AstroChemical Newsletter #34

August 2018

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Abstracts

Discovery of interstellar isocyanogen (CNCN): further evidence that dicyanopolyynes are abundant in space

M. Agundez, N. Marcelino, J. Cernicharo

It is thought that dicyanopolyynes could be potentially abundant interstellar molecules, although their lack of dipole moment makes it impossible to detect them through radioastronomical techniques. Recently, the simplest member of this chemical family, cyanogen (NCCN), was indirectly probed for the first time in interstellar space through the detection of its protonated form toward the dense clouds L483 and TMC-1. Here we present a second firm evidence of the presence of NCCN in interstellar space, namely the detection of the metastable and polar isomer isocyanogen (CNCN). This species has been identified in L483 and tentatively in TMC-1 by observing various rotational transitions in the 3 mm band with the IRAM 30m telescope. We derive beam-averaged column densities for CNCN of 1.6e12 cm-2 in L483 and 9e11 cm-2 in TMC-1, which imply fractional abundances relative to H2 in the range (5-9)e-11. While the presence of NCCN in interstellar clouds seems out of doubt owing to the detection of NCCNH+ and CNCN, putting tight constraints on its abundance is still hampered by the poor knowledge of the chemistry that links NCCN with NCCNH+ and especially with CNCN. We estimate that NCCN could be fairly abundant, in the range 1e-9 - 1e-7 relative to H2, as other abundant nitriles like HCN and HC3N.

ApJL 2018 861 L22
DOI: 10.3847/2041-8213/aad089
Full-text URL: https://arxiv.org/abs/1806.10328

The ALMA-PILS survey: first detection of methyl isocyanide (CH3NC) in a solar-type protostar

H. Calcutt, M. R. Fiechter E. R. Willis H. S. P. Müller, R. T. Garrod, J. K. Jørgensen, S. F. Wampfler, T. L. Bourke, A. Coutens, M. N. Drozdovskaya, N. F. W. Ligterink, L. E. Kristensen

Context. Methyl isocyanide (CH3NC) is the isocyanide with the largest number of atoms confirmed in the interstellar medium (ISM), but it is not an abundant molecule, having only been detected towards a handful of objects. Conversely, its isomer, methyl cyanide (CH3CN), is one of the most abundant complex organic molecules detected in the ISM, with detections in a variety of low- and high-mass sources. Aims. The aims of this work are to determine the abundances of methyl isocyanide in the solar-type protostellar binary IRAS 16293– 2422 and understand the stark abundance differences observed between methyl isocyanide and methyl cyanide in the ISM. Methods. We use ALMA observations from the Protostellar Interferometric Line Survey (PILS) to search for

methyl isocyanide and compare its abundance with that of its isomer methyl cyanide. We use a new line catalogue from the Cologne Database for Molecular Spectroscopy (CDMS) to identify methyl isocyanide lines. We also model the chemistry with an updated version of the three-phase chemical kinetics model MAGICKAL, presenting the first chemical modelling of methyl isocyanide to date. Results. We detect methyl isocyanide for the first time in a solar-type protostar, IRAS 16293–2422 B, and present upper limits for its companion protostar, IRAS 16293–2422 A. Methyl isocyanide is found to be at least 20 times more abundant in source B compared to source A, with a CH3CN/CH3NC abundance ratio of 200 in IRAS 16293–2422 B and >5517 in IRAS 16293–2422 A. We also present the results of a chemical model of methyl isocyanide chemistry in both sources, and discuss the implications on methyl isocyanide formation mechanisms and the relative evolutionary stages of both sources. The chemical modelling is unable to match the observed CH3CN/CH3NC abundance ratio towards the B source at densities representative of that source. The modelling, however, is consistent with the upper limits for the A source. There are many uncertainties in the formation and destruction pathways of methyl isocyanide, and it is therefore not surprising that the initial modeling attempts do not reproduce observations. In particular, it is clear that some destruction mechanism of methyl isocyanide which does not destroy methyl cyanide is needed. Furthermore, these initial model results suggest that the final density plays a key role in setting the abundance ratio. The next steps are therefore to obtain further detections of methyl isocyanide in more objects, as well as undertaking more detailed physico-chemical modeling of sources such as IRAS 16293-2422.

Accepted in A&A
DOI: 10.1051/0004-6361/201833140
Full-text URL: http://arxiv.org/abs/1807.02909

Measurements of diffusion of volatiles in amorphous solid water: application to interstellar medium environments

J. He, S. Emtiaz, G. Vidali

The diffusion of atoms and molecules in ices covering dust grains in dense clouds in interstellar space is an important but poorly characterized step in the formation of complex molecules in space. Here we report the measurement of diffusion of simple molecules in amorphous solid water (ASW), an analog of interstellar ices, which are amorphous and made mostly of water molecules. The new approach that we used relies on measuring in situ the change in band strength and position of mid-infrared features of OH dangling bonds as molecules move through pores and channels of ASW. We obtained the Arrhenius pre-exponents and activation energies for diffusion of CO, O2, N2, CH4, and Ar in ASW. The diffusion energy barrier of H2 and D2 were also measured, but only upper limits were obtained. These values constitute the first comprehensive set of diffusion parameters of simple molecules on the pore surface of ASW, and can be used in simulations of the chemical evolution of ISM environments, thus replacing unsupported estimates. We also present a set of argon temperature programmed desorption experiments to determine the desorption energy distribution of argon on non-porous ASW.

ApJ accepted
Full-text URL: http://arxiv.org/abs/1806.06980

X-ray photodesorption from water ice in protoplanetary disks and X-ray-dominated regions

R. Dupuy, M. Bertin, G. Féraud, M. Hassenfratz, X. Michaut, T. Putaud, L. Philippe, P. Jeseck, M. Angelucci, R. Cimino, V. Baglin, C. Romanzin & J.-H. Fillion

Water is the main constituent of interstellar ices, and it plays a key role in the evolution of many regions of the interstellar medium, from molecular clouds to planet-forming disks. In cold regions of the interstellar medium, water is expected to be completely frozen out onto the dust grains. Nonetheless, observations indicate the presence of cold water vapour, implying that non-thermal desorption mechanisms are at play. Photodesorption by ultraviolet photons has been proposed to explain these observations, with the support of extensive experimental and theoretical work on ice analogues. In contrast, photodesorption by X-rays, another viable mechanism, has been little studied. The potential of this process to desorb key molecules such as water, intact rather than fragmented or ionized, remains unexplored. We experimentally investigated X-ray photodesorption from water ice, monitoring all desorbing species. We found that desorption of neutral water is efficient, while ion desorption is minor. We derived yields that can be implemented in astrochemical models. These results open up the possibility of taking into account the X-ray photodesorption process in the modelling of protoplanetary disks or X-ray-dominated regions.

Nature Astronomy (2018)
DOI: 10.1038/s41550-018-0532-y
Full-text URL: https://arxiv.org/abs/1807.03725

Nitrogen fractionation in high-mass star-forming cores across the Galaxy

L. Colzi, F. Fontani, V. M. Rivilla, Á. Sánchez-Monge, L. Testi, M. T. Beltrán, P. Caselli

The fractionation of nitrogen (N) in star-forming regions is a poorly understood process. To put more stringent observational constraints on the N-fractionation, we have observed with the IRAM-30-m telescope a large sample of 66 cores in massive star-forming regions. We targeted the (1–0) rotational transition of HN13C, HC15N, H13CN and HC15N, and derived the 14N/15N ratio for both HCN and HNC. We have completed this sample with that already observed by Colzi et al. (2018a), and thus analysed a total sample of 87 sources. The 14N/15N ratios are distributed around the Proto-Solar Nebula value with a lower limit near the TA value (about 272). We have also derived the 14N/15N ratio as a function of the Galactocentric distance and deduced a linear trend based on unprecedented statistics. The Galactocentric dependences that we have found are consistent, in the slope, with past works but we have found a new local 14N/15N value of about 400, i.e. closer to the Prosolar Nebula value. A second analysis was done, and a parabolic Galactocentric trend was found. Comparison with Galactic chemical evolution models shows that the slope until 8 kpc is consistent with the linear analysis, while the flattening trend above 8 kpc is well reproduced by the parabolic analysis.

Monthly Notices of the Royal Astronomical Society, Volume 478, Issue 3, Pages 3693–3720
DOI: 10.1093/mnras/sty1027
Full-text URL: https://arxiv.org/abs/1804.05717

First Detection of the Simplest Organic Acid in a Protoplanetary Disk

C.Favre, D. Fedele, D. Semenov, S. Parfenov, C. Codella, C. Ceccarelli, E. A. Bergin, E. Chapillon, L. Testi, F. Hersant, B. Lefloch, F. Fontani, G. A. Blake, L. I. Cleeves, C. Qi, K. R. Schwarz, V. Taquet

The formation of asteroids, comets, and planets occurs in the interior of protoplanetary disks during the early phase of star formation. Consequently, the chemical composition of the disk might shape the properties of the emerging planetary system. In this context, it is crucial to understand whether and what organic molecules are synthesized in the disk. In this Letter, we report the first detection of formic acid (HCOOH) toward the TW Hydrae protoplanetary disk. The observations of the trans-HCOOH 6(1,6)–5(1,5) transition were carried out at 129 GHz with Atacama Large Millimeter/Submillimeter Array (ALMA). We measured a disk-averaged gas-phase t-HCOOH column density of about (2–4)×10^12 cm-2, namely as large as that of methanol. HCOOH is the first organic molecule containing two oxygen atoms detected in a protoplanetary disk, a proof that organic chemistry is very active, albeit difficult to observe, in these objects. Specifically, this simplest acid stands as the basis for synthesis of more complex carboxylic acids used by life on Earth.

2018, ApJL, 862, L2
DOI: 10.3847/2041-8213/aad046
Full-text URL: https://arxiv.org/abs/1807.05768

The role of external far-ultraviolet irradiation in the survival of astrophysical ices in Elias 29

W. R. M. Rocha, S. Pilling

The survival of astrophysical ices in star-forming regions depends on the suitability of temperature, density and radiation conditions. In this article, the role of the interstellar radiation field (ISRF) on ices in Elias 29 is addressed. This object is the most luminous protostar in the rho Oph E molecular cloud and is surrounded by many young stellar objects only a few arcmin distant. In addition, two other bright BV stars (S1 and HD 147889) enhance the external irradiation in Elias 29. This study was carried out using the Monte Carlo radiative transfer code RADMC-3D assuming internal and external irradiation. As result, we found that HD 147889 dominates the ISRF, rather than the closest protostars, and contributes to enhancing the external irradiation by 44 times the standard value. Furthermore, remarkable effects are observed in the far-infrared (FIR) spectrum, as well as in the near-infrared (near-IR) image. Additionally, the snowline positions of volatile compounds, such as CO, O2, N2 and CH4, are redefined to a toroidal-shaped morphology in the envelope, with low far-ultraviolet (FUV) flux (10^−7 erg cm^−2 s^−1). In such a scenario, the formation of complex molecules as the result of hydrogenation or oxygenation of volatile species is expected to be severely affected.

Monthly Notices of the Royal Astronomical Society, Volume 478, Issue 4, 21 August 2018, Pages 5190–5198
DOI: 10.1093/mnras/sty1492
Full-text URL: https://arxiv.org/abs/1806.01769

Sulphur-bearing molecules in AGB stars II: Abundances and distributions of CS and SiS

T. Danilovich, S. Ramstedt, D. Gobrecht, L. Decin, E. De Beck, H. Olofsson

We surveyed 20 AGB stars of different chemical types using the APEX telescope, and

combined this with an IRAM 30 m and APEX survey of CS and SiS emission towards over 30 S-type stars. For those stars with detections, we performed radiative transfer modelling to determine abundances and abundance distributions. We detect CS towards all the surveyed carbon stars, some S-type stars, and the highest mass-loss rate oxygen-rich stars (>5×1e-6 Msol yr−1). SiS is detected towards the highest mass-loss rate sources of all chemical types (>8×1e-7 Msol yr−1). We find CS peak fractional abundances ranging from ~ 4×1e-7 to ~ 2×1e-5 for the carbon stars, from ~ 3×1e-8 to ~ 1×1e-7 for the oxygen-rich stars and from ~ 1×1e-7 to ~ 8×1e-6 for the S-type stars. We find SiS peak fractional abundances ranging from ~ 9×1e-6 to ~ 2×1e-5 for the carbon stars, from ~ 5×1e-7 to ~ 2×1e-6 for the oxygen-rich stars, and from ~ 2×1e-7 to ~ 2×1e-6 for the S-type stars. We derived Si32S/Si34S = 11.4 for AI Vol, the only star for which we had a reliable isotopologue detection. Overall, we find that wind density plays an important role in determining the chemical composition of AGB CSEs. It is seen that for oxygen-rich AGB stars both CS and SiS are detected only in the highest density circumstellar envelopes and their abundances are generally lower than for carbon-rich AGB stars by around an order of magnitude. For carbon-rich and S-type stars SiS was also only detected in the highest density circumstellar envelopes, while CS was detected consistently in all surveyed carbon stars and sporadically among the S-type stars.

accepted in A&A
DOI: 10.1051/0004-6361/201833317
Full-text URL: https://arxiv.org/abs/1807.05144

Rate constants for the formation of CS by radiative association

R. C. Forrey, J. F. Babb, P. C. Stancil and B. M. McLaughlin

Rate constants for the formation of carbon monosulfide (CS) by radiative association are calculated using accurate molecular data. The rate constants include both direct and indirect formation processes. The indirect processes (inverse rotational and electronic predissociation) are evaluated for conditions of local thermodynamic equilibrium (LTE) and also in the non-LTE limit of zero radiation temperature and atomic density. Phenomenological rate constants for CS formation in realistic astrophysical environments are expected to lie in-between these limiting cases. An analytic formula is used to fit the rate constants for convenient use in astrophysical models. The impact of the results on various astrophysical environments is briefly discussed.

MNRAS 479, pp 4727-4734, 2018
DOI: 10.1093/mnras/sty1739
Full-text URL: https://doi.org/10.1093/mnras/sty1739

Announcements

Staff astronomer position at the IRAM 30-meter telescope

http://www.iram-institute.org/EN/job-offer.php?id=50 IRAM is an international research organization for millimeter and submillimeter astronomy supported by the CNRS (France), the Max-Planck Gesellschaft (Germany), and the IGN (Spain). IRAM operates two world-class research facilities, a 30-meter single-dish telescope in the Spanish Sierra Nevada and the mm/submm interferometer NOEMA in the French Alps. The scientific capabilities of the 30-meter telescope are continuously enhanced with state-of-the-art technology such as for EMIR, the multi-wavelength heterodyne frontend, and

with the recent commissioning of the new large field-of-view continuum 1mm/2mm camera NIKA2. IRAM is also preparing for new multi-beam heterodyne-arrays for the 30-meter telescope. IRAM is seeking a senior staff astronomer at IRAM/Granada and the 30-meter telescope. The candidate must have a PhD and a solid experience in observational millimeter/ submillimeter/far-infrared astronomy. With recent and planned upgrades of the instrumentation of the 30m telescope, the control system of the telescope, i.e. the software controlling its various components, needs to be adapted and enhanced. Thorough and proven programming experience is a requirement for this position. Knowledge of Fortran 90 is an asset. The astronomer shall support this work in the framework of the Science Operations Group in Granada and in close collaboration with the GILDAS software development team in Granada and Grenoble. In addition, the successful candidate shall support science operation at the telescope by providing assistance to visiting astronomers. He/she will typically spend about one week every six weeks at the observatory. This support work shall in total account for 50% of the working time. During the remaining 50% of the time, the candidate is expected to actively pursue his/her astronomical research. Review of applications will begin mid August 2018 and the search will continue until the position is filled. The appointment is initially for three years with the possibility of extension. Applications should be sent as one pdf file to the IRAM personnel department, jobs-scsu@iram.fr, and should include a cover letter indicating motivation and qualifications, a curriculum vitae with a list of publications, and a short research statement. Applicants should arrange for two letters of reference to be sent to the personnel department. Inquiries should be addressed to the station manager Carsten Kramer. Posting date: June, 16, 2018 – Closing date: August, 16, 2018

One Postdoctoral Research Position in Millimeter Astronomy for NOEMA

http://www.iram-institute.org/EN/job-offer.php?id=51 IRAM is an international research organization for millimeter and submillimeter astronomy supported by the CNRS (France), the Max-Planck Gesellschaft (Germany), and the IGN (Spain). The organization operates two world-class research facilities, the IRAM 30-meter telescope in Spain, and NOEMA, the largest millimeter interferometer of the northern hemisphere in the French Alps. By the end of 2020, NOEMA will have twelve antennas and offer ten times the sensitivity and twice the spatial resolution of the former Plateau de Bure interferometer. The institute also houses one of the nodes of the European ALMA science support center. IRAM is seeking a qualified candidate for a position in the NOEMA Science Operations Group (SOG). The successful candidate is expected to invest 50% of the time on an astronomical research program, in collaboration with astronomers within and outside IRAM, and 50% to contribute to the overall SOG mission. The ideal candidate will take part in a range of activities to support the integration and science verification of NOEMA subsystems, provide assistance to the scientific operation of NOEMA as an astronomer on duty, support the broader user community in the preparation of proposals and observations, and provide technical expertise to visiting astronomers in the analysis and interpretation of data obtained with the NOEMA interferometer. Depending on experience and skills, the successful candidate may also take part in software developments aimed at extending NOEMA's capabilities. The current position offers the opportunity for astronomers to work with world-class research facilities and pursue their career in a very dynamic and competitive field of research. IRAM's research programs cover a wide range of subjects from ISM chemistry, planetary science, young stellar objects, late stage stellar evolution, to extragalactic research at low and high redshift. We are seeking qualified candidates with a PhD (or close to completion), preferably with a demonstrated observational experience and a strong interest in (sub)millimeter wave interferometry. Good English

communication skills and a strong sense of team spirit are essential attributes. Aptitude and interest in developing software applications and working experience in an international research environment are an asset. Applicants must possess a driver's license. Interested candidates should send their curriculum vitae, bibliography, a brief statement of research interests, an outline of future plans, and arrange for three letters of reference. Applications received before September 03, 2018 will be given full consideration, but will continue to be accepted until the position is filled. The appointment is for two years with the possibility of extension, and could start as early as possible. Applications and reference letters are to be submitted by email to the IRAM personnel department. Questions should be directed to the Head of the Astronomy and Science Support Group (neri@iram.fr).

Exploring the Infrared Universe: The Promise of SPICA -- Crete (Greece), 20-23 May 2019

The infrared wavelength range is key to understand the origin and evolution of galaxies, stars and planetary systems, which are obscured by dust during a large part of their life cycles. With a large cold mirror and a sensitive suite of instruments, SPICA, recently selected as a candidate for ESA’s Cosmic Visions program, stands poised to revolutionize these fields by providing ultra-deep spectroscopy in the 12-230 µm range, as well as imaging (17-37 µm and 100-350 µm) and polarimetry (100-350 µm). With launch planned for 2030, SPICA will complement current and upcoming facilities, filling the spectral gap between JWST and ALMA, while providing a huge leap over previous infrared space missions. We would like to invite the international astronomical community to participate in the conference, Exploring the Infrared Universe: The Promise of SPICA, which will take place on the island of Crete on 20-23 May 2019. At this conference, participants will learn about the capabilities and current design of SPICA, which includes a significant Guest Observer program, while discussing the exciting scientific promise of the mission. Up to date information about the SPICA mission and its instruments can be found at http://www.spica-mission.org, in addition to links to a set of whitepapers recently published in the journal PASA, that focus on some of extragalactic science enabled by SPICA. Topics to be addressed at the meeting include: -The rise of metals and dust across cosmic time -Feedback and feeding processes in galaxy evolution -Star formation and the baryon cycle in galaxies -Magnetic fields and turbulence in star formation -Protoplanetary disks and the formation of habitable planets -Debris disks, planetary systems, and the Solar system Confirmed invited speakers include: Susanne Aalto, Yuri Aikawa, Françoise Combes, Bill Dent, Edith Falgarone, Davide Fedele, Andrea Ferrara, Javier Goicoechea, Masateru Ishiguro, Patrick Koch, Leon Koopmans, Ilse de Looze, Roberto Maiolino, Thomas Müller, Tohru Nagao, Klaus Pontoppidan, Alexandra Pope, and Peter Roelfsema. For further information about the conference, please visit http://www.spica2019.org/ Looking forward to seeing you in Crete! The scientific organizing committee: Lee Armus, Marc Audard, Vassilis Charmandaris, Yasuo Doi, Eiichi Egami, David Elbaz, Martin Giard, Matt Griffin, Carlotta Gruppioni, Doug Johnstone, Inga Kamp, Hidehiro Kaneda, Ciska Kemper, Kotaro Kohno, Sue Madden, Mikako Matsuura, Stefanie Milam, Paco Najarro, Takashi Onaka, Luigi Spinoglio, Floris van der Tak (chair), Jan Tauber

Ph.D. in Astrochemistry

http://phd.sns.it/it/astrochemistry/ The increasing investments in astrochemistry in Europe and the growing need for top level scientists that can participate in research programs has prompted the Scuola Normale Superiore to open in 2018-2019 for the first time in Italy 4 positions in a 4-year PhD course in Astrochemistry, as part of the activities of the Interuniversity Center STAR (Systems and Theories for Astrochemical Research) in partnership with the University of Bologna and the University of Naples

Federico II. The PhD course, which provides this year a joint-degree with the University of Naples Federico II, aims at offering a basic education in one of the most fascinating and rapidly growing fields of research, which is expected to gain increasing momentum in the coming years. Astrochemistry spans the disciplines of chemistry, physics, planetary science, chemical biology, astronomy, and computational science. Scientists trained in astrochemistry perform experimental and computational studies (including quantum chemical calculations) to generate data for interpreting or explaining astronomical observations, to provide input data for models, and to test theories about the formation and evolution of large and small molecules in various astrophysical environments. Research in astrochemistry includes one of the biggest and most fascinating challenges of modern science: understanding the origin of life. Astrochemists investigate the molecular basis of the evolution of the Universe: the formation of small molecules in space, their conversion into complex molecular systems, the transformation/destruction of the latter, the effects of the interaction between radiation and molecules in different environments. In addition, astrochemists seek to retrieve information on molecular excitation, radiative transfer, and kinematics by studying molecules in the interstellar, circumstellar and pre-galactic gas, in proto-stellar disks, stars and planetary surface or atmosphere. In line with the objectives of the Interuniversity Center STAR, the PhD course aims at training students for competitive research in one of the several fields related to Astrochemistry: • Experimental and theoretical studies: ranging from molecular spectroscopy to organic synthesis, to chemical reactivity, to photochemistry; • Astronomical observations: ranging from the detection of molecules in the interstellar medium to the characterization of planetary atmospheres; • Modeling: ranging from the derivation of molecular abundances in the astronomical object under consideration to the characterization of the physical properties of the latter. PhD students will acquire: a) problem-solving skills and an interest in solving basic and applied research problems; b) critical thinking and analytical skills to design and validate laboratory and computational models and analyze and interpret data results; c) a capacity in designing experiments and applying computer software to solve new categories of problems; d) skills in the experimental determination of complex reaction mixtures and mechanisms under UV irradiation conditions, both in the gas phase and on surface . To fulfill these goals, students training will be supported by: • Highly innovative and multidisciplinary research projects; • National and international collaborations; • Innovative, state-of-the art experimental and high-performance computing resources; • National and international workshops and training schools; • Research periods abroad. Contact: cristina.puzzarini@unibo.it

Workshop Oxygen in Space, October 16-17, 2018, Cergy France

http://laboratoires.u-cergy.fr/~lerma/OxygenInSpace/index.html After hydrogen, oxygen is the second most abundant reactive element. The reductionoxidation reaction is one of the pillars of chemistry, on Earth and in space. The present workshop focuses on the role and form of oxygen in astrophysical environments. During two days, the elusive presence of molecular oxygen in the Interstellar Medium and its unexpectedly high abundance in comets will be discussed. A session devoted to proxy molecules such as NO, SO and sulfur-substituted molecules will take place. The last part of the workshop will be devoted to the hydrogenated forms of oxygen (such as water and methanol), with a special attention to their deuterated isotopologues. Observational, modelling, and laboratory aspects will be included in the discussion. The workshop will be located at the Maison Internationale de la Recherche in Neuville-sur-Oise, 45 minutes by train from the center of Paris (France). The participation is free of fees and is limited to 60 participants, by order of registration which is open. About half of the time will be devoted to contributions and posters. Confirmed speakers :Aurore Bacmann (IPAG,

France), Dominique BockelŽe-Morvan (Observatoire de Paris, France), Claudio Codella (Osservatorio di Arcetri, Italy), Ewine van Dishoeck (Leiden Observatory, NL), Kostas Giapis (California Institute of Technology, USA), Paul F. Goldsmith (NASA JPL, Pasadena, USA), Marco Minissale (Aix-Marseille UniversitŽ, France), Vianney Taquet (Osservatorio di Arcetri, Italy),Valentine Wakelam Symposium: The workshop will be followed by the Symposium honoring Paul F. Goldsmith: "Velocity-Resolved Far-Infrared Imaging Spectroscopy of the Future", which will take place at the Paris Observatory on October 18-19.

First Annoucement IAU Symposium 350 on Laboratory Astrophysics

First Announcement Please save the date! The First International Astronomical Union Symposium on Laboratory Astrophysics, IAUS 350: Laboratory Astrophysics: from Observations to Interpretation, will be held in Cambridge, UK, from 14 - 19 April 2019. The active synergy between astronomical observation, laboratory experiment and theoretical modeling has been reinforced at the 2015 IAU General Assembly by the creation of a new IAU Commission (CB5) on Laboratory Astrophysics (https://www.iau.org/science/scientific_bodies/commissions/B5/). In this meeting we hope to build on this momentum and bring together active researchers in observational astronomy, space missions, experimental and theoretical laboratory astrophysics and astrochemistry to discuss the major topics and challenges that face today's Astronomy. We expect that interactions between researchers will result in a solid roadmap for future research that will lead to advances in our understanding of astronomical observations and guide the design of future observational instruments. You can read more on the objectives of the Symposium at https://www.iau.org/science/meetings/proposals/loi/2019/1991/. To register your interest in this meeting, please send an email to IAUS350-labastro2019@open.ac.uk. You will then receive regular updates on the meeting. On behalf of the Organizing Committee for IAUS 350, Farid Salama President IAU Commission B5 IAUS 350 SOC: Farid Salama (Chair), USA, Paul Barklem, Sweden, Helen Fraser, UK, Thomas Henning, Germany, Christine Joblin, France, Sun Kwok, China, Harold Linnartz, Netherlands, Lyudmila Mashonkina, Russia, Tom Millar, UK, Osama Shalabiea, Egypt, Gianfranco Vidali, USA, Feilu Wang, China, Giulio Del- Zanna, UK