

# AstroChemical Newsletter #60

November 2020

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## Abstracts

### A 3 mm Chemical Exploration of Small Organics in Class I YSOs

**Romane Le Gal, Karin I. Öberg, Jane Huang, Charles J. Law, François Ménard, Bertrand Lefloch, Charlotte Vastel, Ana Lopez-Sepulcre, Cécile Favre, Eleonora Bianchi, Cecilia Ceccarelli**

There is mounting evidence that the composition and structure of planetary systems are intimately linked to their birth environments. During the past decade, several spectral surveys probed the chemistry of the earliest stages of star formation and of late planet-forming disks. However, very little is known about the chemistry of intermediate protostellar stages, i.e. Class I Young Stellar Objects (YSOs), where planet formation may have already begun. We present here the first results of a 3mm spectral survey performed with the IRAM-30m telescope to investigate the chemistry of a sample of seven Class I YSOs located in the Taurus star-forming region. These sources were selected to embrace the wide diversity identified for low-mass protostellar envelope and disk systems. We present detections and upper limits of thirteen small (i.e. molecules with no more than 3 atoms) C, N, O, and S carriers - namely CO, HCO<sup>+</sup>, HCN, HNC, CN, N<sub>2</sub>H<sup>+</sup>, C<sub>2</sub>H, CS, SO, HCS<sup>+</sup>, C<sub>2</sub>S, SO<sub>2</sub>, OCS - and some of their D, <sup>13</sup>C, <sup>15</sup>N, <sup>18</sup>O, <sup>17</sup>O, and <sup>34</sup>S isotopologues. Together, these species provide constraints on gas-phase C/N/O ratios, D- and <sup>15</sup>N-fractionation, source temperature and UV exposure, as well as the overall S-chemistry. We find substantial evidence of chemical differentiation among our source sample, some of which can be traced back to Class I physical parameters, such as the disk-to-envelope mass ratio (proxy for Class I evolutionary stage), the source luminosity, and the UV-field strength. Overall, these first results allow us to start investigating the astrochemistry of Class I objects, however, interferometric observations are needed to differentiate envelope versus disk chemistry.

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### Probing Low-Energy Resonances in Water-Hydrogen Inelastic Collisions

**A. Bergeat, S. B. Morales, C. Naulin, L. Wiesenfeld, A. Faure**

Molecular scattering at collisional energies of the order of 10–100 /cm (corresponding to kinetic temperatures in the 15–150 K range) provides insight into the details of the scattering process and, in particular, of the various resonances that appear in inelastic cross sections. In this Letter, we present a detailed experimental and theoretical study

of the rotationally inelastic scattering of ground-state ortho-D<sub>2</sub>O by ground-state para-H<sub>2</sub> in the threshold region of the D<sub>2</sub>O(000) → (202) transition at 35.9 /cm. The measurements were performed with a molecular crossed beam apparatus with variable collision angle, thence with variable collisional energy. Calculations were carried out with the coupled-channel method combined with a dedicated high-level D<sub>2</sub>O-H<sub>2</sub> intermolecular potential. Our theoretical cross section 000 → 202 is found to display several resonance peaks in perfect agreement with the experimental work, in their absolute positions and relative intensities. We show that those peaks are mostly due to shape resonances, characterized here for the first time for a polyatomic molecule colliding with a diatom.

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Full-text URL: <https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.125.143402>

## The chemical structure of young high-mass star-forming clumps: (II) parsec-scale CO depletion and deuterium fraction of HCO<sup>+</sup>

**S. Feng, D. Li, P. Caselli, F. Du, Y. Lin, O. Sipilä, H. Beuther, Patricio Sanhueza, K. Tatematsu, S. Y. Liu, Q. Zhang, Y. Wang, T. Hogge, I. Jimenez-Serra, X. Lu, T. Liu, K. Wang, Z. Y. Zhang, S. Zahorecz, G. Li, H. B. Liu, and J. Yuan**

The physical and chemical properties of cold and dense molecular clouds are key to understanding how stars form. Using the IRAM 30 m and NRO 45 m telescopes, we carried out a Multiwavelength line-Imaging survey of the 70 μm-dArk and bright cLOUDs (MIAO). At a linear resolution of 0.1–0.5 pc, this work presents a detailed study of parsec-scale CO depletion and HCO<sup>+</sup> deuterium (D-) fractionation toward four sources (G11.38+0.81, G15.22–0.43, G14.49–0.13, and G34.74–0.12) included in our full sample. In each source with T < 20 K and n<sub>H</sub> ~ 1e4–1e5 cm<sup>-3</sup>, we compared pairs of neighboring 70 μm bright and dark clumps and found that (1) the H<sub>2</sub> column density and dust temperature of each source show strong spatial anticorrelation; (2) the spatial distribution of CO isotopologue lines and dense gas tracers, such as 1–0 lines of H<sub>13</sub>CO<sup>+</sup> and DCO<sup>+</sup>, are anticorrelated; (3) the abundance ratio between C<sub>18</sub>O and DCO<sup>+</sup> shows a strong correlation with the source temperature; (4) both the C<sub>18</sub>O depletion factor and D-fraction of HCO<sup>+</sup> show a robust decrease from younger clumps to more evolved clumps by a factor of more than 3; and (5) preliminary chemical modeling indicates that chemical ages of our sources are ~8e4 yr, which is comparable to their free-fall timescales and smaller than their contraction timescales, indicating that our sources are likely dynamically and chemically young.

The Astrophysical Journal, 901:145 (24pp), 2020 October 1

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## Seeds of Life in Space (SOLIS). IX. Chemical Segregation of SO<sub>2</sub> and SO toward the Low-mass Protostellar Shocked Region of L1157

**S. Feng, C. Codella, C. Ceccarelli, P. Caselli, A. Lopez-Sepulcre, R. Neri, F. Fontani, L. Podio, B. Lefloch, H. B. Liu, R. Bachiller, and S. Viti**

We present observations of SO and SO<sub>2</sub> lines toward the shocked regions along the L1157 chemically rich outflow, taken in the context of the Seeds of Life in Space IRAM

Northern Extended Millimeter Array Large Program, and supported by data from the Submillimeter Array and IRAM-30 m telescope at 1.1–3.6 mm wavelengths. We simultaneously analyze, for the first time, all of the brightest shocks in the blueshifted lobe, namely, B0, B1, and B2. We found the following. (1) SO and SO<sub>2</sub> may trace different gas, given that the large(-scale) velocity gradient analysis indicates for SO<sub>2</sub> a volume density ( $1e5$ – $1e6$  cm<sup>-3</sup>) denser than that of the gas emitting in SO by a factor up to an order of magnitude. (2) Investigating the 0.1 pc scale field of view, we note a tentative gradient along the path of the precessing jet. More specifically,  $c(\text{SO}/\text{SO}_2)$  decreases from the B0–B1 shocks to the older B2. (3) At a linear resolution of 500–1400 au, a tentative spatial displacement between the two emitting molecules is detected, with the SO peak closer (with respect to SO<sub>2</sub>) to the position where the recent jet is impinging on the B1 cavity wall. Our astrochemical modeling shows that the SO and SO<sub>2</sub> abundances evolve on timescales less than about 1000 years. Furthermore, the modeling requires high abundances ( $2e-6$ ) of both H<sub>2</sub>S/H and S/H injected in the gas phase due to the shock occurrence, so prefrozen OCS only is not enough to reproduce our new observations.

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Full-text URL: <https://arxiv.org/abs/2005.04629>

## The Chemical Structure of Young High-mass Star-forming Clumps. I. Deuteration

S. Feng, P. Caselli, K. Wang, Y. Lin, H. Beuther, and O. Sipilä

The chemical structure of high-mass star nurseries is important for a general understanding of star formation. Deuteration is a key chemical process in the earliest stages of star formation because its efficiency is sensitive to the environment. Using the IRAM-30 m telescope at 1.3–4.3 mm wavelengths, we have imaged two parsec-scale high-mass protostellar clumps (P1 and S) that show different evolutionary stages but are located in the same giant filamentary infrared dark cloud G28.34+0.06. Deep spectral images at subparsec resolution reveal the dust and gas physical structures of both clumps. We find that (1) the low-J lines of N<sub>2</sub>H<sup>+</sup>, HCN, HNC, and HCO<sup>+</sup> isotopologues are subthermally excited; and (2) the deuteration of N<sub>2</sub>H<sup>+</sup> is more efficient than that of HCO<sup>+</sup>, HCN, and HNC by an order of magnitude. The deuteration of these species are enriched toward the chemically younger clump S compared with P1, indicating that this process favors the colder and denser environment ( $T_{\text{kin}} \sim 14$  K,  $N(\text{NH}_3) \sim 9e15$  cm<sup>-2</sup>). In contrast, single deuteration of NH<sub>3</sub> is insensitive to the environmental difference between P1 and S; and (3) single deuteration of CH<sub>3</sub>OH (>10%) is detected toward the location where CO shows a depletion of  $\sim 10$ . This comparative chemical study between P1 and S links the chemical variations to the environmental differences and shows chemical similarities between the early phases of high- and low-mass star-forming regions.

The Astrophysical Journal, 883:202 (23pp), 2019 October 1

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Full-text URL: <https://arxiv.org/abs/1909.00209>

## Rate Constants of the CN + Toluene Reaction from 15 to 294 K and Interstellar Implications

Joey Messinger, Divita Gupta, Ilsa R. Cooke, Mitchio Okumura, Ian R. Sims

CN is known for its fast reactions with hydrocarbons at low temperatures, but relatively

few studies have focused on the reactions between CN and aromatic molecules. The recent detection of benzonitrile in the interstellar medium, believed to be produced by the reaction of CN and benzene, has ignited interest in studying these reactions. Here, we report rate constants of the CN + toluene (C<sub>7</sub>H<sub>8</sub>) reaction between 15 and 294 K using a CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme; reaction kinetics in uniform supersonic flow) apparatus coupled with the pulsed laser photolysis-laser-induced fluorescence (PLP-LIF) technique. We also present the stationary points on the potential energy surface of this reaction to study the available reaction pathways. We find the rate constant does not change over this temperature range, with an average value of  $(4.1 \pm 0.2) \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$ , which is notably faster than the only previous measurement at 105 K. While the reason for this disagreement is unknown, we discuss the possibility that it is related to enhanced multiphoton effects in the previous work.

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## Gas-phase formation of acetaldehyde: review and new theoretical computations

**F. Vazart, C. Ceccarelli, N. Balucani, E. Bianchi, D. Skouteris**

Among all the interstellar complex organic molecules (iCOMs), acetaldehyde is one of the most widely detected species. The question of its formation route(s) is, therefore, of a major interest regarding astrochemical models. In this paper, we provide an extensive review of the gas-phase formation paths that were, or are, reported in the literature and the major astrochemical databases. Four different gas-phase formation routes stand out : (1) CH<sub>3</sub>OCH<sub>3</sub> + H<sup>+</sup> / CH<sub>3</sub>CHOH<sup>+</sup> + e<sup>-</sup>, (2) C<sub>2</sub>H<sub>5</sub> + O(3P), (3) CH<sub>3</sub>OH + CH and (4) CH<sub>3</sub>CH<sub>2</sub>OH + OH / CH<sub>3</sub>CHOH + O(3P). Paths (2) and (3) were not studied neither via laboratory or theoretical works in the low temperature and density regime valid for the ISM. Thus, we carried out new accurate quantum chemistry computations. A theoretical kinetics study at low temperatures (7-300 K), adopting the RRKM scheme, was also performed. We confirm that reaction (2) is efficient in forming acetaldehyde in the 7-300 temperature range ( $\alpha = 1.21 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$  and  $\beta = 0.16$ ). On the contrary, our new computations disprove the formation of acetaldehyde through reaction (3) ( $\alpha = 1.84, 0.67 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$  and  $\beta = -0.07, -0.95$ ). Path (1) was showed to be inefficient too by recent computations, while path (4) was formerly considered for glycolaldehyde formation, having acetaldehyde as a by-product. In conclusions, of the four above paths only two, the (2) and (4), are potentially efficient gas-phase reaction routes for the formation of acetaldehyde and we encourage astrochemical modellers to only consider them. Comparison with astronomical observations suggest that path (4) may actually play the major role.

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## Discovery of HC<sub>3</sub>O<sup>+</sup> in space: The chemistry of O-bearing species in TMC-1

**J. Cernicharo, N. Marcelino, M. Agundez, Y. Endo, C. Cabezas, C. Bermudez, B. Tercero, P. de Vicente**

Using the Yebes 40m and IRAM 30m radio telescopes, we detected a series of

harmonically related lines with a rotational constant  $B_0=4460.590 \pm 0.001$  MHz and a distortion constant  $D_0=0.511 \pm 0.005$  kHz towards the cold dense core TMC-1. High-level-of-theory ab initio calculations indicate that the best possible candidate is protonated tricarbon monoxide, HC3O+. We have succeeded in producing this species in the laboratory and observed its  $J = 2-1$  and  $3-2$  rotational transitions. Hence, we report the discovery of HC3O+ in space based on our observations, theoretical calculations, and laboratory experiments. We derive an abundance ratio  $N(\text{C3O})/N(\text{HC3O}+) = 7$ . The high abundance of the protonated form of C3O is due to the high proton affinity of the neutral species. The chemistry of O-bearing species is modelled, and predictions are compared to the derived abundances from our data for the most prominent O-bearing species in TMC-1.

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## Chemical evolution during the formation of a protoplanetary disk

**A. Coutens, B. Commerçon, V. Wakelam**

The chemical composition of protoplanetary disks is expected to impact the composition of the forming planets. Characterizing the diversity of chemical composition in disks and the physicochemical factors that lead to this diversity is consequently of high interest. The aim of this study is to investigate the chemical evolution from the prestellar phase to the formation of the disk, and to determine the impact that the chemical composition of the cold and dense core has on the final composition of the disk. We performed 3D nonideal magneto-hydrodynamic (MHD) simulations of a dense core collapse using the adaptive-mesh-refinement RAMSES code. For each particle ending in the young rotationally supported disk, we ran chemical simulations with the three-phase gas-grain chemistry code Nautilus. Two different sets of initial abundances, which are characteristic of cold cores, were considered. The final distributions of the abundances of common species were compared to each other, as well as with the initial abundances of the cold core. We find that the spatial distributions of molecules reflect their sensitivity to the temperature distribution. The main carriers of the chemical elements in the disk are usually the same as the ones in the cold core, except for the S-bearing species, where HS is replaced by H<sub>2</sub>S<sub>3</sub>, and the P-bearing species, where atomic P leads to the formation of PO, PN, HCP, and CP. However, the abundances of less abundant species change over time. This is especially the case for "large" complex organic molecules (COMs) such as CH<sub>3</sub>CHO, CH<sub>3</sub>NH<sub>2</sub>, CH<sub>3</sub>OCH<sub>3</sub>, and HCOOCH<sub>3</sub> which see their abundances significantly increase during the collapse. These COMs often present similar abundances in the disk despite significantly different abundances in the cold core. In contrast, the abundances of many radicals decrease with time. A significant number of species still show the same abundances in the cold core and the disk, which indicates efficient formation of these molecules in the cold core. This includes H<sub>2</sub>O, H<sub>2</sub>CO, HNC, and "small" COMs such as CH<sub>3</sub>OH, CH<sub>3</sub>CN, and NH<sub>2</sub>CHO. We computed the MHD resistivities within the disk for the full gas-grain chemical evolution and find results in qualitative agreement with the literature assuming simpler chemical networks. In conclusion, the chemical content of prestellar cores is expected to affect the chemical composition of disks. The impact is more or less important depending on the type of species. Users of stand-alone chemical models of disks should pay special attention to the initial abundances they choose.

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## Tentative detection of HC5NH<sup>+</sup> in TMC-1

**N. Marcelino, M. Agundez, B. Tercero, C. Cabezas, C. Bermudez, J. D. Gallego, P. de Vicente, J. Cernicharo**

Using the Yebes 40m radio telescope, we report the detection of a series of seven lines harmonically related with a rotational constant  $B_0=1295.81581 \pm 0.00026$  MHz and a distortion constant  $D_0=27.3 \pm 0.5$  Hz towards the cold dense cloud TMC-1. Ab initio calculations indicate that the best possible candidates are the cations HC5NH<sup>+</sup> and NC4NH<sup>+</sup>. From a comparison between calculated and observed rotational constants and other arguments based on proton affinities and dipole moments, we conclude that the best candidate for a carrier of the observed lines is the protonated cyanodiacetylene cation, HC5NH<sup>+</sup>. The HC5N/HC5NH<sup>+</sup> ratio derived in TMC-1 is 240, which is very similar to the HC3N/HC3NH<sup>+</sup> ratio. Results are discussed in the framework of a chemical model for protonated molecules in cold dense clouds.

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## Discovery of HC4NC in TMC-1: A study of the isomers of HC3N, HC5N, and HC7N

**J. Cernicharo, N. Marcelino, M. Agundez, C. Bermudez, C. Cabezas, B. Tercero, J. R. Pardo**

We present a study of the isocyano isomers of the cyanopolyynes HC3N, HC5N, and HC7N in TMC-1 and IRC+10216 carried out with the Yebes 40m radio telescope. This study has enabled us to report the detection, for the first time in space, of HCCCCNC in TMC-1 and to give upper limits for HC6NC in the same source. In addition, the deuterated isotopologues of HCCNC and HNCCC were detected, along with all <sup>13</sup>C substitutions of HCCNC, also for the first time in space. The abundance ratios of HC3N and HC5N, with their isomers, are very different in TMC-1 and IRC+10216, namely,  $N(\text{HC5N})/N(\text{HC4NC})$  is 300 and  $>2100$ , respectively. We discuss the chemistry of the metastable isomers of cyanopolyynes in terms of the most likely formation pathways and by comparing observational abundance ratios between different sources.

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Full-text URL: <https://arxiv.org/abs/2009.07686>

## Interstellar nitrile anions: Detection of C3N<sup>-</sup> and C5N<sup>-</sup> in TMC-1

**J. Cernicharo, N. Marcelino, J. R. Pardo, M. Agundez, B. Tercero, P. de Vicente, C. Cabezas, C. Bermudez**

We report on the first detection of C3N<sup>-</sup> and C5N<sup>-</sup> towards the cold dark core TMC-1 in the Taurus region, using the Yebes 40 m telescope. The observed C3N/C3N<sup>-</sup> and C5N/C5N<sup>-</sup> abundance ratios are 140 and 2, respectively; that is similar to those found in the circumstellar envelope of the carbon-rich star IRC+10216. Although the formation mechanisms for the neutrals are different in interstellar (ion-neutral reactions) and circumstellar clouds (photodissociation and radical-neutral reactions), the similarity of

the C3N/C3N- and C5N/C5N- abundance ratios strongly suggests a common chemical path for the formation of these anions in interstellar and circumstellar clouds. We discuss the role of radiative electronic attachment, reactions between N atoms and carbon chain anions C<sub>n</sub><sup>-</sup>, and that of H<sup>-</sup> reactions with HC3N and HC5N as possible routes to form C<sub>n</sub>N<sup>-</sup>. The detection of C5N<sup>-</sup> in TMC-1 gives strong support for assigning to this anion the lines found in IRC+10216, as it excludes the possibility of a metal-bearing species, or a vibrationally excited state. New sets of rotational parameters have been derived from the observed frequencies in TMC-1 and IRC+10216 for C5N<sup>-</sup> and the neutral radical C5N.

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Full-text URL: <https://arxiv.org/abs/2009.03240>

## Observations of the Onset of Complex Organic Molecule Formation in Interstellar Ices

**L. Chu, K. Hodapp, A. Boogert**

Isolated dense molecular cores are investigated to study the onset of complex organic molecule formation in interstellar ice. Sampling three cores with ongoing formation of low-mass stars (B59, B335, and L483) and one starless core (L694-2) we sample lines of sight to nine background stars and five young stellar objects (YSOs; A<sub>K</sub> ~0.5 - 4.7). Spectra of these stars from 2-5 μm with NASA's Infrared Telescope Facility (IRTF) simultaneously display signatures from the cores of H<sub>2</sub>O (3.0 μm), CH<sub>3</sub>OH (C-H stretching mode, 3.53 μm) and CO (4.67 μm) ices. The CO ice is traced by nine stars in which five show a long wavelength wing due to a mixture of CO with polar ice (CO<sub>r</sub>), presumably CH<sub>3</sub>OH. Two of these sight lines also show independent detections of CH<sub>3</sub>OH. For these we find the ratio of the CH<sub>3</sub>OH:CO<sub>r</sub> is 0.55±0.06 and 0.73±0.07 from L483 and L694-2, respectively. The detections of both CO and CH<sub>3</sub>OH for the first time through lines of sight toward background stars observationally constrains the conversion of CO into CH<sub>3</sub>OH ice. Along the lines of sight most of the CO exists in the gas phase and ≤15% of the CO is frozen out. However, CH<sub>3</sub>OH ice is abundant with respect to CO (~50%) and exists mainly as a CH<sub>3</sub>OH-rich CO ice layer. Only a small fraction of the lines of sight contains CH<sub>3</sub>OH ice, presumably that with the highest density. The high conversion of CO to CH<sub>3</sub>OH can explain the abundances of CH<sub>3</sub>OH ice found in later stage Class 1 low mass YSO envelopes (CH<sub>3</sub>OH:CO<sub>r</sub> ~ 0.5-0.6). For high mass YSOs and one Class 0 YSO this ratio varies significantly implying local variations can affect the ice formation. The large CH<sub>3</sub>OH ice abundance indicates that the formation of complex organic molecules is likely during the pre-stellar phase in cold environments without higher energy particle interactions (e.g. cosmic rays).

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## Rotational spectra of vibrationally excited AlO and TiO in oxygen rich stars

**T. Danilovich, C. A. Gottlieb, L. Decin, A. M. S. Richards, K. L. K. Lee, T. Kaminski, N. A. Patel, K. H. Young, and K. M. Menten**

Rotational transitions in vibrationally excited AlO and TiO — two possible precursors of dust — were observed in the 300 GHz range (1 mm wavelength) towards the oxygen rich AGB stars R Dor and IK Tau with ALMA, and vibrationally excited AlO was observed towards the red supergiant VY CMa with the SMA. The J=11-10 transition of TiO in the

$v=1$  and  $2$  levels, and the  $N=9-8$  transition in the  $v=2$  level of AIO were identified towards R Dor; the  $J=11-10$  line of TiO was identified in the  $v=1$  level towards IK Tau; and two transitions in the  $v=1$  and  $2$  levels of AIO were identified towards VY CMa. The newly-derived high vibrational temperature of TiO and AIO in R Dor of  $1800 \pm 200$  K, and prior measurements of the angular extent confirm that the majority of the emission is from a region within  $\leq 2R^*$  of the central star. A full radiative transfer analysis of AIO in R Dor yielded a fractional abundance of  $\sim 3\%$  of the solar abundance of Al. From a similar analysis of TiO a fractional abundance of  $\sim 78\%$  of the solar abundance of Ti was found. The observations provide indirect evidence that TiO is present in a rotating disk close to the star. Further observations in the ground and excited vibrational levels are needed to determine whether AIO, TiO, and TiO<sub>2</sub> are seeds of the Al<sub>2</sub>O<sub>3</sub> dust in R Dor, and perhaps in the gravitationally bound dust shells in other AGB stars with low mass loss rates.

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## Cosmic ray tracks in astrophysical ices: Modeling with the Geant4-DNA Monte Carlo Toolkit

**Christopher N. Shingledecker, Sebastien Incerti, Alexei Ivlev, Dimitris Emfietzoglou, Ioanna Kyriakou, Anton Vasyunin, Paola Caselli**

Cosmic rays are ubiquitous in interstellar environments, and their bombardment of dust-grain ice mantles is a possible driver for the formation of complex, even prebiotic molecules. Yet, critical data that are essential for accurate modeling of this phenomenon, such as the average radii of cosmic-ray tracks in amorphous solid water (ASW) remain unconstrained. It is shown that cosmic ray tracks in ASW can be approximated as a cylindrical volume with an average radius that is mostly independent of the initial particle energy. Interactions between energetic ions and both a low-density amorphous (LDA) and high-density amorphous (HDA) ice target are simulated using the Geant4-DNA Monte Carlo toolkit, which allows for tracking secondary electrons down to subexcitation energies in the material. We find the peak track core radii,  $r_{cyl}$ , for LDA and HDA ices to be 9.9 nm and 8.4 nm, respectively - somewhat less than double the value of 5 nm often assumed in astrochemical models.

ApJ, accepted

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## Anharmonic Frequencies and Spectroscopic Constants of OAlOH and AlOH: Strong Bonding but Unhindered Motion

**Ryan C. Fortenberry, Tarek Trabelsi, and Joseph S. Francisco**

The astrophysical buildup of premineral nanocrystals from atoms to the smallest network-covalent solids will require observations of various small molecules containing the most common elements in minerals including aluminum and oxygen. The present work utilizes high-level quantum chemical quartic force field (QFF) approaches to produce anharmonic vibrational frequencies and spectroscopic constants for such species. The computed  $B_{eff}$  for the astrochemically known AlOH molecule at 15780.5 MHz is a mere 40 MHz above the experimental value implying that the  $B_{eff}$  for OAlOH at 5580.9 MHz is similarly accurate. The additional 7.31 D dipole moment in OAlOH implies that this molecule is a viable target for interstellar observation. Unlike the other anharmonic vibrational frequencies reported in this work, the Al-O-H bending frequencies in both AlOH and OAlOH are poorly described in the present QFF results.



However, this failing actually highlights the fact that these bends are exceptionally floppy yet with counterintuitive exceedingly strong bonding. The Al–O bond energies are 128.2 and 107.2 kcal/mol, respective of AlOH and OAlOH, while the barriers to linearity are meager 16.6 and 380.7 cm<sup>-1</sup> (0.1 and 1.1 kcal/mol).

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## Laboratory gas-phase vibrational spectra of [C<sub>3</sub>H<sub>3</sub>]<sup>+</sup> isomers and isotopologues by IRPD spectroscopy

**A. N. Marimuthu, D. Sundelin, S. Thorwirth, B. Redlich, W. D. Geppert, S. Brünken**

Gas phase vibrational spectra of [C<sub>3</sub>H<sub>3</sub>]<sup>+</sup> isomers and their fully deuterated isotopologues measured in a cryogenic 22-pole ion trap are presented. The widely tunable free electron laser for infrared experiments, FELIX, was employed to cover the frequency range 500–2400 cm<sup>-1</sup>, complemented with an OPO/OPA system covering 2800–3400 cm<sup>-1</sup>. Spectral assignments for both the linear and cyclic isomeric form (H<sub>2</sub>C<sub>3</sub>H<sup>+</sup> and c-C<sub>3</sub>H<sub>3</sub><sup>+</sup>, respectively) are made based on various high-level computational studies. The effect of ion source conditions and different precursors (allene and propargyl chloride) for the preferential production of a specific isomer is discussed. The perturbation of the vibrational band position due to complexation with neon in the recorded infrared-predissociation (IRPD) spectra are also reported in this study.

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## Prestellar grain-surface origins of deuterated methanol in comet 67P/Churyumov-Gerasimenko

**Maria N. Drozdovskaya, Isaac R. H. G. Schroeder, I. Martin Rubin, Kathrin Altwegg, Ewine F. van Dishoeck, Beatrice M. Kulterer, Johan De Keyser, Stephen A. Fuselier, Michael Combi**

Deuterated methanol is one of the most robust windows astrochemists have on the individual chemical reactions forming deuterium-bearing molecules and the physicochemical history of the regions where they reside. The first-time detection of mono- and di-deuterated methanol in a cometary coma is presented for comet 67P/Churyumov-Gerasimenko using Rosetta-ROSINA data. D-methanol (CH<sub>3</sub>OD and CH<sub>2</sub>DOH combined) and D<sub>2</sub>-methanol (CH<sub>2</sub>DOD and CHD<sub>2</sub>OH combined) have an abundance of 5.5±0.46 and 0.00069±0.00014 per cent relative to normal methanol. The data span a methanol deuteration fraction (D/H ratio) in the 0.71–6.6 per cent range, accounting for statistical corrections for the location of D in the molecule and including statistical error propagation in the ROSINA measurements. It is argued that cometary CH<sub>2</sub>DOH forms from CO hydrogenation to CH<sub>3</sub>OH and subsequent H-D substitution reactions in CH<sub>3</sub>-R. CHD<sub>2</sub>OH is likely produced from deuterated formaldehyde. Meanwhile, CH<sub>3</sub>OD and CH<sub>2</sub>DOD, could form via H-D exchange reactions in OH-R in the presence of deuterated water ice. Methanol formation and deuteration is argued to occur at the same epoch as D<sub>2</sub>O formation from HDO, with formation of mono-deuterated water, hydrogen sulfide, and ammonia occurring prior to that. The cometary D-methanol/methanol ratio is demonstrated to agree most

closely with that in prestellar cores and low-mass protostellar regions. The results suggest that cometary methanol stems from the innate cold (10-20 K) prestellar core that birthed our Solar System. Cometary volatiles individually reflect the evolutionary phases of star formation from cloud to core to protostar.

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## Announcements

### Postdoctoral Research Associate positions

The University of Virginia (UVA) invites applications for Postdoctoral Research Associate positions as part of the interdisciplinary Virginia Initiative on Cosmic Origins (VICO).

The incumbents will lead ambitious, independent research programs related to Cosmic Origins science, expected to align with the wide range of research at UVA, as well as at the National Radio Astronomy Observatory (NRAO) on the grounds of the University.

The relevant themes include star formation, planet formation and evolution, planetary science, astrochemistry, quantum chemistry and astrobiology, from both theoretical and observational perspectives. See [www.cosmicorigins.space](http://www.cosmicorigins.space) for more information.

The Postdoctoral Research Associates will participate in departmental activities and promote collaboration both within VICO and with its partner institutes, Chalmers University of Technology, Gothenburg, Sweden and the Center for Astrochemical Studies at the Max Planck Institute for Extraterrestrial Physics (MPE), Garching, Germany.

There are two types of research programs being advertised this year: 1) Virginia Cosmic Origins Program; (2) Virginia-Chalmers Cosmic Origins Program. Applicants should indicate in their cover letter if they have preferences among these research programs.

**QUALIFICATION REQUIREMENTS:** Applicants are required to have a Ph.D. in astrophysics, astrochemistry, astrobiology or related disciplines by the appointment start date.

**APPLICATION PROCEDURE:** Apply online at [https://uva.wd1.myworkdayjobs.com/en-US/UVAJobs/job/Charlottesville-VA/Virginia-Cosmic-Origins-Postdoctoral-Research-Associate\\_R0018893](https://uva.wd1.myworkdayjobs.com/en-US/UVAJobs/job/Charlottesville-VA/Virginia-Cosmic-Origins-Postdoctoral-Research-Associate_R0018893) and attach as a single PDF document a cover letter; curriculum vitae; list of publications; summary of previous and current research (limited to 3 pages, including references); research proposal (limited to 3 pages text plus up to 2 pages of references/figures). Applicants should also arrange for 3 letters of recommendation to be submitted to [vico-postdoc@virginia.edu](mailto:vico-postdoc@virginia.edu).

**APPLICATION DEADLINE:** Applications must be received by December 15, 2020 to be considered. The University will perform background checks on all new hires prior to employment

All positions will start at UVA and are initially a one-year appointment, with renewal for an additional two one-year increments for the Virginia position, contingent upon satisfactory performance and available funding, and an additional three one-year increments for the Virginia-Chalmers position, contingent upon satisfactory performance and available funding (Years 3 and 4 would be at Chalmers).

Questions regarding the position should be directed to: Eric Herbst ([eh2ef@virginia.edu](mailto:eh2ef@virginia.edu)), Jonathan Tan ([jct6e@virginia.edu](mailto:jct6e@virginia.edu)), Ilse Cleaves ([lic3f@virginia.edu](mailto:lic3f@virginia.edu)), Rob Garrod ([rg5qp@virginia.edu](mailto:rg5qp@virginia.edu)) or Zhi-Yun Li ([z14h@virginia.edu](mailto:z14h@virginia.edu)). Questions regarding the application process should be directed to Richard Haverstrom, Faculty Search Advisor, at [rkh6j@Virginia.EDU](mailto:rkh6j@Virginia.EDU).

A competitive salary and benefits package is offered at University of Virginia. For more information on the benefits available to postdoctoral associates at UVA, visit [postdoc.virginia.edu](http://postdoc.virginia.edu) and [hr.virginia.edu/benefits](http://hr.virginia.edu/benefits). The positions also include travel funds and opportunities for dissemination, networking, and international collaboration. Additional information about VICO can be found at <http://cosmicorigins.space/> The University of Virginia, including the UVA Health System and the University Physician's Group are fundamentally committed to the diversity of our faculty and staff. We believe diversity is excellence expressing itself through every person's perspectives and lived experiences. We are equal opportunity and affirmative action employers. All qualified applicants will receive consideration for employment without regard to age, color, disability, gender identity, marital status, national or ethnic origin, political affiliation, race, religion, sex (including pregnancy), sexual orientation, veteran status, and family medical or genetic information. Included Benefits: Benefits Included

The University of Virginia, including the UVA Health System which represents the UVA Medical Center, Schools of Medicine and Nursing, UVA Physician's Group and the Claude Moore Health Sciences Library, are fundamentally committed to the diversity of our faculty and staff. We believe diversity is excellence expressing itself through every person's perspectives and lived experiences. We are equal opportunity and affirmative action employers. All qualified applicants will receive consideration for employment without regard to age, color, disability, gender identity or expression, marital status, national or ethnic origin, political affiliation, race, religion, sex (including pregnancy), sexual orientation, veteran status, and family medical or genetic information.

## **Postdoctoral Position in Merged-Fast-Beams Astrochemical Studies**

The Columbia Astrophysics Laboratory (CAL) invites applications for a Postdoctoral Research Scientist (PdRS) in the group of Dr. Daniel Wolf Savin. The main goal of the project is to perform merged-fast-beams studies of deuterating reactions that form key molecules used to probe the properties of prestellar cores and protoplanetary disks. The successful candidate will be appointed and based at Columbia. Appointments are for one year, with the possibility of renewal for up to two additional years contingent on the availability of funds and mutual satisfaction.

The successful candidate will have a Ph.D. or the equivalent degree in Physics, Chemistry, Astrophysics, or a related field, with an emphasis in molecular physics. Desired laboratory skills include experience with ion sources, fast ion beams, ion optics, ultra-high vacuum techniques, infrared lasers, apparatus design and construction, single particle detectors and associated electronics, analog and digital signal processing, data reduction, and statistical and systematic error propagation. Desired computer skills include programming, multidimensional data analysis, LabView, 3D CAD, SIMION, Mathematica, or similar, Linux OS, and Windows OS.

The successful candidate will have a strong background in at least some of the areas listed above, a proven research ability, and evidence of future research potential. The candidate is expected to be able to work well independently and cooperatively with a team and to communicate the results of his/her research both orally and in writing. Demonstrated written and oral communication skills are highly desirable. Questions regarding this position can be addressed to Dr. Savin at [dws26@columbia.edu](mailto:dws26@columbia.edu). Applicants should submit a cover letter, curriculum vitae (including a list of publications) and statement of past research. In addition, they should arrange to have three letters of reference sent directly by the writers to Dr. Savin. Applications will be considered only after all of the requested material has been received. Applications and letters should be submitted by email to [dws26@columbia.edu](mailto:dws26@columbia.edu). Screening of applicants will begin immediately and will continue until the position has been filled.

Columbia is an Equal Opportunity Employer/Disability/Veteran Employer. CAL values a

diverse workforce and culture of inclusion, which are keys to attracting and engaging the brightest minds to further our record of scientific excellence and groundbreaking innovations. Applications from women, minorities, and other underrepresented groups are strongly encouraged.

## **PhD position in the Experimental Biophysics and Space Sciences group, Physics Department, Freie Universität Berlin (Germany)**

(Deadline extended 16/11/2020)

We offer a research assistant position in the “Experimental Biophysics and Space Sciences” group in the Physics Department of Freie Universität Berlin. The position is part of the project 'Finding Life', funded by the Freigeist program of the Volkswagen Foundation, and focuses on how we can potentially detect life on another planet. Within the framework of the project, it is planned to mimic exotic planetary and atmospheric conditions in the laboratory in order to study their impact on the stability of spectroscopic signatures of potential biomarkers and molecules, which are associated to life. The project is embedded in international collaborations with partner in Europe and the US, and it is linked to projects on an outside exposure platform on the International Space Station in order to investigate the molecular stability of biosignatures in space. We offer a creative and inspiring environment for experimental approaches and interesting research in the fields of planetary and biophysics, astrochemistry, planetary and space sciences. Moreover, we highly encourage the development of new ideas and projects and provide opportunities to do so.

-Job description: We are looking for highly motivated candidates with an interest in interdisciplinary research in the fields of biophysics, astrophysics, astrochemistry, astrobiology and space sciences. A main task of the project is the design, planning and realisation of experiments for simulating planetary conditions in the laboratory; therefore, we envisage a significant portion of the time being spent working in the laboratory. The selected candidate will analyse, present (conferences) and publish (peer-reviewed literature) spectroscopic and mass-spectrometric data from the planetary simulations. Due to the international links and collaborations, it is required to plan, conduct and synchronise experiments with project partners, which will include interactions with the German Space Agency (DLR), the European Space and Technology Centre (ESTEC/ESA) and NASA Ames Research Center.

-Requirements: Master degree (or equivalent) in Physics, Chemistry, Biology or related disciplines.

Further information and contact at: [https://www.fu-berlin.de/universitaet/beruf-karriere/jobs/wiss/20\\_fb-physik/PH-2020-Freigeist-PhD\\_E.html](https://www.fu-berlin.de/universitaet/beruf-karriere/jobs/wiss/20_fb-physik/PH-2020-Freigeist-PhD_E.html)