

# AstroChemical Newsletter #65

April 2021

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## Abstracts

### OH mid-infrared emission as a diagnostic of H<sub>2</sub>O UV photodissociation. I. Model and application to the HH 211 shock

**Benoît Tabone, Marc C. van Hemert, Ewine F. van Dishoeck, John H. Black**

Water is an important molecule in interstellar and circumstellar environments. Previous observations of mid-infrared rotational lines of OH suggest that these lines may be used to probe the photodissociation of water. In this work, cross sections for the photodissociation of H<sub>2</sub>O resolving the state of the OH fragment are collected and incorporated in a new molecular excitation code called GROSBETA, which includes radiative pumping, collisional (de)excitation, and prompt emission (i.e., following the production of OH in excited states). We find that the OH rotational line intensities in the range 9–16 μm, covering rotational transitions with  $N_{up}=18$  to 45, are proportional to the column density of H<sub>2</sub>O photodissociated per second by photons in the range 114–143 nm and do not depend on other local properties. Provided an independent measurement of the column density of water is available, the strength of the local UV radiation field can be deduced with good accuracy. In contrast, the OH lines at longer far-infrared wavelengths are primarily produced by IR radiative pumping and collisions. Our model successfully reproduces the OH mid-IR lines in the 10–16 μm range observed by Spitzer toward the tip of the HH 211 bow-shock and shows that the jet shock irradiates its surroundings, exposing H<sub>2</sub>O to a UV photon flux that is about 5000 times larger than the standard interstellar radiation field. We also find that chemical pumping by the reaction H<sub>2</sub><sup>+</sup> + O may supplement the excitation of lines in the range 16–30 μm. The mid-infrared lines of OH constitute a powerful diagnostic for inferring the photodissociation rate of water and thus the UV field water is exposed to. Future JWST-MIRI observations will be able to map the photodestruction rate of H<sub>2</sub>O in various dense and irradiated environments and provide robust estimates of the local UV radiation field.

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### The initial gas-phase sulfur abundance in the Orion Molecular Cloud from sulfur radio recombination lines

**Javier R. Goicoechea, Sara Cuadrado**

The abundances of chemical elements and their depletion factors are essential parameters for understanding the composition of the gas and dust that are ultimately incorporated into stars and planets. Sulfur is an abundant but peculiar element in the sense that, despite being less volatile than other elements (e.g., carbon), it is not a major constituent of dust grains in diffuse interstellar clouds. Here, we determine the gas-phase carbon-to-sulfur abundance ratio,  $[C]/[S]$ , and the sulfur abundance  $[S]$  in a dense star-forming cloud from new radio recombination lines (RRLs) detected with the Yebes 40m telescope - at relatively high frequencies ( $\sim 40$  GHz  $\sim 7$  mm) and angular resolutions (down to 36") - in the Orion Bar, a rim of the Orion Molecular Cloud (OMC). We detect nine C $n\alpha$  RRLs (with  $n=51$  to 59) as well as nine narrow line features separated from the C $n\alpha$  lines by  $\Delta v = -8.4 \pm 0.3$  km s<sup>-1</sup>. Based on this velocity separation, we assign these features to sulfur RRLs, with little contribution of RRLs from the more condensable elements Mg, Si, or Fe. Sulfur RRLs lines trace the photodissociation region (PDR) of the OMC. In these predominantly neutral gas layers, up to  $A_V \sim 4$ , the ions C<sup>+</sup> and S<sup>+</sup> lock in most of the C and S gas-phase reservoir. We determine a relative abundance of  $[C]_{\text{Ori}}/[S]_{\text{Ori}} = 10.4 \pm 0.6$  and, adopting the same  $[C]_{\text{Ori}}$  measured in the translucent gas toward star  $\theta^{1}$  Ori B, an absolute abundance of  $[S]_{\text{Ori}} = (1.4 \pm 0.4) \times 10^{-5}$ . This value is consistent with emission models of the observed sulfur RRLs if  $N(S^+) \sim 7 \times 10^{17}$  cm<sup>-2</sup> (beam-averaged). The  $[S]_{\text{Ori}}$  is the "initial" sulfur abundance in the OMC, before an undetermined fraction of the  $[S]_{\text{Ori}}$  goes into molecules and ice mantles in the cloud interior. The inferred abundance  $[S]_{\text{Ori}}$  matches the solar abundance, thus implying that there is little depletion of sulfur onto rocky dust grains, with  $D(S) = 0.0 \pm 0.2$  dex.

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### Laboratory-based sticking coefficients for ices on a variety of small-grain analogues

**C. Laffon, D. Ferry, O. Grauby and P. Parent**

Abundances and the partitioning between ices and gases in gas-grain chemistry are governed by adsorption and desorption on grains. Understanding of astrophysical observations relies on laboratory measurements of adsorption and desorption rates on dust grain analogues. On flat surfaces, gas adsorption probabilities (or sticking coefficients) have been found to be close to unity for most gases. Here we report a strong decrease in the sticking coefficients of H<sub>2</sub>O and CO<sub>2</sub> on substrates

more akin to cosmic dust, such as submicrometre-sized particles of carbon and olivine, bare or covered with ice. This effect results from the local curvature of the grains, and then extends to larger grains made of aggregated small particles, such as fluffy or porous dust in more evolved media (for example, circumstellar disks). The main astrophysical implication is that accretion rates of gases are reduced accordingly, slowing the growth of cosmic ices. Furthermore, volatile species that are not adsorbed on a grain at their freeze-out temperature will persist in the gas phase, which will impact gas–ice partitions. We also found that thermal desorption of H<sub>2</sub>O is not modified by grain size, and thus the temperature of snowlines should be independent of the dust size distribution.

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## Water in star-forming regions (WISH): physics and chemistry from clouds to disks as probed by Herschel spectroscopy

**E.F. van Dishoeck, L.E. Kristensen and the WISH team.**

Data and results from the WISH key program are summarized, designed to provide a legacy data set to address its physics and chemistry. WISH targeted ~80 sources along the two axes of luminosity and evolutionary stage: from low- to high-mass protostars and from pre-stellar cores to protoplanetary disks. Lines of H<sub>2</sub>O, HDO, OH, CO and [O I] were observed with the HIFI and PACS instruments, complemented by molecules that probe UV, X-ray or grain chemistry. Most of the far-infrared water emission from protostars is found to be compact, originating from warm outflowing and shocked gas at high density and temperature in at least two physical components. This gas is not probed by low-J CO lines, only by J>14. Water is a significant, but not dominant, coolant. Its abundance is universally low, of order H<sub>2</sub>O/H<sub>2</sub>=2E-6, pointing to shock and outflow cavity models that include UV radiation at 100-1000 times the ISRF. In cold quiescent pre-stellar cores and envelopes, the water abundance structure is accurately probed through velocity-resolved line profiles, confirming basic chemistry networks. The gaseous HDO/H<sub>2</sub>O ratio of 0.025, much higher than that of bulk ice, is representative of the outer photodesorbed ice layers and cold chemistry. Water abundances in the inner hot cores are high, but with variations from 5E-6 to 2E-4. Combined analyses of water gas and ice show that up to 50% of the oxygen budget may be missing, with possible explanations discussed. Water vapor emission from disks is weak, indicating that water ice is locked up in larger pebbles early on and that these pebbles have settled and drifted inward by the Class II stage. Quantitatively, many oceans of water ice are available. Extragalactic low-J H<sub>2</sub>O emission is mostly compact and collisionally excited. Prospects for future mid- to far-infrared missions are given.

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## Infrared action spectroscopy of doubly charged PAHs and their contribution to the aromatic infrared bands

**S. Banhatti, J. Palotás, P. Jusko, B. Redlich, J. Oomens, S. Schlemmer, and S. Brünken**

The so-called aromatic infrared bands (AIBs) are attributed to emission of polycyclic aromatic hydrocarbons (PAHs). The observed variations towards different regions in space are believed to be caused by contributions of different classes of PAH molecules, i.e. with respect to their size, structure, and charge state. Laboratory spectra of members of these classes are needed to compare to observations and to benchmark quantum-chemically computed spectra of these species. In this paper we present the experimental infrared spectra of three different PAH dications, naphthalene<sup>2+</sup>, anthracene<sup>2+</sup> and phenanthrene<sup>2+</sup>, in the vibrational fingerprint region 500 - 1700 cm<sup>-1</sup>. The dications were produced by electron impact ionization of the vapors with 70 eV electrons, and remained stable against dissociation and Coulomb explosion. The vibrational spectra were obtained by infrared pre-dissociation of the PAH<sup>2+</sup> complexed with neon in a 22-pole cryogenic ion trap setup coupled to a free-electron infrared laser at the FELIX Laboratory. We performed anharmonic DFT calculations for both singly and doubly charged states of the three molecules. The experimental band positions showed excellent agreement with the calculated band positions of the singlet electronic ground state for all three doubly charged species, indicating its higher stability over the triplet state. The presence of several strong combination bands and additional weaker features in the recorded spectra, especially in the 10-15 μm region of the mid-IR spectrum, required anharmonic calculations to understand their effects on the total integrated intensity for the different charge states. These measurements, in tandem with theoretical calculations, will help in the identification of this specific class of doubly-charged PAHs as carriers of AIBs

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## Photolysis of acetonitrile in a water-rich ice as a source of complex organic molecules: CH<sub>3</sub>CN and H<sub>2</sub>O:CH<sub>3</sub>CN ices

**M. Bulak, D. M. Paardekooper, G. Fedoseev and H. Linnartz**

Context. Many C-, O-, and H-containing complex organic molecules (COMs) have been observed in the interstellar medium (ISM) and their formation has been investigated in laboratory experiments. An increasing number of recent detections of

large N-bearing COMs motivates our experimental investigation of their chemical origin. Aims. We investigate the potential role of acetonitrile (CH<sub>3</sub>CN) as a parent molecule to N-bearing COMs, motivated by its omnipresence in the ISM and structural similarity to another well-known precursor species, CH<sub>3</sub>OH. The aim of the present work is to characterize the chemical complexity that can result from vacuum UV photolysis of a pure CH<sub>3</sub>CN ice and a more realistic mixture of H<sub>2</sub>O:CH<sub>3</sub>CN. Methods. The CH<sub>3</sub>CN ice and H<sub>2</sub>O:CH<sub>3</sub>CN ice mixtures were UV irradiated at 20 K. Laser desorption post ionization time-of-flight mass spectrometry was used to detect the newly formed COMs in situ. We examined the role of water in the chemistry of interstellar ices through an analysis of two different ratios of H<sub>2</sub>O:CH<sub>3</sub>CN (1:1 and 20:1). Results. We find that CH<sub>3</sub>CN is an excellent precursor to the formation of larger nitrogen-containing COMs, including CH<sub>3</sub>CH<sub>2</sub>CN, NCCN/CNCN, and NCCH<sub>2</sub>CH<sub>2</sub>CN. During the UV photolysis of H<sub>2</sub>O:CH<sub>3</sub>CN ice, the water derivatives play a key role in the formation of molecules with functional groups of: imines, amines, amides, large nitriles, carboxylic acids, and alcohols. We discuss possible formation pathways for molecules recently detected in the ISM.

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## Computational Study of the Hydrogenation Sequence of the Phosphorous Atom on Interstellar Dust Grains

G. Molpeceres & J. Kästner

The detection of phosphorous bearing molecules in interstellar environments constitutes a fundamental task for understanding the formation of prebiotic molecules, but also a challenge. In cold interstellar environments, where rich chemistry is expected to happen, only PN and PO have been detected. Phosphine (PH<sub>3</sub>) must also play an essential role in these regions since P is expected to deplete onto dust grains significantly and hydrogenation reactions are dominant in such environments. Surface chemistry on dust grains shows a particular idiosyncrasy where an equilibrium between competitive reactions, photoconversion processes, and desorption are in continuous interplay, modifying both the dust composition and the gas composition. In this study, we theoretically study in detail the interconversion of P to PH<sub>3</sub> via subsequent additions of H on cold dust grains analogs. For all reactions, we provide binding energy of the adsorbates, reaction energies, and when present, activation barriers and tunneling corrected rate constants. We also present an estimate of the desorption temperature of these species based on transition state theory. Using recently available experimental results on PH<sub>3</sub> desorption via chemical reactions, we conclude that all the intermediate products of the hydrogenation sequence to phosphine may be released to the gas phase.

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## Binding energies and sticking coefficients of H<sub>2</sub> on crystalline and amorphous CO ice

G. Molpeceres, V. Zaverkin, N. Watanabe & J. Kästner

Our results show that the binding energy for the H<sub>2</sub>/CO system is low on average, -157 K for amorphous CO and -266 K for crystalline CO. This carries several implications for the rest of the work. H<sub>2</sub> binding to crystalline CO is stronger by 109 K than to amorphous CO, while amorphous CO shows a wider H<sub>2</sub> binding energy distribution. Sticking coefficients are never unity and vary strongly with surface temperature, but less so with ice phase, with values between 0.95 and 0.17. With the values of this study, between 17 and 25 % of a beam of H<sub>2</sub> molecules at room temperature would stick to the surface, depending on the temperature of the surface and the ice phase. Residence times vary by several orders of magnitude between crystalline and amorphous CO, with the latter showing residence times on the order of seconds at 5 K. H<sub>2</sub> may diffuse before desorption in amorphous ices, which might help to accommodate it in deeper binding sites.

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## Discovery of allenyl acetylene, H<sub>2</sub>CCCHCCH, in TMC-1. A study of the isomers of C<sub>5</sub>H<sub>4</sub>

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

We present the discovery in TMC-1 of allenyl acetylene, H<sub>2</sub>CCCHCCH, through the observation of nineteen lines with a signal-to-noise ratio ~4-15. For this species, we derived a rotational temperature of 7 +/- 1 K and a column density of (1.2 +/- 0.2)e13 cm<sup>-2</sup>. The other well known isomer of this molecule, methyl diacetylene (CH<sub>3</sub>C<sub>4</sub>H), has also been observed and we derived a similar rotational temperature, Trot = 7.0 +/- 0.3 K, and a column density for its two states (A and E) of (6.5 +/- 0.3)e12 cm<sup>-2</sup>. Hence, allenyl acetylene and methyl diacetylene have a similar abundance. Remarkably, their abundances are close to that of vinyl acetylene (CH<sub>2</sub>CHCCH). We also searched for the other isomer of C<sub>5</sub>H<sub>4</sub>, HCCCH<sub>2</sub>CCH (1,4-pentadiyne), but only a 3sigma upper limit of 2.5e12 cm<sup>-2</sup> to the column density can be established. These results have been compared to state-of-the-art chemical models for TMC-1, indicating the important role of these hydrocarbons in its chemistry. The rotational parameters of allenyl acetylene have been improved by fitting the existing laboratory data together with the frequencies of the transitions observed in TMC-1.

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## Discovery of CH<sub>2</sub>CHCCH and detection of HCCN, HC<sub>4</sub>N, CH<sub>3</sub>CH<sub>2</sub>CN, and, tentatively, CH<sub>3</sub>CH<sub>2</sub>CCH in TMC-1

J. Cernicharo, M. Agúndez, C. Cabezas, N. Marcelino, B. Tercero, J. R. Pardo, J. D. Gallego, F. Tercero, J. A. López-Pérez, P. de Vicente

We present the discovery in TMC-1 of vinyl acetylene, CH<sub>2</sub>CHCCH, and the detection, for the first time in a cold dark cloud, of HCCN, HC<sub>4</sub>N, and CH<sub>3</sub>CH<sub>2</sub>CN. A tentative detection of CH<sub>3</sub>CH<sub>2</sub>CCH is also reported. The column density of vinyl acetylene is  $(1.2 \pm 0.2) \times 10^{13}$  cm<sup>-2</sup>, which makes it one of the most abundant closed-shell hydrocarbons detected in TMC-1. Its abundance is only three times lower than that of propylene, CH<sub>3</sub>CHCH<sub>2</sub>. The column densities derived for HCCN and HC<sub>4</sub>N are  $(4.4 \pm 0.4) \times 10^{11}$  cm<sup>-2</sup> and  $(3.7 \pm 0.4) \times 10^{11}$  cm<sup>-2</sup>, respectively. Hence, the HCCN/HC<sub>4</sub>N abundance ratio is  $1.2 \pm 0.3$ . For ethyl cyanide we derive a column density of  $(1.1 \pm 0.3) \times 10^{11}$  cm<sup>-2</sup>. These results are compared with a state-of-the-art chemical model of TMC-1, which is able to account for the observed abundances of these molecules through gas-phase chemical routes.

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## Discovery of the propargyl radical (CH<sub>2</sub>CCH) in TMC-1: one of the most abundant radicals ever found and a key species for cyclization to benzene in cold dark clouds

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

We present the first identification in interstellar space of the propargyl radical (CH<sub>2</sub>CCH). This species was observed in the cold dark cloud TMC-1 using the Yebes 40m telescope. The six strongest hyperfine components of the 2,0,2-1,0,1 rotational transition, lying at 37.46–GHz, were detected with signal-to-noise ratios in the range 4.6–12.3 sigma. We derive a column density of  $8.7 \times 10^{13}$  cm<sup>-2</sup> for CH<sub>2</sub>CCH, which translates to a fractional abundance relative to H<sub>2</sub> of  $8.7 \times 10^{-9}$ . This radical has a similar abundance to methyl acetylene, with an abundance ratio CH<sub>2</sub>CCH/CH<sub>3</sub>CCH close to one. The propargyl radical is thus one of the most abundant radicals detected in TMC-1, and it is probably the most abundant organic radical with a certain chemical complexity ever found in a cold dark cloud. We constructed a gas-phase chemical model and find calculated abundances that agree with, or fall two orders of magnitude below, the observed value depending on the poorly constrained low-temperature reactivity of CH<sub>2</sub>CCH with neutral atoms. According to the chemical model, the propargyl radical is essentially formed by the C + C<sub>2</sub>H<sub>4</sub> reaction and by the dissociative recombination of C<sub>3</sub>H<sub>n</sub><sup>+</sup> ions with n = 4–6. The propargyl radical is believed to control the synthesis of the first aromatic ring in combustion processes, and it probably plays a key role in the synthesis of large organic molecules and cyclization processes to benzene in cold dark clouds.

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## Chemical compositions of five Planck cold clumps

V. Wakelam, P. Gratier, M. Ruaud, R. Le Gal, L. Majumdar, J.-C. Loison, and K. M. Hickson

**Aims.** Interstellar molecules form early in the evolutionary sequence of interstellar material that eventually forms stars and planets. To understand this evolutionary sequence, it is important to characterize the chemical composition of its first steps. **Methods.** In this paper, we present the result of a 2 and 3 mm survey of five cold clumps identified by the Planck mission. We carried out a radiative transfer analysis on the detected lines in order to put some constraints on the physical conditions within the cores and on the molecular column densities. We also performed chemical models to reproduce the observed abundances in each source using the gas-grain model Nautilus. **Results.** Twelve molecules were detected: H<sub>2</sub>CO, CS, SO, NO, HNO, HCO<sup>+</sup>, HCN, HNC, CN, CCH, CH<sub>3</sub>OH, and CO. Here, CCH is the only carbon chain we detected in two sources. Radiative transfer analyses of HCN, SO, CS, and CO were performed to constrain the physical conditions of each cloud with limited success. The sources have a density larger than  $1 \times 10^4$  cm<sup>-3</sup> and a temperature lower than 15 K. The derived species column densities are not very sensitive to the uncertainties in the physical conditions, within a factor of 2. The different sources seem to present significant chemical differences with species abundances spreading over one order of magnitude. The chemical composition of these clumps is poorer than the one of Taurus Molecular Cloud 1 Cyanopolyne Peak (TMC-1 CP) cold core. Our chemical model reproduces the observational abundances and upper limits for 79 to 83% of the species in our sources. The 'best' times for our sources seem to be smaller than those of TMC-1, indicating that our sources may be less evolved and explaining the smaller abundances and the numerous non-detections. Also, CS and HCN are always overestimated by our models.

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## Dissociative electron attachment cross sections for ro-vibrationally excited NO molecule and N-

## anion formation

V. Laporta, I. F. Schneider and J. Tennyson

Motivated by the huge need for data for non-equilibrium plasma modeling, a theoretical investigation of dissociative electron attachment to the NO molecule is performed. The calculations presented here are based on the local-complex-potential approach, taking into account five NO<sup>-</sup> resonances. Three specific channels of the process are studied, including the production of excited nitrogen atoms N(2D) and of its anions N<sup>-</sup>. Interpretation of the existing experimental data and their comparison with our theoretical result are given. A full set of ro-vibrationally-resolved cross sections and the corresponding rate coefficients are reported. In particular, a relatively large cross sections for N<sup>-</sup> ion formation at low energy of the incident electron and for vibrationally excited NO target are predicted. Finally, molecular rotation effects are discussed.

Plasma Sources Sci. Technol. 29, 10LT01 (2020)

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## ALMA Observations of Massive Clouds in the Central Molecular Zone: Ubiquitous Protostellar Outflows

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We observe 1.3-mm spectral lines at 2000-AU resolution toward four massive molecular clouds in the Central Molecular Zone of the Galaxy to investigate their star formation activities. We focus on several potential shock tracers that are usually abundant in protostellar outflows, including SiO, SO, CH<sub>3</sub>OH, H<sub>2</sub>CO, HC<sub>3</sub>N, and HNCO. We identify 43 protostellar outflows, including 37 highly likely ones and 6 candidates. The outflows are found toward both known high-mass star forming cores and less massive, seemingly quiescent cores, while 791 out of the 834 cores identified based on the continuum do not have detected outflows. The outflow masses range from less than 1-M<sub>⊙</sub> to a few tens of M<sub>⊙</sub>, with typical uncertainties of a factor of 70. We do not find evidence of disagreement between relative molecular abundances in these outflows and in nearby analogs such as the well-studied L1157 and NGC7538S outflows. The results suggest that i) protostellar accretion disks driving outflows ubiquitously exist in the CMZ environment, ii) the large fraction of candidate starless cores is expected if these clouds are at very early evolutionary phases, with a caveat on the potential incompleteness of the outflows, iii) high-mass and low-mass star formation is ongoing simultaneously in these clouds, and iv) current data do not show evidence of difference between the shock chemistry in the outflows that determines the molecular abundances in the CMZ environment and in nearby clouds.

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## Announcements

### Southern Sources with EXES/SOFIA: A Community Chat

The SOFIA Science Center is soliciting input from the astrochemistry community to evaluate the potential scientific impact unlocked of Southern observations with EXES/SOFIA in the next few years ((4.5 – 28.3 μm, R=5000-100000). . This webinar on Tuesday, March 30, 2021 - 8:30am to 10:00am PDT is an opportunity for anyone to present ideas about high-impact EXES observations of Southern sources, which will be used as inputs to the development of a long-term Southern deployment strategy, supporting Cycle 10 and beyond. .

Registration is free but necessary in order to join the webinar (<https://events.r20.constantcontact.com/register/eventReg?oeidk=a07ehnlb57d3d93a5c&oseq=&c=&ch=>)

### Postdoctoral and PhD positions in star formation and astrochemistry, IRAP (Toulouse, France)

Applications are invited for a postdoctoral position and a PhD position in star formation and astrochemistry at the Institute of Research in Astrophysics and Planetology (IRAP, Toulouse). The successful applicants will work with Dr Audrey Coutens in the framework of the ERC project Chemtrip (grant agreement 949278), whose ultimate goal is to reconstruct the physico-chemical evolution from the deeply embedded protostellar stage to the planet forming disk stage, through multi-source analyses of high angular resolution observations combined with chemical modeling studies.

Postdoctoral position: The postdoctoral researcher will investigate the evolution of the chemical complexity in solar-type protostars with ALMA and NOEMA observations. This is a 2-year position with the possibility of an extension with a third year (upon performance). The starting date can be as early as September 2021 (preferred) and should not be later than December 2021. The candidates must have a PhD in astrophysics or in a closely related discipline. They should have some expertise in radio/(sub)millimeter observations, preferably in the areas of star formation and/or astrochemistry. Experience in the reduction and analysis of interferometric data is an advantage. Experience with radiative transfer codes is also appreciated. Teamwork ability is essential. Interested candidates should send a cover letter, a curriculum vitae, a publication list, and a brief statement of research interests to [audrey.coutens@irap.omp.eu](mailto:audrey.coutens@irap.omp.eu). They should also arrange for two letters of reference to be sent separately to the same address. The deadline is 23 April 2021. Later applications will be considered until the position is filled. Questions about this position should be sent to Audrey Coutens ([audrey.coutens@irap.omp.eu](mailto:audrey.coutens@irap.omp.eu)).

PhD position: The PhD student will characterize the variation of the isotopic fractionation of various molecules in solar-type protostars. The student will work on already existing NOEMA and ALMA data of solar-type protostars as well as new data that will be gathered during the thesis. The identification of the processes responsible for the isotopic fractionation will be done in collaboration with chemical modeling experts. The PhD thesis will be supervised by Dr Audrey Coutens and Dr Charlotte Vastel. The position is a 3-year appointment and can start from 1 September 2021. The successful applicant must have a Master's degree in astrophysics or physics by the time of enrollment. Previous experience in radio/(sub)millimeter observations, astrochemistry, and python programming are appreciated. Teamwork ability is essential. A high level of written and spoken English is expected. Applications should be sent to [audrey.coutens@irap.omp.eu](mailto:audrey.coutens@irap.omp.eu) and [charlotte.vastel@irap.omp.eu](mailto:charlotte.vastel@irap.omp.eu). They should include: a cover letter, a detailed curriculum vitae and transcripts and rankings obtained during the university curriculum (levels L3, M1 and M2 or equivalent). The applicants should arrange for 2 letters of reference (ideally one from the supervisor of the research internship and one from the person in charge of the last academic year (usually M2)) to be sent separately to the same addresses. The deadline is 27 May 2021. More information on the PhD position can be found here : [https://www.adum.fr/as/ed/voirproposition.pl?langue=&site=sdu2e&matricule\\_prop=34733](https://www.adum.fr/as/ed/voirproposition.pl?langue=&site=sdu2e&matricule_prop=34733). Additional questions should be sent to Audrey Coutens ([audrey.coutens@irap.omp.eu](mailto:audrey.coutens@irap.omp.eu)).

### **PhD position in Astrophysics, fall 2021 at LERMA (France)**

A PhD position in laboratory astrophysics is open in September 2021 at LERMA. Title : "The rôle of radicals in the growth of the molecular complexity on interstellar dust grains".

More informations : <https://cylerma.cyu.fr/version-francaise/actualites>

### **Ph. D position at the Laboratoire d'Astrophysique de Bordeaux/Institut des Sciences Moléculaires (France): WaterStars, from observation to experiments on water in space**

Scientific subject: Water is the third most abundant molecule in the interstellar medium. It has been observed in various objects, but it is only in the extended atmosphere of the envelope of O-rich evolved stars that the very rich spectrum of rotational, vibrational and ro-vibrational transitions of water is observed, and sometimes in surprisingly excited energy states. To understand the excitation of water in these environments, it is necessary to model the excitation of water not only by the radiation from the central star and by radiative coupling with the background radiation, but also by collisions with its most abundant partners (H<sub>2</sub>, He, H, e<sup>-</sup>). This implies knowing the collision rates for pure rotational transitions within the first four excited vibrational states ( $v_1=1$ ,  $v_2=1$ , 2 and  $v_3=1$ ) as well as the rotational transitions between the ground state and these excited states. The first objective is therefore to obtain these collision rates. The second is to include these in an advanced radiative transfer code to reproduce the ALMA observations (ATOMIUM consortium, (<https://fys.kuleuven.be/ster/research-projects/aerosol/atomium/atomium>) and interpret them. The crossed molecular beam experiment in Bordeaux allows the study of inelastic collisions down to very low collision energies, where quantum effects may be observed. The experimental studies will be used to validate theoretical methods in order to provide reliable data to astrophysicists. The first objective of the thesis will be to extend our first experimental studies on H<sub>2</sub>O and D<sub>2</sub>O + H<sub>2</sub> to vibrationally excited water molecules. To model the emission of water lines from highly excited levels we will use a radiative transfer code published by Gray, Baudry et al (2016). The next step will be to include the results of the experimental or theoretical work done at the ISM, i.e. to incorporate the new collision rates, and to extend the code to the first four vibrational levels of water in an attempt to model all the lines observed in ATOMIUM. Additional information: The Ph.D. student will work mainly at ISM, together with Fabrice Herpin (LAB) and Astrid Bergeat (ISM) and other WATERSTARS team members, in close collaboration with the ATOMIUM team. More information on the Laboratoire d'Astrophysique de Bordeaux and Institut des Sciences Moléculaires can be found at <https://astrophys.u-bordeaux.fr> and <http://www.ism.u-bordeaux.fr>, respectively. The 3-year paid thesis contract requires a Master's degree in Astronomy, Physics or Physical Chemistry (or equivalent), obtained before the start of the contract. The start date of the thesis will be between 1 October 2021 and 1 March 2022. Applications should include a brief description of research interests and a summary of previous experience relevant to the subject, a CV, copies of Master's and Bachelor's degrees, Master's certificates or transcripts and internships, as well as contact details of the Master's supervisor and internship supervisors. Applications are open until the vacancy is filled and should be sent to Fabrice Herpin ([fabrice.herpin@u-bordeaux.fr](mailto:fabrice.herpin@u-bordeaux.fr)) or Astrid Bergeat ([astrid.bergeat@u-bordeaux.fr](mailto:astrid.bergeat@u-bordeaux.fr)). A complete description of the position can be found at <https://www.ism.u-bordeaux.fr/spip.php?article354> Funding details: secured financing (ANR Ph-D fellowship)