss some astrophysical implications that show the importance of calculating BEs using more realistic interstellar ice surfaces to have reliable values for inclusion in the astrochemical models.

## A novel framework to study the impact of binding energy distributions on the chemistry of dust grains

Grassi, T.; Bovino, S.; Caselli, P.; Bovolenta, G.; Vogt-Geisse, S.; Ercolano, B.

The evaporation of molecules from dust grains is crucial to understand some key aspects of the star- and the planet-formation processes. During the warm-up phase the presence of young protostellar objects induces molecules to evaporate from the dust surface into the gas phase, enhancing its chemical complexity. Similarly, in circumstellar disks, the position of the so-called snow-lines is determined by evaporation, with important consequences for the formation of planets. The amount of molecules that are desorbed depends on the interaction between the species and the grain surface, which is controlled by the binding energy. Recent theoretical and experimental works point towards a distribution of values for this parameter instead of the single value often employed in astrochemical models. We present here a new "multi-binding energy" framework, to assess the effects that a distribution of binding energies has on the amount of species bound to the grains. We find that the efficiency of the surface chemistry is significantly influenced by this process with crucial consequences on the theoretical estimates of the desorbed species.

Accepted A&A  
Full-text URL: <https://arxiv.org/abs/2009.03900>

## Detection of Interstellar HC<sub>4</sub>NC and an Investigation of Isocyanopolyne Chemistry under TMC-1 Conditions

C. Xue, E. Willis, R. Loomis, K. Lee, A. Burkhardt, C. Shingledecker, S. Charnley, M. Cordiner, S. Kalenskii, M. McCarthy, E. Herbst, A. Remijan, and B. McGuire

We report an astronomical detection of HC<sub>4</sub>NC for the first time in the interstellar medium with the Green Bank Telescope toward the TMC-1 molecular cloud with a minimum significance of 10.5 $\sigma$ . The total column density and excitation temperature of HC<sub>4</sub>NC are determined to be 3.29x1e11 cm<sup>-2</sup> and 6.7 K, respectively, using Markov chain Monte Carlo analysis. In addition to HC<sub>4</sub>NC, HCCNC is distinctly detected whereas no clear detection of HC<sub>6</sub>NC is made. We propose that the dissociative recombination of the protonated cyanopolyne, HC<sub>5</sub>NH<sup>+</sup>, and the protonated isocyanopolyne, HC<sub>4</sub>NCH<sup>+</sup>, are the main formation mechanisms for HC<sub>4</sub>NC while its destruction is dominated by reactions with simple ions and atomic carbon. With the proposed chemical networks, the observed abundances of HC<sub>4</sub>NC and HCCNC are reproduced satisfactorily.

2020 Astrophysical Journal Letters 900, L9  
DOI: [10.3847/2041-8213/aba631](https://doi.org/10.3847/2041-8213/aba631)  
Full-text URL: <https://arxiv.org/abs/2008.12345>

## Early Science from GOTHAM: Project Overview, Methods, and the Detection of Interstellar Propargyl Cyanide (HCCCH<sub>2</sub>CN) in TMC-1

B. McGuire, A. Burkhardt, R. Loomis., C. Shingledecker, K. Lee, S. Charnley, M. Cordiner, E. Herbst, S. Kalenskii, E. Momjian, E. Willis, C. Xue, A. Remijan, and M. McCarthy

We present an overview of the GBT Observations of TMC-1: Hunting Aromatic Molecules Large Program on the Green Bank Telescope. This and a related program were launched to explore the depth and breadth of aromatic chemistry in the interstellar medium at the earliest stages of star formation, following our earlier detection of benzonitrile (c-C<sub>6</sub>H<sub>5</sub>CN) in TMC-1. In this work, details of the observations, use of archival data, and data reduction strategies are provided. Using these observations, the interstellar detection of propargyl cyanide (HCCCH<sub>2</sub>CN) is described, as well as the accompanying laboratory spectroscopy. We discuss these results, and the survey project as a whole, in the context of investigating a previously unexplored reservoir of complex, gas-phase molecules in pre-stellar sources. A series of companion papers describe other new astronomical detections and analyses.

2020 Astrophysical Journal Letters 900, L10  
DOI: [10.3847/2041-8213/aba632](https://doi.org/10.3847/2041-8213/aba632)  
Full-text URL: <https://arxiv.org/abs/2008.12349>

## Diffusive Hydrogenation Reactions of CO Embedded in Amorphous Solid Water at Elevated Temperatures ~70 K

Masashi Tsuge, Hiroshi Hidaka, Akira Kouchi, and Naoki Watanabe

The surface processes on interstellar dust grains have an important role in the chemical evolution in molecular clouds. Hydrogenation reactions on ice surfaces have been extensively investigated and are known to proceed at low temperatures mostly below 20 K. In contrast, information about the chemical processes of molecules within an ice mantle is lacking. In this work, we investigated diffusive hydrogenation reactions of carbon monoxide (CO) embedded in amorphous solid water (ASW) as a model case and discovered that the hydrogenation of CO efficiently proceeds to yield H<sub>2</sub>CO and CH<sub>3</sub>OH even

above 20 K when CO is buried beneath ASW. The experimental results suggest that hydrogen atoms diffuse through the cracks of ASW and have a sufficient residence time to react with embedded CO. The hydrogenation reactions occurred even at temperatures up to ~70 K. Cracks collapse at elevated temperatures but the occurrence of hydrogenation reactions means that the cracks would not completely disappear and remain large enough for penetration by hydrogen atoms. Considering the hydrogen-atom fluence in the laboratory and molecular clouds, we suggest that the penetration of hydrogen and its reactions within the ice mantle occur in astrophysical environments.

2020 ApJ 900 187

DOI: [10.3847/1538-4357/abab9b](https://doi.org/10.3847/1538-4357/abab9b)

Full-text URL: <https://iopscience.iop.org/article/10.3847/1538-4357/abab9b>

## Rotational spectrum simulations of asymmetric tops in an astrochemical context

Santos, J. C., Rocha, A. B., Oliveira, R. R.

Rotational spectroscopy plays a major role in the field of observational astrochemistry, enabling the detection of more than 200 species including a plethora of complex organic molecules in different space environments. Those line detections allow correctly determining the sources and physical properties, as well as exploring their morphology, evolutionary stage, and chemical evolution pathways. In this context, quantum chemistry is a powerful tool to the investigation of the molecular inventory of astrophysical environments, guiding laboratory experiments and assisting in both line assignments and extrapolation of the experimental data to unexplored frequency ranges. In the present work, we start by briefly reviewing the rotational model Hamiltonian for asymmetric tops beyond the rigid-rotor approximation, including rotational-vibrational, centrifugal, and anharmonic effects. Then, aiming at further contributing to the recording and analysis of laboratory microwave spectroscopy by means of accessible, less demanding quantum chemical methods, we performed density functional theory (DFT) calculations of the spectroscopic parameters of astrochemically relevant species, followed by their rotational spectrum simulations. Furthermore, dispersion-correction effects combined with different functionals were also investigated. Case studies are the asymmetric tops H<sub>2</sub>CO, H<sub>2</sub>CS, c-HCOOH, t-HCOOH, and HNCO. Spectroscopic parameter predictions were overall very close to experiment, with mean percentage errors smaller than 1% for zeroth order and ~ 5% for first-order constants. We discuss the implications and impacts of those constants on spectrum simulations, and compare line-frequency predictions at millimeter wavelengths. Moreover, theoretical spectroscopic parameters of c-HCOOH and HNCO are introduced for the first time in this work.

Accepted in Journal of Molecular Modeling

DOI: [10.1007/s00894-020-04523-0](https://doi.org/10.1007/s00894-020-04523-0)

Full-text URL: <http://doi.org/10.1007/s00894-020-04523-0>

## Structure and Spectroscopic Properties of Hydrocalcium Isocyanide Isomers: Plausible Astronomical Ca-bearing Molecules

P. Redondo, A. Largo, C. Barrientos

Recently, the first Ca-bearing molecule discovered in space, calcium isocyanide, CaNC, has been detected in the IRC+10216 circumstellar envelope. Related to CaNC are closed-shell stable molecules of [C, Ca, H, N] composition. One of the isomers with this composition is hydrocalcium isocyanide, HCaNC, which belongs to the hydrometal isocyanide/cyanide group of compounds, among which hydromagnesium isocyanide, HMgNC, is, to date, the only one detected in space. In this work, we have performed a study of the [C, Ca, H, N] isomers that are systems of possible interstellar interest by using quantum theoretical methodologies. The analysis of the relative energies predicts three low-lying isomers: c-HCa-NC (1A'), hydrocalcium isocyanide, HCaNC (1Σ), and hydrocalcium cyanide, HCaCN (1Σ). At the composite level, HCaNC (1Σ) and HCaCN (1Σ) were located 0.87 and 4.84 kcal mol<sup>-1</sup>, respectively, above the c-HCa-NC (1Σ) isomer. Interconversion processes between these isomers have been studied to analyze their stability. Isomer HCaNC is characterized as a transition state and thus directly isomerizes to the c-HCa-NC minimum. The isomerization process of HCaCN → c-HCa-NC shows a small barrier of about 0.76 kcal mol<sup>-1</sup> (~382 K) above HCaCN, at the highest level of theory employed in this work, suggesting that HCaCN could easily isomerize into the most stable isomer, c-HCa-NC. Our results predict two low-lying isomers, namely, c-HCa-NC (1A') and hydrocalcium cyanide, HCaCN (1Σ), as possible candidates for experimental or radioastronomical detection. For these isomers, we provide predictions for their vibrational and rotational spectroscopic parameters that could aid in their eventual characterization in the laboratory or in space.

2020, ApJ, 899, 135

DOI: [10.3847/1538-4357/aba747](https://doi.org/10.3847/1538-4357/aba747)

Full-text URL: <http://doi.org/10.3847/1538-4357/aba747>

## Stable isomeric structures of the pyridine cation (C<sub>5</sub>H<sub>5</sub>N<sup>•+</sup>) and protonated pyridine (C<sub>5</sub>H<sub>5</sub>NH<sup>+</sup>) elucidated by cold ion infrared spectroscopy

Daniël B. Rap, Aravindh N. Marimuthu, Britta Redlich, and Sandra Brünken

Cold ion action spectroscopy is applied to record the gas phase infrared fingerprint spectra of mass-selected C<sub>5</sub>H<sub>5</sub>N<sup>•+</sup> and C<sub>5</sub>H<sub>5</sub>NH<sup>+</sup> cations using an infrared free electron laser. The structures of the cations are deduced from the experimental spectra using anharmonic vibrational frequencies from density functional theory calculations. A very good agreement between experimental and theoretical infrared frequencies is observed. The dominant structure of the C<sub>5</sub>H<sub>5</sub>N<sup>•+</sup> cation is

assigned to the aromatic pyridine radical cation form. Additionally, a minor contribution of the lower energetic  $\alpha$ -dystonic isomer is observed. The  $C_5H_5NH^+$  cation is ascribed to the aromatic pyridinium cation where protonation has taken place on the nitrogen atom. The rare-gas tag used in the action spectroscopic method has a negligible effect on the vibrational frequencies. The observed species, with now accurately determined vibrational frequencies, are good candidates for future rotational spectroscopic studies and infrared observations in astronomical sources such as interstellar clouds or Titan's atmosphere.

J. Mol. Spectrosc. 373 (2020) 111357

DOI: [10.1016/j.jms.2020.111357](https://doi.org/10.1016/j.jms.2020.111357)

Full-text URL: <https://doi.org/10.1016/j.jms.2020.111357>

## Gas-phase kinetics of CH<sub>3</sub>CHO with OH radicals between 11.7 and 177.5 K

S. Blázquez, D. González, E.M. Neeman, B. Ballesteros, M. Agúndez, A. Canosa, J. Albaladejo, J. Cernicharo, and E. Jiménez.

Gas-phase reactions in the interstellar medium (ISM) are a source of molecules in this environment. The knowledge of the rate coefficient for neutral–neutral reactions as a function of temperature,  $k(T)$ , is essential to improve astrochemical models. In this work, we have experimentally measured  $k(T)$  for the reaction between the OH radical and acetaldehyde, both present in many sources of the ISM. Laser techniques coupled to a CRESU system were used to perform the kinetic measurements. The obtained modified Arrhenius equation is  $k(T = 11.7–177.5 \text{ K}) = (1.2 \pm 0.2) \times 10^{-11} (T/300 \text{ K})^{-(1.8 \pm 0.1)} \exp\{-\{(28.7 \pm 2.5)/T\}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>. The  $k(T)$  value of the title reaction has been measured for the first time below 60 K. No pressure dependence of  $k(T)$  was observed at ca. 21, 50, 64 and 106 K. Finally, a pure gas-phase model indicates that the title reaction could become the main CH<sub>3</sub>CO formation pathway in dark molecular clouds, assuming that CH<sub>3</sub>CO is the main reaction product at 10 K.

Phys. Chem. Chem. Phys., 22[36], 20562-20572 (2020).

DOI: [10.1039/d0cp03203d](https://doi.org/10.1039/d0cp03203d)

Full-text URL: <https://pubs.rsc.org/en/content/articlelanding/2020/cp/d0cp03203d#!divAbstract>

## Announcements

### PhD position in experimental astrochemistry and planetary science

At the University of Bern, Switzerland, a PhD project under supervision of Dr. Niels Ligterink is available on the investigation of molecules in ices that are present in star-forming regions and on Solar System bodies. Using laboratory experiments that make use of Laser Desorption Mass Spectrometry and cryogenic cooling techniques, chemical reactions and physical processes in these ices are studied. The full description of the position and how to apply can be found at:

[here](#)

For questions, please send an email to: [niels.ligterink@csh.unibe.ch](mailto:niels.ligterink@csh.unibe.ch)

### Special Research topic on Astrochemistry in "Frontiers in Astronomy and Space Sciences"

An article collection on "RNA World Hypothesis and the Origin of Life: Astrochemistry Perspective" is presently open to contributions.

Article submission is possible until February 22nd, 2021 with a short abstract to be sent by November 25th, 2020.

Contributions should focus on one of the main following subtopics:

1. State-of-the-art radio and terahertz receivers for precision spectroscopy of molecules in protostellar and protoplanetary systems: high spectral resolving power and ultrahigh sensitivity large single-aperture far-infrared/submm/mm telescopes or interferometers.
2. High-resolution rotational spectroscopy (MW/mm/submm experimental perspective) and quantum chemistry theoretical underpinnings.
3. Experimental and theoretical studies of elementary reactions at very low temperatures. Role of Terahertz molecular spectroscopy, with special attention to ultra-cold isolated molecular ions: carbocations and carbanions, in chemical reactivity.

More scientific details and information about the submission process can be found at the following [webpage](#)

or by contacting the topic editors:

Ashraf Ali: [ashrali100@gmail.com](mailto:ashrali100@gmail.com)

David Leisawitz: [david.t.leisawitz@nasa.gov](mailto:david.t.leisawitz@nasa.gov)

André Canosa: [andre.canosa@univ-rennes1.fr](mailto:andre.canosa@univ-rennes1.fr)