AstroChemical Newsletter #68

July 2021

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

Neutral–neutral synthesis of organic molecules in cometary comae

M. A. Cordiner & S. B. Charnley

Remote and in-situ observations of cometary gases have revealed the presence of a wealth of complex organic molecules, including carbon chains, alcohols, imines and the amino acid glycine. Such chemical complexity in cometary material implies that impacts by comets could have supplied reagents for prebiotic chemistry to young planetary surfaces. However, the assumption that some of the molecules observed in cometary comae at millimetre wavelengths originate from ices stored inside the nucleus has not yet been proven. In fact, the comae of moderately-active comets reach sufficient densities within a few thousand kilometers of the nucleus for an active (solar radiation-driven) photochemistry to ensue. Here we present results from our latest chemical-hydrodynamic models incorporating an updated reaction network, and show that the commonly-observed HC3N (cyanoacetylene) and NH2CHO (formamide) molecules can be efficiently produced in cometary comae as a result of two-body, neutral-neutral, gas-phase reactions involving well-known coma species. In the presence of a near-nucleus distributed source of CN (similar to that observed by the Rosetta spacecraft at comet 67P), we find that sufficient HC3N and NH2CHO can be synthesized to match the abundances of these molecules previously observed in Oort cloud comets. The precise coma origins of these (and other) complex organic molecules can be verified through radio interferometric mapping, for example, using the Atacama Large Millimeter/submillimeter Array (ALMA).

Monthly Notices of the Royal Astronomical Society, Volume 504, Issue 4, July 2021, Pages 5401–5408
DOI: 10.1093/mnras/stab1123
Full-text URL: https://arxiv.org/abs/2104.07577

TMC-1, the starless core sulfur factory: Discovery of NCS, HCCS, H2CCS, H2CCCS, and C4S and detection of C5S

J. Cernicharo, C. Cabezas, M. Agundez, B. Tercero, J. R. Pardo, N. Marcelino, J. D. Gallego, F. Tercero, J. A. Lopez-Perez, P. de Vicente

We report the detection of the sulfur-bearing species NCS, HCCS, H2CCS, H2CCCS, and C4S for the first time in space. These molecules were found towards TMC-1 through the observation of several lines for each species. We also report the detection of C5S for the first time in a cold cloud through the observation of five lines in the 31-50 GHz range. The derived column densities are N(NCS) = (7.8 +/- 0.6)e11 cm-2, N(HCCS) = (6.8 +/- 0.6)e11 cm-2, N(H2CCS) = (7.8 +/- 0.8)e11 cm-2, N(H2CCCS) =

(3.7 +/- 0.4)e11 cm-2, N(C4S) = (3.8 +/- 0.4)e10 cm-2, and N(C5S) = (5.0 +/- 1.0)e10 cm-2. The observed abundance ratio between C3S and C4S is 340, that is to say a factor of approximately one hundred larger than the corresponding value for CCS and C3S. The observational results are compared with a state-of-the-art chemical model, which is only partially successful in reproducing the observed abundances. These detections underline the need to improve chemical networks dealing with S-bearing species.

A&A, 648, L3 (2021)
DOI: 10.1051/0004-6361/202140642
Full-text URL: https://arxiv.org/abs/2103.12431

Cumulene carbenes in TMC-1: Astronomical discovery of l-H2C5

C. Cabezas, B. Tercero, M. Agúndez, N. Marcelino, J. R. Pardo, P. de Vicente and J. Cernicharo

We report the first detection in space of the cumulene carbon chain l-H2C5. A total of eleven rotational transitions, with Jup = 7-10 and Ka = 0 and 1, were detected in TMC-1 in the 31.0-50.4 GHz range using the Yebes 40m radio telescope. We derive a column density of (1.8 +/-0.5)e10 cm-2. In addition, we report observations of other cumulene carbenes detected previously in TMC-1, to compare their abundances with the newly detected cumulene carbene chain. We find that l-H2C5 is ~4.0 times less abundant than the larger cumulene carbene l-H2C6, while it is ~300 and ~500 times less abundant than the shorter chains l-H2C3 and l-H2C4. We discuss the most likely gas-phase chemical routes to these cumulenes in TMC-1 and stress that chemical kinetics studies able to distinguish between different isomers are needed to shed light on the chemistry of CnH2 isomers with n > 3.

A&A 650, L9 (2021)
DOI: 10.1051/0004-6361/202141274
Full-text URL: https://arxiv.org/abs/2106.00635

Quantum study of reaction O (3P) + H2 (v,j) → OH + H: OH formation in strongly UV-irradiated gas

A. Veselinova, M. Agundez, J. R. Goicoechea, M. Menendez, A. Zanchet, E. Verdasco, P. G. Jambrina, F. J. Aoiz

The reaction between atomic oxygen and molecular hydrogen is an important one in astrochemistry as it regulates the abundance of the hydroxyl radical and serves to open the chemistry of oxygen in diverse astronomical environments. However, the existence of a high activation barrier in the reaction with ground state oxygen atoms limits its efficiency in cold gas. In this study we calculate the dependence of the reaction rate coefficient on the rotational and vibrational state of H2 and evaluate the impact on the abundance of OH in interstellar regions strongly irradiated by far-UV photons, where H2 can be efficiently pumped to excited vibrational states. We use a recently calculated potential energy surface and carry out time-independent quantum mechanical scattering calculations to compute rate coefficients for the reaction O(3P) + H2(v,j) -> OH + H, with H2 in vibrational states v = 0-7 and rotational states j = 0-10. We find that the reaction becomes significantly faster with increasing vibrational quantum number of H2, although even for high vibrational states of H2 (v = 4-5) for which the reaction is barrierless, the rate coefficient does not strictly attain the collision limit and still maintains a positive dependence with temperature. We implemented the calculated state-specific rate coefficients in the Meudon PDR code to model the Orion Bar PDR and evaluate the impact on the abundance of the OH radical. We find the fractional abundance of OH is enhanced by up to one order of magnitude in regions of the cloud corresponding to Av = 1.3-2.3, compared to the use of a thermal rate coefficient for O + H2, although the impact on the column density of OH is modest, of about 60 %. The calculated rate coefficients will be useful to model and interpret JWST observations of OH in strongly UV-illuminated environments.

A&A, 648, A76 (2021)
DOI: 10.1051/0004-6361/202140428
Full-text URL: https://arxiv.org/abs/2103.03810

First detection of doubly deuterated methyl acetylene (CHD2CCH and CH2DCCD)

M. Agundez, E. Roueff, C. Cabezas, J. Cernicharo, N. Marcelino

We report the first detection in space of the two doubly deuterated isotopologues of methyl acetylene. The species CHD2CCH and CH2DCCD were identified in the dense core L483 through nine and eight, respectively, rotational lines in the 72-116 GHz range using the IRAM 30m telescope. The astronomical frequencies observed here were combined with laboratory frequencies from the literature measured in the 29-47 GHz range to derive more accurate spectroscopic parameters for the two isotopologues. We derive beam-averaged column densities of (2.7 +/- 0.5)e12 cm-2 for CHD2CCH and (2.2 +/- 0.4)e12 cm-2 for CH2DCCD, which translate to abundance ratios CH3CCH/CHD2CCH = 34 +/- 10 and CH3CCH/CH2DCCD = 42 +/- 13. The doubly deuterated isotopologues of methyl acetylene are only a few times less abundant than the singly deuterated ones, concretely around 2.4 times less abundant than CH3CCD. The abundances of the different deuterated isotopologues with respect to CH3CCH are reasonably accounted for by a gas-phase chemical model in which deuteration occurs from the precursor ions C3H6D+ and C3H5D+, when the ortho-to-para ratio of molecular hydrogen is sufficiently low. This points to gas-phase chemical reactions, rather than grain-surface processes, as responsible for the formation and deuterium fractionation of CH3CCH in L483. The abundance ratios CH2DCCH/CH3CCD = 3.0 +/- 0.9 and CHD2CCH/CH2DCCD = 1.25 +/- 0.37 observed in L483 are consistent with the statistically expected values of three and one, respectively, with the slight overabundance of CHD2CCH compared to CH2DCCD being well explained by the chemical model.

A&A, 649, A171 (2021)
DOI: 10.1051/0004-6361/202140843
Full-text URL: https://www.aanda.org/articles/aa/abs/2021/05/aa40843-21/aa40843-21.html

Pure hydrocarbon cycles in TMC-1: Discovery of ethynyl cyclopropenylidene, cyclopentadiene and indene

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

We report the detection for the first time in space of three new pure hydrocarbon cycles in TMC-1: c-C3HCCH (ethynyl cyclopropenylidene), c-C5H6 (cyclopentadiene) and c-C9H8 (indene). We derive a column density of 3.1e11 cm-2 for the former cycle and similar values, in the range (1-2)e13 cm-2, for the two latter molecules. This means that cyclopentadiene and indene, in spite of their large size, are exceptionally abundant, only a factor of five less abundant than the ubiquitous cyclic hydrocarbon c-C3H2. The high abundance found for these two hydrocarbon cycles, together with the high abundance previously found for the propargyl radical (CH2CCH) and other hydrocarbons like vinyl and allenyl acetylene (Agundez et al. 2021; Cernicharo et al. 2021a,b), start to allow us to quantify the abundant content of hydrocarbon rings in cold dark clouds and to identify the intermediate species that are probably behind the in situ bottom-up synthesis of aromatic cycles in these environments. While c-C3HCCH is most likely formed through the reaction between the radical CCH and c-C3H2, the high observed abundances of cyclopentadiene and indene are difficult to explain through currently proposed chemical mechanisms. Further studies are needed to identify how are five- and six-membered rings formed under the cold conditions of clouds like TMC-1.

A&A, 649, L15 (2021)
DOI: 10.1051/0004-6361/202141156
Full-text URL: https://arxiv.org/abs/2104.13991

O-bearing complex organic molecules at the cyanopolyyne peak of TMC-1: detection of C2H3CHO, C2H3OH, HCOOCH3, and CH3OCH3

M. Agundez, N. Marcelino, B. Tercero, C. Cabezas, P. de Vicente, J. Cernicharo

We report the detection of the oxygen-bearing complex organic molecules propenal (C2H3CHO), vinyl alcohol (C2H3OH), methyl formate (HCOOCH3), and dimethyl ether (CH3OCH3) toward the cyanopolyyne peak of the starless core TMC-1. These molecules are detected through several emission lines in a deep Q-band line survey of TMC-1 carried out with the Yebes 40m telescope. These observations reveal that the cyanopolyyne peak of TMC-1, which is the prototype of cold dark cloud rich in carbon chains, contains also O-bearing complex organic molecules like HCOOCH3 and CH3OCH3, which have been previously seen in a handful of cold interstellar clouds. In addition, this is the first secure detection of C2H3OH in space and the first time that C2H3CHO and C2H3OH are detected in a cold environment, adding new pieces in the puzzle of complex organic molecules in cold sources. We derive column densities of (2.2 +/- 0.3)e11 cm-2, (2.5 +/- 0.5)e12 cm-2, (1.1 +/- 0.2)e12 cm-2, and (2.5 +/- 0.7)e12 cm-2 for C2H3CHO, C2H3OH, HCOOCH3, and CH3OCH3, respectively. Interestingly, C2H3OH has an abundance similar to that of its well known isomer acetaldehyde (CH3CHO), with C2H3OH/CH3CHO ~ 1 at the cyanopolyyne peak. We discuss potential formation routes to these molecules and recognize that further experimental, theoretical, and astronomical studies are needed to elucidate the true mechanism of formation of these O-bearing complex organic molecules in cold interstellar sources.

A&A, 649, L4 (2021)
DOI: 10.1051/0004-6361/202140978
Full-text URL: https://arxiv.org/abs/2104.11506

The sulphur saga in TMC-1: Discovery of HCSCN and HCSCCH

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

We report the detection, for the first time in space, of cyano thioformaldehyde (HCSCN) and propynethial (HCSCCH) towards the starless core TMC-1. Cyano thioformaldehyde presents a series of prominent a- and b-type lines, which are the

strongest previously unassigned features in our Q-band line survey of TMC-1. Remarkably, HCSCN is four times more abundant than cyano formaldehyde (HCOCN). On the other hand, HCSCCH is five times less abundant than propynal (HCOCCH). Surprisingly, we find an abundance ratio HCSCCH/HCSCN of 0.25, in contrast with most other ethynyl-cyanide pairs of molecules for which the CCH-bearing species is more abundant than the CN-bearing one. We discuss the formation of these molecules in terms of neutral-neutral reactions of S atoms with CH2CCH and CH2CN radicals as well as of CCH and CN radicals with H2CS. The calculated abundances for the sulphur-bearing species are, however, significantly below the observed values, which points to an underestimation of the abundance of atomic sulphur in the model or to missing formation reactions, such as ion-neutral reactions.

A&A 650, L14 (2021)
DOI: 10.1051/0004-6361/202141297
Full-text URL: https://arxiv.org/abs/2105.12996

Sublimation of Laboratory Ices Millimeter/Submillimeter Experiment (SubLIME): Structure-specific Identifications of Products from UV-photolyzed Methanol Ice

K. M. Yocum, S. N. Milam, P. A. Gerakines, and S. L. Widicus Weaver

Submillimeter/far-IR spectroscopy was used to detect and quantify organic molecules sublimated after the ultraviolet photolysis (at 12 K) and warm-up (up to 300 K) of a methanol (CH3OH) ice sample. Eleven sublimated photoproducts were uniquely identified: carbon monoxide (CO), formaldehyde (H2CO), ketene (C2H2O), acetaldehyde (CH3CHO), ethylene oxide (CH2OCH2), vinyl alcohol (CH2CHOH), ethanol (CH3CH2OH), dimethyl ether (CH3OCH3), methyl formate (HCOOCH3), glycolaldehyde (HOCH2CHO), and acetone ((CH3)2CO). Two additional products were detected in the photolyzed ice by Fourier-transform infrared (FTIR) spectroscopy: carbon dioxide (CO2) and methane (CH4). The rotational temperatures and gas densities were calculated for the organics containing two or more C atoms via a rotation diagram analysis, and the gas-phase submillimeter/far-IR technique was used in tandem with mass spectrometry and FTIR spectroscopy of the ice during photolysis. The abundance ratios of the sublimated species (normalized to methanol) were compared to those observed in hot cores (Orion-KL, Sagittarius B2(N), and IRAS 16293-2422(B)) and in comets C/2014 Q2 (Lovejoy) and 67P/Churyumov–Gerasimenko.

K. M. Yocum et al. 2021, ApJ, 913, 61.
DOI: 10.3847/1538-4357/abf14e
Full-text URL: https://doi.org/10.3847/1538-4357/abf14e

Formation of complex organic molecules in molecular clouds: acetaldehyde, vinyl alcohol, ketene, and ethanol via the “energetic” processing of C2H2 ice

K.-J. Chuang, G. Fedoseev, C. Scirè, G. A. Baratta, C. Jäger, Th. Henning, H. Linnartz and M. E. Palumbo

Context. The simultaneous detection of organic molecules of the form C2HnO, such as ketene (CH2CO), acetaldehyde (CH3CHO), and ethanol (CH3CH2OH), toward early star-forming regions offers hints of a shared chemical history. Several reaction routes have been proposed and experimentally verified under various interstellar conditions to explain the formation pathways involved. Most noticeably, the non-energetic processing of C2H2 ice with OH-radicals and H-atoms was shown to provide formation routes to ketene, acetaldehyde, ethanol, and vinyl alcohol (CH2CHOH) along the H2O formation sequence on grain surfaces in translucent clouds. Aims. In this work, the non-energetic formation scheme is extended with laboratory measurements focusing on the energetic counterpart, induced by cosmic rays penetrating the H2O-rich ice mantle. The focus here is on the H+ radiolysis of interstellar C2H2:H2O ice analogs at 17 K. Methods. Ultra-high vacuum experiments were performed to investigate the 200 keV H+ radiolysis chemistry of predeposited C2H2:H2O ices, both as mixed and layered geometries. Fourier-transform infrared spectroscopy was used to monitor in situ newly formed species as a function of the accumulated energy dose (or H+ fluence). The infrared spectral assignments are further confirmed in isotope labeling experiments using H218O. Results. The energetic processing of C2H2:H2O ice not only results in the formation of (semi-) saturated hydrocarbons (C2H4 and C2H6) and polyynes as well as cumulenes (C4H2 and C4H4), but it also efficiently forms O-bearing COMs, including vinyl alcohol, ketene, acetaldehyde, and ethanol, for which the reaction cross-section and product composition are derived. A clear composition transition of the product, from H-poor to H-rich species, is observed as a function of the accumulated energy dose. Furthermore, the astronomical relevance of the resulting reaction network is discussed.

2021, Astronomy & Astrophysics, 650, p.A85.
DOI: 10.1051/0004-6361/202140780
Full-text URL: https://arxiv.org/abs/2104.09434

Efficiency of non-thermal desorptions in cold-core conditions. Testing the sputtering of grain mantles induced by cosmic rays

V. Wakelam, E. Dartois, M. Chabot, S. Spezzano, D. Navarro-Almaida, J.-C. Loison, and A. Fuente

Under cold conditions in dense cores, gas-phase molecules and atoms are depleted from the gas-phase to the surface of interstellar grains. Considering the time scales and physical conditions within these cores, a portion of these molecules has to be brought back into the gas-phase to explain their observation by milimeter telescopes. We tested the respective efficiencies of the different mechanisms commonly included in the models. We also tested the addition of sputtering of ice grain mantles via a collision with cosmic rays in the electronic stopping power regime. The ice sputtering induced by cosmic rays has been added to the Nautilus gas-grain model while the other processes were already present. Each of these processes were tested on a 1D physical structure determined by observations in TMC1 cold cores. The resulting 1D chemical structure was also compared to methanol gas-phase abundances observed in these cores. We found that all species are not sensitive in the same way to the non-thermal desorption mechanisms, and the sensitivity also depends on the physical conditions. Thus, it is mandatory to include all of them. Chemical desorption seems to be essential in reproducing the observations for H densities smaller than 4e4cm-3, whereas sputtering is essential above this density. The models are, however, systematically below the observed methanol abundances. A more efficient chemical desorption and a more efficient sputtering could better reproduce the observations. In conclusion, the sputtering of ices by cosmic-rays collisions may be the most efficient desorption mechanism at high density (a few 1e4cm-3 under the conditions studied here) in cold cores, whereas chemical desorption is still required at smaller densities. Additional works are needed on both mechanisms to assess their efficiency with respect to the main ice composition.

Accepted for publication in A&A
DOI: 10.1051/0004-6361/202039855
Full-text URL: http://arxiv.org/abs/2106.08621

Constraining Spatial Densities of Early Ice Formation in Small Dense Molecular Cores from Extinction Maps

L. Chu, K. Hodapp

Tracing dust in small dense molecular cores is a powerful tool to study the conditions required for ices to form during the pre-stellar phase. To study these environments, five molecular cores were observed: three with ongoing low-mass star formation (B59, B335, and L483) and two starless collapsing cores (L63 and L694-2). Deep images were taken in the infrared JHK bands with the United Kingdom Infrared Telescope (UKIRT) WFCAM (Wide Field Camera) instrument and IRAC channels 1 and 2 on the Spitzer Space Telescope. These five photometric bands were used to calculate extinction along the line of sight toward background stars. After smoothing the data, we produced high spatial resolution extinction maps (~13-29") . The maps were then projected into the third dimension using the AVIATOR algorithm implementing the inverse Abel transform. The volume densities of the total hydrogen were measured along lines of sight where ices (H_2O, CO, and CH_3OH) have previously been detected. We find that lines of sight with pure CH_3OH or a mixture of CH_3OH with CO have maximum volume densities above 1.0x1e5 cm^{-3}. These densities are only reached within a small fraction of each of the cores (~0.3-2.1%). CH_3OH presence may indicate the onset of complex organic molecule formation within dense cores and thus we can constrain the region where this onset can begin. The maximum volume densities toward star-forming cores in our sample (~$1.2\text{-}1.7e^6$ cm^{-3}) are higher than those toward starless cores (~$3.5\text{-}9.5e^5$ cm^{-3}).

Accepted to the Astrophysical Journal
Full-text URL: http://arxiv.org/abs/2106.08333

Detection of the cyanomidyl radical (HNCN): a new interstellar species with the NCN backbone

V. M. Rivilla, I. Jiménez-Serra, J. García de la Concepción, J. Martín-Pintado, L. Colzi, L. F. Rodríguez-Almeida, B. Tercero, F. Rico-Villas, S. Zeng, S. Martín, M. A. Requena-Torres, P. de Vicente

We report here the first detection in the interstellar medium of the cyanomidyl radical (HNCN). Using the Yebes 40m and the IRAM 30m telescopes, we have targeted the doublets of the N=2−1, 4−3, 5−4, 6−5, and 7−6 transitions of HNCN toward the molecular cloud G+0.693-0.027. We have detected three unblended lines of HNCN, these are the N=6−5 doublet and one line of the N=4−3 transition. Additionally we present one line of the N=5−4 transition partially blended with emission from other species. The Local Thermodynamic Equilibrium best fit to the data gives a molecular abundance of (0.91±0.05)e−10 with respect to H_2. The relatively low abundance of this species in G+0.693-0.027, and its high reactivity, suggest that HNCN is possibly produced by gas-phase chemistry. Our work shows that this highly reactive molecule is present in interstellar space, and thus it represents a plausible precursor of larger prebiotic molecules with the NCN backbone such as cyanamide (NH_2CN), carbodiimide (HNCNH) and formamidine (NH_2CHNH).

Accepted in Monthly Notices of the Royal Astronomical Society Letters
Full-text URL: https://arxiv.org/abs/2106.09652

Astrochemical Pathways to Complex Organic and Prebiotic Molecules: Experimental Perspectives for In Situ Solid-State Studies

Daniele Fulvio, Alexey Potapov, Jiao He and Thomas Henning

A deep understanding of the origin of life requires the physical, chemical, and biological study of prebiotic systems and the comprehension of the mechanisms underlying their evolutionary steps. In this context, great attention is paid to the class of interstellar molecules known as “Complex Organic Molecules” COMs), considered as possible precursors of prebiotic species. Although COMs have already been detected in different astrophysical environments (such as interstellar clouds, protostars, and protoplanetary disks) and in comets, the physical–chemical mechanisms underlying their formation are not yet fully understood. In this framework, a unique contribution comes from laboratory experiments specifically designed to mimic the conditions found in space. We present a review of experimental studies on the formation and evolution of COMs in the solid state, i.e., within ices of astrophysical interest, devoting special attention to the in situ detection and analysis techniques commonly used in laboratory astrochemistry. We discuss their main strengths and weaknesses and provide a perspective view on novel techniques, which may help in overcoming the current experimental challenges.

Life 2021, 11, 568
DOI: 10.3390/life11060568
Full-text URL: https://www.mdpi.com/2075-1729/11/6/568

ALMA observations of doubly deuterated water: Inheritance of water from the prestellar environment

S. S. Jensen, J. K. Jørgensen, L. E. Kristensen, A. Coutens, E. F. van Dishoeck, K. Furuya, D. Harsono, M. V. Persson

Establishing the origin of the water D/H ratio in the Solar System is central to our understanding of the chemical trail of water during the star and planet formation process. Recent modeling suggests that comparisons of the D2O/HDO and HDO/H2O ratios are a powerful way to trace the chemical evolution of water and, in particular, determine whether the D/H ratio is inherited from the molecular cloud or established locally. We seek to determine the D2O column density and derive the D2O/HDO ratios in the warm region toward the low-mass Class 0 sources B335 and L483. The results are compared with astrochemical models and previous observations to determine their implications for the chemical evolution of water. We present ALMA observations of the D2O transition at 316.8 GHz toward B335 and L483 at <0.5" (< 100 au) resolution, probing the inner warm envelope gas. The column densities of D2O, HDO, and H182O are determined by synthetic spectrum modeling and direct Gaussian fitting, under the assumption of a single excitation temperature and similar spatial extent for the three water isotopologs. D2O is detected toward both sources in the inner warm envelope. The derived D2O/HDO ratios is (1.0±0.2)e−2 for L483 and (1.4±0.1)e−2 for B335. The high D2O/HDO ratios are a strong indication of chemical inheritance of water from the prestellar phase down to the inner warm envelope. This implies that the local cloud conditions in the prestellar phase, such as temperatures and timescales, determine the water chemistry at later stages and could provide a source of chemical differentiation in young systems. In addition, the observed D2O/H2O ratios support an observed dichotomy in the deuterium fractionation of water toward isolated and clustered protostars, namely, a higher D/H ratio toward isolated sources.

A&A 650, A172 (2021)
DOI: 10.1051/0004-6361/202140560
Full-text URL: https://arxiv.org/abs/2104.13411

Announcements

Two 4 yrs PhD positions in the field of astrochemistry

VACANCY 1: Ice Spectroscopy, in the laboratory and with JWST

We have a 4 yrs (1+3 yrs) PhD vacancy to work with IRASIS, one of the ice setups in the laboratory for astrophysics at Leiden Observatory and data interpretation of upcoming JWST ice data. Laboratory and observational work are roughly 70-30.

The project comprises the systematic vibrational characterization of astrophysically relevant molecules embedded in chemically related ice matrices. This work is in support of JWST data that will become available through more than 150 hours of guaranteed observing time within MIRI-GTO, Early Release Science (ICE AGE), and GO programs.

We are looking for an enthusiastic person, with a good background in experimental physics/chemistry and a strong interest in astronomical data interpretation. The successful candidate has recently obtained her/his master degree or will do very soon. Very good English skills are a prerequisite.

The work is performed in the Laboratory for Astrophysics at Leiden Observatory at Leiden Observatory under supervision of Profs. Harold Linnartz, Ewine van Dishoeck and Dr. Melissa McClure. The candidate will be will be part of a larger international team studying the physical and chemical structure and evolution of protostars and planet-forming disks with JWST and ALMA.

We take applications up to July 6 and aim for a start in early 2022.

Please send your application (motivation letter, cv, grades), together with the names of two persons who can provide a letter of recommendation to ewine@strw.leidenuniv.nl, linnartz@strw.leidenuniv.nl and mcclure@strw.leidenuniv.nl.

Leiden Observatory is a lively institute carrying out observational, interpretative and theoretical research in the fields of the star and planet formation, astrochemistry, laboratory astrophysics, exoplanets, the formation, dynamics and evolution of (high-redshift) galaxies and their nuclei, and cosmology.

The links below provide additional information. More detailed info can be provided upon request.

- Laboratory for astrophysics: http://www.laboratory-astrophysics.eu
- ERS ICE AGE: http://jwst-iceage.org/
- MIRI GTO programme: https://www.stsci.edu/jwst/science-execution/program-information?id=1290
- Leiden Observatory: http://wwww.local.strw.leidenuniv.nl

VACANCY 2: Computationally unraveling energy dissipation on CO ices

We have a 4 yrs (1+3 yrs) PhD vacancy to work on energy dissipation of CO ices within an astrochemical framework at the Theoretical Chemistry department of Leiden University. A strong link with ongoing work at the Laboratory for Astrophysics (LfA) at Leiden Observatory is foreseen and there will be the possibility of applying for beam time at the FELIX facility at Radboud University Nijmegen for complementary experimental work.

The project comprises the implementation of a force field for initially pure CO ices in python (Atomic Simulation Environment) to allow the systematic characterization of the energy flow of particular vibrational modes into the ice cluster. This project is envisioned to expand by studying the influence of including isotope effects and implementing periodic boundary conditions such that also bulk crystaline ices can be studied.

We are looking for an enthusiastic person, with a good background in programming with python (or other languages), a physics or chemistry degree and a strong interest in astrochemistry. Experience or affinity with experimental work is preferred, but not strictly required. The successful candidate has recently obtained a master degree or will do very soon. Very good English skills are a prerequisite.

The work will be performed at the Leiden Institute of Chemistry (LIC) under supervision of Dr. Thanja Lamberts in collaboration with Dr. Jörg Meyer (LIC) and Prof. Harold Linnartz (LfA). Within the Theoretical Chemistry group ample knowledge transfer is expected in the field of solid-state computational chemistry. Through linking with Leiden Observatory the candidate will be in close connection with state-of-the-art research on various aspects of astrochemistry, ranging from the Laboratory perspective to observations with JWST and ALMA.

We take applications up to July 6 and aim for a start in early 2022.

Please send your application (motivation letter, cv, grades), together with the names of two persons who can provide a letter of recommendation to Dr. Lamberts (a.l.m.lamberts@lic.leidenuniv.nl) with Prof. Linnartz in CC (linnartz@strw.leidenuniv.nl).

The chemistry and life science research in the Leiden Institute of Chemistry (LIC) is organized around two major research areas: 'Chemical Biology' and 'Energy & Sustainability'. The institute's research themes illustrate the central position of chemistry between biology, medicine and physics. The various research topics carried out within these themes are ideal for executing interdisciplinary research. For more information, see www.universiteitleiden.nl/en/science and http://workingat.leiden.edu/

More detailed info can be provided upon request.

Splinter session: Impact of Cosmic Rays on the Physics and Chemistry of Dense Molecular Gas

The splinter session "Impact of Cosmic Rays on the Physics and Chemistry of Dense Molecular Gas" will be held as part of the Astronomische Gesellschaft 2021 conference. This conference will be virtual this year. This splinter session is meant to bring together experts in astrochemistry, star formation, and cosmic-ray transport.

Important dates:
Splinter session date: Monday September 13, 09:00-13:00 CEST (UTC+2)
Abstract submission deadline: August 15, 2021

Abstract:

Cosmic rays (CRs) are energetic charged particles that are accelerated in extreme environments. In dense molecular gas that is shielded from external UV radiation, the ionization of atoms and molecules by CRs plays a crucial role in driving chemical and physical processes as well as in affecting the emission of ionic, atomic and molecular lines. At high column densities, CRs ionize H2 initiating a diverse chemistry through fast ion-neutral reactions. The interaction of CRs with the dense gas induces UV photons via H2 electronic excitation. These influence the chemistry in icy grain mantles, as does the deposition of energy by direct CR bombardment. In chemical models, the above processes are controlled by the so-called “cosmic-ray ionization rate”, ζ, making it one of the most important parameters for the underlying physics and chemistry of dense gas. In molecular clouds, ζ is most sensitive to the flux of low-energy CRs (1–100 MeV). However, the transport of low-energy CRs through dense gas is poorly constrained, and estimates of ζ in such regions are highly uncertain. Furthermore, recent observations in dense cores suggest a conflict with current cosmic-ray transport models. Therefore, understanding both the transport of CRs and the chemistry they

drive is vital. During this splinter session, we will bring together researchers across a range of communities, including astrochemists and cosmic-ray transport modellers. These communities do not often meet together, despite how intertwined the research can be. We will focus on talks by junior researchers and develop an interdisciplinary session. We anticipate a fruitful discussion which will help the astrochemical, star formation and high-energy astrophysics communities.
Important questions that will be discussed during this session will be:

- What is the impact of cosmic-rays on gas- and ice-phase chemistry, particularly in regions with high cosmic-ray ionization rates?
- What are the best observations and calibrations to constrain the cosmic-ray ionization rate?
- How do low-energy cosmic rays transport through dense molecular gas? What observations need to be done to constrain this?
- Is there an observable correlation between the star-formation rate and the cosmic-ray ionization rate?
- Looking forward: what kinds of observational facilities and instruments and theoretical models are needed to constrain the transport of low-energy cosmic rays and the cosmic-ray ionization rate in dense gas?