

# AstroChemical Newsletter #11

September 2016

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## Abstracts

### [The ALMA Protostellar Interferometric Line Survey \(PILS\): First results from an unbiased submillimeter wavelength line survey of the Class 0 protostellar binary IRAS 16293-2422 with ALMA](#)

**J. K. Jørgensen, M. H. D. van der Wiel, A. Coutens, J. M. Lykke, H. S. P. Müller, E. F. van Dishoeck, H. Calcutt, P. Bjerkeli, T. L. Bourke, M. N. Drozdovskaya, C. Favre, E. C. Fayolle, R. T. Garrod, S. K. Jacobsen, K. I. Öberg, M. V. Persson and S. F. Wampfler**

The inner regions of the envelopes surrounding young protostars are characterised by a complex chemistry, with prebiotic molecules present on the scales where protoplanetary disks eventually may form. This paper introduces a systematic survey, "Protostellar Interferometric Line Survey (PILS)" of the Class 0 protostellar binary IRAS 16293-2422 using the Atacama Large Millimeter/submillimeter Array (ALMA). The survey covers the full frequency range from 329 to 363 GHz (0.8 mm) with additional targeted observations at 3.0 and 1.3 mm. More than 10,000 features are detected toward one component in the protostellar binary. Glycolaldehyde, its isomers, methyl formate and acetic acid, and its reduced alcohol, ethylene glycol, are clearly detected. For ethylene glycol both lowest state conformers, aGg' and gGg', are detected, the latter for the first time in the ISM. The abundance of glycolaldehyde is comparable to or slightly larger than that of ethylene glycol. In comparison to the Galactic Center, these two species are over-abundant relative to methanol, possibly an indication of formation at low temperatures in CO-rich ices. Both <sup>13</sup>C and deuterated isotopologues of glycolaldehyde are detected, also for the first time ever in the ISM. For the deuterated species, a D/H ratio of approximately 5% is found with no differences between the deuteration in the different functional groups of glycolaldehyde. Measurements of the <sup>13</sup>C-species lead to a <sup>12</sup>C:<sup>13</sup>C ratio of approximately 30, lower than the typical ISM value. This low ratio may reflect an enhancement of <sup>13</sup>CO in the ice due to either ion-molecule reactions in the gas before freeze-out or differences in the temperatures where <sup>12</sup>CO and <sup>13</sup>CO ices sublimate. The results reinforce the importance of low-temperature grain surface chemistry for the formation of prebiotic molecules seen here in the gas after sublimation of the entire ice mantle.

Accepted for publication in Astronomy and Astrophysics

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### [Striations in molecular clouds: Streamers or MHD waves?](#)

**Tritsis A., Tassis K.**

Dust continuum and molecular observations of the low column density parts of molecular clouds have revealed the presence of elongated structures which appear to be well aligned with the

magnetic field. These so-called striations are usually assumed to be streams that flow towards or away from denser regions. We perform ideal magnetohydrodynamic (MHD) simulations adopting four models that could account for the formation of such structures. In the first two models striations are created by velocity gradients between ambient, parallel streamlines along magnetic field lines. In the third model striations are formed as a result of a Kelvin-Helmholtz instability perpendicular to field lines. Finally, in the fourth model striations are formed from the nonlinear coupling of MHD waves due to density inhomogeneities. We assess the validity of each scenario by comparing the results from our simulations with previous observational studies and results obtained from the analysis of CO ( $J = 1 - 0$ ) observations from the Taurus molecular cloud. We find that the first three models cannot reproduce the density contrast and the properties of the spatial power spectrum of a perpendicular cut to the long axes of striations. We conclude that the nonlinear coupling of MHD waves is the most probable formation mechanism of striations.

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## Constraint on a Cosmological Variation in the Proton-to-electron Mass Ratio from Electronic CO Absorption

**M. Daprà, M. L. Niu, E. J. Salumbides, M. T. Murphy, W. Ubachs**

Carbon monoxide (CO) absorption in the sub-damped Lyman- $\alpha$  absorber at redshift  $z=2.69$ , toward the background quasar SDSS J123714.60+064759.5 (J1237+0647), was investigated for the first time in order to search for a possible variation of the proton-to-electron mass ratio,  $\mu$ , over a cosmological time-scale. The observations were performed with the Very Large Telescope/Ultraviolet and Visual Echelle Spectrograph with a signal-to-noise ratio of 40 per 2.5 km/s per pixel at  $\sim 5000$  Å. Thirteen CO vibrational bands in this absorber are detected: the  $A1\Pi - X1\Sigma^+$  ( $v',0$ ) for  $v'=0-8$ ,  $B1\Sigma^+ - X1\Sigma^+$  (0,0),  $C1\Sigma^+ - X1\Sigma^+$  (0,0), and  $E1\Pi - X1\Sigma^+$  (0,0) singlet-singlet bands and the  $d3\Delta - X1\Sigma^+$  (5,0) singlet-triplet band. An updated database including the most precise molecular inputs needed for a  $\mu$ -variation analysis is presented for rotational levels  $J=0-5$ , consisting of transition wavelengths, oscillator strengths, natural lifetime damping parameters, and sensitivity coefficients to a variation of the proton-to-electron mass ratio. A comprehensive fitting method was used to fit all the CO bands at once and an independent constraint of  $d\mu/\mu = (0.7 \pm 1.6 \pm 0.5) \times 10^{-5}$  was derived from CO only. A combined analysis using both molecular hydrogen and CO in the same J1237+0647 absorber returned a final constraint on the relative variation of  $d\mu/\mu = (-5.6 \pm 5.6 \pm 3.1) \times 10^{-6}$ , which is consistent with no variation over a look-back time of  $\sim 11.4$  Gyrs.

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## Analytical methods for measuring the parameters of interstellar gas using methanol observations

**S. V. Kalenskii, S. Kurtz**

The excitation of methanol in the absence of external radiation is analyzed, and LTE methods for probing interstellar gas considered. It is shown that rotation diagrams correctly estimate the gas kinetic temperature only if they are constructed using lines whose upper levels are located in the same K-ladders, such as the  $J(0)-J(-1)$  E lines at 157 GHz, the  $J(1)-J(0)$  E lines at 165 GHz, and the  $J(2)-J(1)$  E lines at 25 GHz. The gas density must be no less than  $10E7$  cm $^{-3}$ . Rotation

diagrams constructed from lines with different  $K$  values for their upper levels (e.g.,  $2(K) - 1(K)$  at 96 GHz,  $3(K) - 2(K)$  at 145 GHz,  $5(K) - 4(K)$  at 241 GHz significantly underestimate the temperature, but enable estimation of the density. In addition, diagrams based on the 96 GHz lines can be used to estimate the methanol column density within a factor of about two to five. It is suggested that rotation diagrams should be used in the following manner. First, two rotation diagrams should be constructed, one from the lines at 96, 145, or 241 GHz, and another from the lines at 157, 165, or 25 GHz. The former diagram is used to estimate the gas density. If the density is about  $10E7 \text{ cm}^{-3}$  or higher, the latter diagram reproduces the temperature fairly well. If the density is around  $10E6 \text{ cm}^{-3}$ , the temperature obtained from the latter diagram should be multiplied by a factor of 1.5–2. If the density is about  $10E5 \text{ cm}^{-3}$  or lower, then the latter diagram yields a temperature that is lower than the kinetic temperature by a factor of three or more, and should be used only as a lower limit for the kinetic temperature. The errors in the methanol column density determined from the integrated intensity of a single line can be more than an order of magnitude, even when the gas temperature is well known. However, if the  $J(0) - (J - 1)(0)E$  lines, as well as the  $J(1) - (J - 1)(1)A+$  or  $A-$  lines are used, the relative error in the column density is no more than a factor of a few.

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## 13C Isotopic Fractionation of HC3N in Star-Forming Regions -Low-Mass Star Forming Region L1527 and High-Mass Star Forming Region G28.28-0.36-

**Kotomi Taniguchi, Masao Saito, Hiroyuki Ozeki**

We observed the  $J=9-8$  and  $10-9$  rotational lines of three  $^{13}\text{C}$  isotopologues of  $\text{HC}_3\text{N}$  in L1527 and G28.28-0.36 with the 45-m radio telescope of the Nobeyama Radio Observatory in order to constrain the main formation mechanisms of  $\text{HC}_3\text{N}$  in each source. The abundance ratios of the three  $^{13}\text{C}$  isotopologues of  $\text{HC}_3\text{N}$  are found to be 0.9 (0.2) : 1.00 : 1.29 (0.19) (1sigma) and 1.0 (0.2) : 1.00 : 1.47 (0.17) (1sigma) for  $[\text{H}^{13}\text{CCCN}]$ :  $[\text{HC}^{13}\text{CCN}]$ :  $[\text{HCC}^{13}\text{CN}]$  in L1527 and G28.28-0.36, respectively. We recognize a similar  $^{13}\text{C}$  isotopic fractionation pattern that the abundances of  $\text{H}^{13}\text{CCCN}$  and  $\text{HC}^{13}\text{CCN}$  are comparable, and  $\text{HCC}^{13}\text{CN}$  is more abundant than the others. Based on the results, we discuss the main formation pathway of  $\text{HC}_3\text{N}$ . The  $^{13}\text{C}$  isotopic fractionation pattern derived from our observations can be explained by the neutral-neutral reaction between  $\text{C}_2\text{H}_2$  and  $\text{CN}$  in both the low-mass (L1527) and high-mass (28.28-0.36) star forming regions.

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## Laboratory rotational ground state transitions of $\text{NH}_3\text{D}^+$ and $\text{CF}^+$

**A. Stoffels, L. Kluge, S. Schlemmer, S. Brünken**

This paper reports accurate laboratory frequencies of the rotational ground state transitions of two astronomically relevant molecular ions,  $\text{NH}_3\text{D}^+$  and  $\text{CF}^+$ . Spectra in the millimetre-wave band were recorded by the method of rotational state-selective attachment of He atoms to the molecular ions stored and cooled in a cryogenic ion trap held at 4 K. The lowest rotational transition in the A state (ortho state) of  $\text{NH}_3\text{D}^+$  ( $J, K = 1, 0 - 0, 0$ ), and the two hyperfine components of the ground state transition of  $\text{CF}^+$  ( $J = 1 - 0$ ) were measured with a relative

precision better than  $10^{-7}$ ). For both target ions, the experimental transition frequencies agree with recent observations of the same lines in different astronomical environments. In the case of  $\text{NH}_3\text{D}^+$  the high-accuracy laboratory measurements lend support to its tentative identification in the interstellar medium. For  $\text{CF}^+$  the experimentally determined hyperfine splitting confirms previous quantum-chemical calculations and the intrinsic spectroscopic nature of a double-peaked line profile observed in the  $J = 1 - 0$  transition towards the Horsehead photon-dominated region (PDR).

A&A in press

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## Compression and ablation of the photo-irradiated molecular cloud the Orion Bar

**Javier R. Goicoechea, Jerome Pety, Sara Cuadrado, Jose Cernicharo, Edwige Chapillon, Asunción Fuente, Maryvonne Gerin, Christine Joblin, Nuria Marcelino, Paolo Pilleri**

The Orion Bar is the archetypal edge-on molecular cloud surface illuminated by strong ultraviolet radiation from nearby massive stars. Our relative closeness to the Orion nebula (about 1,350 light years away from Earth) means that we can study the effects of stellar feedback on the parental cloud in detail. Visible-light observations of the Orion Bar show that the transition between the hot ionized gas and the warm neutral atomic gas (the ionization front) is spatially well separated from the transition between atomic and molecular gas (the dissociation front), by about 15 arcseconds or 6,200 astronomical units (one astronomical unit is the Earth–Sun distance). Static equilibrium models used to interpret previous far-infrared and radio observations of the neutral gas in the Orion Bar (typically at 10–20 arcsecond resolution) predict an inhomogeneous cloud structure comprised of dense clumps embedded in a lower-density extended gas component. Here we report one-arcsecond-resolution millimetre-wave images that allow us to resolve the molecular cloud surface. In contrast to stationary model predictions, there is no appreciable offset between the peak of the  $\text{H}_2$  vibrational emission (delineating the  $\text{H}/\text{H}_2$  transition) and the edge of the observed  $\text{CO}$  and  $\text{HCO}^+$  emission. This implies that the  $\text{H}/\text{H}_2$  and  $\text{C}^+/\text{C}/\text{CO}$  transition zones are very close. We find a fragmented ridge of high-density substructures, photoablative gas flows and instabilities at the molecular cloud surface. The results suggest that the cloud edge has been compressed by a high-pressure wave that is moving into the molecular cloud, demonstrating that dynamical and non-equilibrium effects are important for the cloud evolution.

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## Announcements

### 16 PHD POSITIONS ARE AVAILABLE THROUGH EUROPAH - A NEW MULTI-DISCIPLINARY EUROPEAN TRAINING NETWORK

EUROPAH is a European Training Network (ETN) aimed at studying the “Extensive and Ubiquitous Role of PAHs in the interstellar medium” and has opened a call for PhD students with a deadline of 15th September 2016. The network includes 13 research groups, spread across 10 universities and 3 industrial partners in 6 different countries and will train 16 early stage researchers (PhD students) with starting dates between October 2016 and October 2017. The

project details are available at [www.europah.eu](http://www.europah.eu). The joint scientific research goal is to understand the role that polycyclic aromatic hydrocarbons (PAHs) play in the physics and chemistry of the interstellar medium of galaxies. This will be a highly multidisciplinary network that combines astronomy, molecular physics, molecular spectroscopy, environmental science, quantum chemistry, surface sciences, plasma physics and scientific communication. PAHs are universally ubiquitous and lock-up close to 15% of the elemental carbon in space. They play a key role in maintaining the ionization balance and in the heating of interstellar gas, and are central to the chemical complexity of space and the organic inventory of regions of star and planet formation. On Earth, PAHs are pernicious pollutants affecting the atmosphere and aquatic environments. Understanding PAHs and their multitude of roles in the Universe is thus a key question in both astrophysics and terrestrial chemistry. Candidates must qualify under EU-researcher mobility rules and have a bachelor or masters' degree no more than 4-years old. Check out the project descriptions at [www.europah.eu](http://www.europah.eu) and then forward a 2-page CV and 1-page cover letter, listing your favoured projects in order of preference, to [recruitment@europah.eu](mailto:recruitment@europah.eu) by the deadline: September 15th 2016. Subject to negotiations, EUROPAH will be funded by the European Commission under the Horizon 2020 Marie Skłodowska-Curie Action.

## **IAUS 332: Astrochemistry VII – Through the Cosmos from Galaxies to Planets**

Dear Colleagues, we are please to announce that IAU S332, Astrochemistry VII, will be held in Puerto Varas, in Chile, between 20 and 24 March 2017. The study of astrochemistry has become an important branch of modern astronomy and astrophysics. Molecules are key tools in exploring topics such as star and planet formation, mass loss mechanisms in late-type stars, the origin and evolution of interstellar dust grains, the structure of the interstellar medium in galaxies and the origin of protogalaxies in the early Universe. Facilities such as the Herschel Space Observatory, ALMA, NOEMA, Rosetta and SOFIA are producing results that provide information on densities, temperatures, excitation mechanisms, dynamics in interstellar gas and lead to new research areas such as the habitability of exoplanets, the origin of prebiotic chemistry and astrobiology. At the same time as new observational facilities and instruments are revealing new views of our molecular universe, there has been a concerted effort among physical chemists to provide the large amount of fundamental data required to interpret these observations. The active synergy between astronomical observation, laboratory experiment and theoretical modelling has been reinforced at the latest General Assembly by the creation of a new IAU Commission (B5) on Laboratory Astrophysics, of which laboratory astrochemistry is a component. This meeting is the seventh in a series to discuss astrochemistry. You can find more information on the meeting website: <http://newt.phys.unsw.edu.au/IAUS332/>. The confirmed invited speakers are Kathrin Altwegg, Arnaud Belloche, Simon Casassus, L. Ilseidore Cleeves, Herma Cuppen, Nanase Harada, Suzanne Madden, Nikku (Madhu) Madhusudhan, Stefanie N. Milam, Sergio Pilling, Ian Sims, Ewine van Dishoeck, Satoshi Yamamoto, Leen Decin. Scientific Organising Committee, S332.