

AstroChemical Newsletter #6

April 2016

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Abstracts

Detection of CH₃SH in protostar IRAS 16293-2422

Liton Majumdar, Pierre Gratier, Thomas Vidal, Valentine Wakelam, Jean-Christophe Loison, Kevin M. Hickson, Emmanuel Caux

The nature of the main sulphur reservoir in star forming regions is a long standing mystery. The observed abundance of sulphur-bearing species in dense clouds is only about 0.1 per cent of the same quantity in diffuse clouds. Therefore, the main sulphur species in star forming regions of the interstellar medium are still unknown. IRAS 16293-2422 is one of the regions where production of S-bearing species is favourable due to its conditions which allows the evaporation of ice mantles. We carried out observations in the 3 mm band towards the solar type protostar IRAS 16293-2422 with the IRAM 30m telescope. We observed a single frequency setup with the EMIR heterodyne 3 mm receiver with an Lower Inner (LI) tuning frequency of 89.98 GHz. Several lines of the complex sulphur species CH₃SH were detected. Observed abundances are compared with simulations using the NAUTILUS gas-grain chemical model. Modelling results suggest that CH₃SH has the constant abundance of 4e-9 (compared to H₂) for radii lower than 200 AU and is mostly formed on the surfaces. Detection of CH₃SH indicates that there may be several new families of S-bearing molecules (which could form starting from CH₃SH) which have not been detected or looked for yet.

Monthly Notices of the Royal Astronomical Society, Volume 458, Issue 2, p.1859-1865

DOI: [10.1093/mnras/stw457](https://doi.org/10.1093/mnras/stw457)

Full-text URL: <http://arxiv.org/abs/1602.07619>

Isotopic ratios of H, C, N, O, and S in comets C/2012 F6 (Lemmon) and C/2014 Q2 (Lovejoy)

N. Biver, R. Moreno, D. Bockelée-Morvan, Aa. Sandqvist, P. Colom, J. Crovisier, D.C. Lis, J. Boissier, V. Debout, G. Paubert, S. Milam, A. Hjalmarson, S. Lundin, T. Karlsson, M. Battelino, U. Frisk, D. Murtagh, and the Odin team

The apparition of bright comets C/2012 F6 (Lemmon) and C/2014 Q2 (Lovejoy) in March-April 2013 and January 2015, combined with the improved observational capabilities of submillimeter facilities, offered an opportunity to carry out sensitive compositional and isotopic studies of the volatiles in their coma. We observed comet Lovejoy with the IRAM 30m telescope between 13 and 26 January 2015, and with the Odin submillimeter space observatory on 29 January - 3 February 2015. We detected 22 molecules and several isotopologues. The H₂16O and H₂18O production rates measured with Odin follow a periodic pattern with a period of 0.94 days and an amplitude of ~25%. The inferred isotope ratios in comet Lovejoy are 16O/18O = 499 ± 24 and D/H = 1.4 ± 0.4 × 10⁻⁴ in water, 32S/34S = 24.7 ± 3.5 in CS, all compatible with terrestrial values. The ratio 12C/13C = 109 ± 14 in HCN is marginally higher than terrestrial and 14N/15N = 145 ± 12 in HCN is half the Earth ratio. Several upper limits for D/H or 12C/13C in other molecules are reported. From our observation of HDO in comet C/2014 Q2 (Lovejoy), we report the first D/H ratio in an Oort Cloud comet that is not larger than the terrestrial value. On the other hand, the observation of the same HDO line in the other Oort-cloud comet, C/2012 F6 (Lemmon), suggests a D/H value four times higher. Given the previous measurements of D/H in cometary water, this illustrates that a diversity in the D/H ratio and in the chemical composition, is present even within the same dynamical group of comets, suggesting that current dynamical groups contain comets formed at very different places or times in the early solar system.

Accepted for publication in Astronomy and Astrophysics

DOI: [10.1051/0004-6361/201528041](https://doi.org/10.1051/0004-6361/201528041)

Full-text URL: <http://arxiv.org/abs/1603.05006>

Structure and stability in TMC-1: analysis of NH₃ molecular line and Herschel continuum data

O. Fehér, L. V. Tóth, D. Ward-Thompson, J. Kirk, A. Kraus, V.-M. Pelkonen, S. Pintér, S. Zahorec

We observed high S/N, high velocity resolution NH₃(1,1) and (2,2) emission on an extended map in TMC-1, a filamentary cloud in a nearby quiescent star forming area. By fitting multiple hyperfine-split line profiles to the NH₃(1,1) spectra we derived the velocity distribution of the line components and calculated gas parameters on several positions. Herschel SPIRE continuum observations were reduced and used to calculate the physical parameters of the Planck Galactic Cold Clumps in the region. The Herschel-based column density map of TMC-1 shows a main ridge with two local maxima and a separated peak to the south-west. H₂-column densities and dust temperatures are in the range of 0.5-3.3 × 1e22 cm⁻² and 10.5-12 K, respectively. NH₃-column densities are 2.8-14.2 × 1e14 cm⁻² and H₂-volume densities are 0.4-2.8 × 1e4 cm⁻³. Kinetic temperatures are typically very low with a minimum of 9 K, and a maximum of 13.7 K was found at the Class I protostar IRAS 04381+2540. The kinetic temperatures vary similarly as the dust temperatures in spite of the fact that densities are lower than the critical density for coupling between the gas and dust phase. The k-means clustering method separated four

sub-filaments in TMC-1 in the position-velocity-column density parameter space. They have masses of 32.5, 19.6, 28.9 and 45.9 M_{\odot} , low turbulent velocity dispersion (0.13-0.2 kms^{-1}) and they are close to gravitational equilibrium. We label them TMC-1F1 through F4. TMC-1F1, TMC-1F2 and TMC-1F4 are very elongated, dense and cold. TMC-1F3 is a little less elongated and somewhat warmer, probably heated by IRAS 04381+2540 that is embedded in it. TMC-1F3 is ~ 0.1 pc behind TMC1-F1. Because of its structure, TMC-1 is a good target to test filament evolution scenarios.

accepted for publication in A&A

DOI: [10.1051/0004-6361/201424385](https://doi.org/10.1051/0004-6361/201424385)

Full-text URL: <http://arxiv.org/abs/1603.05844>

Subsurface characterization of 67P/Churyumov-Gerasimenko's Abydos site

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On November 12, 2014, the ESA/Rosetta descent module Philae landed on the Abydos site of comet 67P/Churyumov-Gerasimenko. Aboard this module, the Ptolemy mass spectrometer measured a CO/CO₂ ratio of 0.07 \pm 0.04 which differs substantially from the value obtained in the coma by the Rosetta/ROSINA instrument, suggesting a heterogeneity in the comet nucleus. To understand this difference, we investigated the physico-chemical properties of the Abydos subsurface leading to CO/CO₂ ratios close to that observed by Ptolemy at the surface of this region. We used a comet nucleus model that takes into account different water ice phase changes (amorphous ice, crystalline ice and clathrates), as well as diffusion of molecules throughout the pores of the matrix. The input parameters of the model were optimized for the Abydos site and the ROSINA CO/CO₂ measured ratio is assumed to correspond to the bulk value in the nucleus. We find that all considered structures of water ice are able to reproduce the Ptolemy observation with a time difference not exceeding ~ 50 days, i.e. lower than $\sim 2\%$ on 67P/Churyumov-Gerasimenko's orbital period. The suspected heterogeneity of 67P/Churyumov-Gerasimenko's nucleus is also found possible only if it is constituted of crystalline ices. If the icy phase is made of amorphous ice or clathrates, the difference between Ptolemy and ROSINA's measurements would rather originate from the spatial variations in illumination on the nucleus surface. An eventual new measurement of the CO/CO₂ ratio at Abydos by Ptolemy could be decisive to distinguish between the three water ice structures.

Accepted for publication in The Astrophysical Journal

Full-text URL: <http://arxiv.org/abs/1603.05893>

Reactions of N⁺ ions with H₂ and HD molecules at low temperatures

T. Grodanov, R. McCarroll, E. Roueff

This work is motivated by the necessity to take account both of the nuclear spin symmetries of H₂ and of the spin-orbit interaction of N⁺ ion in order to investigate gas phase reactions in interstellar chemistry, leading to the formation of nitrogenous and deuterated compounds. The main objective in this work is to determine the rate coefficients for each possible initial quantum state of the reactants N⁺(3P_j) + H₂(J) (and their isotopic variants). Only in this way does it become possible both to analyze experimental data and develop realistic application to interstellar chemical models to constrain the gas phase chemistry of ammonia and its isotopologues. A statistical treatment is presented of state selective reactive collisions involving N⁺ ions in fine structure state j with H₂ or HD molecules in a rotation level J of the ground vibration state, leading either to the production of NH⁺ ions and H in the case of the H₂ reactant and to the production of either NH⁺ ions or ND⁺ in the case of the HD reactant. The fine structure states (j=0, 1, 2) of the N⁺ ions are treated on an equal footing with other internal motions. Cross sections for state to state collisions are calculated for collision energies ranging from 0.1 - 30 meV. These cross sections are then averaged over the kinetic energies of the reactants for each (J,j) to obtain the rate coefficients for a range of kinetic temperatures 10-200 K. The exothermicity of the reactions involving N⁺(3P_j) + H₂(J) (and isotopic variants) are derived from the difference ΔE_e between the dissociation energies of the electronic molecular potentials of NH⁺ and H₂. The value $\Delta E_e = 101$ meV is found to satisfactorily reproduce the experiments performed with para and ortho- H₂. This value is used to determine the endothermicity of the N⁺ + HD reaction leading to the formation of ND⁺, and subsequently the rate coefficient. The calculated rate is consistent with the available experimental data. The present results allow for the determination of reaction rate coefficients for any given distribution of specific fine structure and rotational state populations of the reactants. In interstellar conditions, where N⁺ is in its 3P₀ state and para and ortho-H₂ respectively in J= 0 and J=1, our results enable a study of the influence of the ortho/para evolution of molecular hydrogen on the formation of nitrogen compounds.

accepted in Astronomy Astrophysics

DOI: [10.1051/0004-6361/201628092](https://doi.org/10.1051/0004-6361/201628092)

Full-text URL: <http://www.aanda.org/articles/aa/pdf/forth/aa28092-16.pdf>

Quantum-state Dependence of Product Branching Ratios in Vacuum Ultraviolet Photodissociation of N₂

Yu Song, Hong Gao, Yih Chung Chang, D. Hammoutène, H. Ndome, M. Hochlaf, William M. Jackson, and C. Y. Ng

The branching ratios for the N(4S) + N(2D), N(4S) + N(2P), and N(2D) + N(2D) channels are measured for the photodissociation of N₂(X¹ Σ_g^+ ; v''= 0, J'') in the vacuum ultraviolet (VUV) region of 100,808–122,159 cm^{-1} using the VUV-VUV pump-probe approach combined with velocity-map-imaging-photoion detection. No evidence of forming the ground-state N(4S) + N(4S) products is found. No potential barrier is observed for the N(2D) + N(2D) channel, but the

N(4S) + N(2P) channel has a small potential barrier of ≈ 740 cm⁻¹. The branching ratios are found to depend on the symmetry of predissociative N₂ states instead of the total VUV excitation energy, indicating that N₂ photodissociation is nonstatistical. When the branching ratios for N(4S) + N(2D) and N(4S) + N(2P) products are plotted as a function of the VUV excitation energy for the valence N₂ 1Π_u and 1Σ_u⁺ states, oscillations in these ratios are observed demonstrating how these channels are competing with each other. These data can be used to select both the velocity and internal states of the atomic products by picking the quantum state that is excited. High-level ab initio potential energy curves of the excited N₂ states are calculated to provide insight into the mechanisms for the observed branching ratios. The calculations predict that the formation of both N(4S) + N(2D) and N(4S) + N(2P) channels involves potential energy barriers, in agreement with experimental observations. A discussion of the application of the present results to astronomy, planetary sciences, and comets is given.

The Astrophysical Journal, 819:23 (13pp), 2016 March 1

DOI: [10.3847/0004-637X/819/1/23](https://doi.org/10.3847/0004-637X/819/1/23)

Full-text URL: <http://iopscience.iop.org/article/10.3847/0004-637X/819/1/23;jsessionid=ACC2C87AE92A95E8F9A36C78495F8C39.c1.iopscience.cld.iop.org>

Methylacetylene (CH₃CCH) and propene (C₃H₆) formation in cold dense clouds: a case of dust grain chemistry.

Kevin M. Hickson, Valentine Wakelam, Jean-Christophe Loison

We present an extensive review of gas phase reactions producing methylacetylene and propene showing that these relatively abundant unsaturated hydrocarbons cannot be synthesized through gas-phase reactions. We explain the formation of propene and methylacetylene through surface hydrogenation of C₃ depleted onto interstellar ices, C₃ being a very abundant species in the gas phase.

Molecular Astrophysics in Press

Full-text URL: <http://arxiv.org/abs/1603.02703>

Chemical and physical characterization of collapsing low-mass prestellar dense cores

U. Hincelin, B. Commerçon, V. Wakelam, F. Hersant, S. Guilloteau

The first hydrostatic core, also called the first Larson core, is one of the first steps in low-mass star formation, as predicted by theory. With recent and future high performance telescopes, details of these first phases become accessible, and observations may confirm theory and even bring new challenges for theoreticians. In this context, we study from a theoretical point of view the chemical and physical evolution of the collapse of prestellar cores until the formation of the first Larson core, in order to better characterize this early phase in the star formation process. We couple a state-of-the-art hydrodynamical model with full gas-grain chemistry, using different assumptions on the magnetic field strength and orientation. We extract the different components of each collapsing core (i.e., the central core, the outflow, the disk, the pseudodisk, and the envelope) to highlight their specific physical and chemical characteristics. Each component often presents a specific physical history, as well as a specific chemical evolution. From some species, the components can clearly be differentiated. The different core models can also be chemically differentiated. Our simulation suggests some chemical species as tracers of the different components of a collapsing prestellar dense core, and as tracers of the magnetic field characteristics of the core. From this result, we pinpoint promising key chemical species to be observed.

Accepted for publication in ApJ

Full-text URL: <http://arxiv.org/abs/1603.02529>

The Cologne Database for Molecular Spectroscopy, CDMS, in the Virtual Atomic and Molecular Data Centre, VAMDC

Christian P. Endres, Stephan Schlemmer, Peter Schilke, Jürgen Stutzki, Holger S.P. Müller

The Cologne Database for Molecular Spectroscopy, CDMS, was founded 1998 to provide in its catalog section line lists of mostly molecular species which are or may be observed in various astronomical sources by means of (usually) radio astronomical means. The line lists contain transition frequencies with qualified accuracies, intensities, quantum numbers, as well as further auxiliary information. They have been generated from critically evaluated experimental line lists, mostly from laboratory experiments, employing established Hamiltonian models. Separate entries exist for different isotopic species and usually also for different vibrational states. As of December 2015, the number of entries is 792. They are available online as ascii tables with additional files documenting information on the entries. The Virtual Atomic and Molecular Data Centre, VAMDC, was founded more than 5 years ago as a common platform for atomic and molecular data. This platform facilitates exchange not only between spectroscopic databases related to astrophysics or astrochemistry, but also with collisional and kinetic databases. A dedicated infrastructure was developed to provide a common data format in the various databases enabling queries to a large variety of databases on atomic and molecular data at once. For CDMS, the incorporation in VAMDC was combined with several modifications on the generation of CDMS catalog entries. Here we introduce related changes to the data structure and the data content in the CDMS. The new data scheme allows us to incorporate all previous data entries but in addition allows us also to include entries based on new theoretical descriptions. Moreover, the CDMS entries have been transferred into a MySQL database format. These developments within the VAMDC framework have in part been driven by the needs of the astronomical community to be able to deal efficiently with large data sets obtained with

the Herschel Space Telescope or, more recently, with the Atacama Large Millimeter Array.

J. Mol. Spectrosc., Special Issue on Databases; in press

DOI: [10.1016/j.jms.2016.03.005](https://doi.org/10.1016/j.jms.2016.03.005)

Full-text URL: <http://arxiv.org/abs/1603.03264>

Inclusion of ^{13}C and D in protonated acetylene

R.C. Fortenberry, E. Roueff, T.J Lee

The rovibrational spectrum of cyclic, protonated acetylene has been established. The improvement in modern telescopes coupled with the different branching ratios in reaction models welcomes study of ^{13}C -substitution for C_2H_3^+ . Quartic force fields (QFFs) have been previously utilized to predict the anti-symmetric HCCH stretch in standard $c\text{-C}_2\text{H}_3^+$ to within 0.1cm^{-1} of experiment and are employed heretogenerate rovibrational insights for the ^{13}C isotopologues. The zero-point energie are also given for the cyclic and 'Y'-shaped isomers for both ^{13}C and D substitutions. Vibrational intensities and the dipole moments are provided in order to characterize more fully this simple cation.

Chemical Physics Letters, 650, 126, 2016

DOI: [10.1016/j.cplett.2016.02.068](https://doi.org/10.1016/j.cplett.2016.02.068)

Full-text URL: <http://authors.elsevier.com/a/1Sic626nNRS7Y>

Reactivity of OH and CH_3OH between 22 and 64 K: Modelling the gas phase production of CH_3O in Barnard 1b

M. Antinolo, M. Agundez, E. Jimenez, B. Ballesteros, A. Canosa, G. El Dib, J. Albaladejo, and J. Cernicharo

In the last years, ultra-low temperature chemical kinetic experiments have demonstrated that some gas-phase reactions are much faster than previously thought. One example is the reaction between OH and CH_3OH , which has been recently found to be accelerated at low temperatures yielding CH_3O as main product. This finding opened the question of whether the CH_3O observed in the dense core Barnard 1b could be formed by the gas-phase reaction of CH_3OH and OH. Several chemical models including this reaction and grain-surface processes have been developed to explain the observed abundance of CH_3O with little success. Here we report for the first time rate coefficients for the gas-phase reaction of OH and CH_3OH down to a temperature of 22 K, very close to those in cold interstellar clouds. Two independent experimental set-ups based on the supersonic gas expansion technique coupled to the pulsed laser photolysis-laser induced fluorescence technique were used to determine rate coefficients in the temperature range 22-64 K. The temperature dependence obtained in this work can be expressed as $k(22\text{-}64\text{ K}) = (3.6\pm 0.1)e^{-12} (T/300)^{-1.0\pm 0.2} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. Implementing this expression in a chemical model of a cold dense cloud results in $\text{CH}_3\text{O}/\text{CH}_3\text{OH}$ abundance ratios similar or slightly lower than the value of $3e^{-3}$ observed in Barnard 1b. This finding confirms that the gas-phase reaction between OH and CH_3OH is an important contributor to the formation of interstellar CH_3O . The role of grain-surface processes in the formation of CH_3O , although it cannot be fully neglected, remains controversial.

Accepted for publication in The Astrophysical Journal

Full-text URL: <http://arxiv.org/abs/1603.04244>

The interstellar chemistry of $\text{H}_2\text{C}_3\text{O}$ isomers

J.-C. Loison, M. Agúndez, N. Marcelino, V. Wakelam, K. M. Hickson, J. Cernicharo, M. Gerin, E. Roueff, M. Guélin

We present the detection of two $\text{H}_2\text{C}_3\text{O}$ isomers, propynal and cyclopropenone, toward various starless cores and molecular clouds, together with upper limits for the third isomer propadienone. We review the processes controlling the abundances of $\text{H}_2\text{C}_3\text{O}$ isomers in interstellar media showing that the reactions involved are gas-phase ones. We show that the abundances of these species are controlled by kinetic rather than thermodynamic effects.

MNRAS 456, 4101–4110 (2016)

DOI: [10.1093/mnras/stv2866](https://doi.org/10.1093/mnras/stv2866)

Full-text URL: <http://arxiv.org/abs/1512.01582>

The virtual atomic and molecular data centre (VAMDC) consortium

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The Virtual Atomic and Molecular Data Centre (VAMDC) Consortium is a worldwide consortium which federates atomic and molecular databases through an e-science infrastructure and an organisation to support this activity. About 90% of the interconnected databases handle data that are used for the interpretation of astronomical spectra and for modelling in many fields of astrophysics. Recently the VAMDC Consortium has connected databases from the radiation damage and the

plasma communities, as well as promoting the publication of data from Indian institutes. This paper describes how the VAMDC Consortium is organised for the optimal distribution of atomic and molecular data for scientific research. It is noted that the VAMDC Consortium strongly advocates that authors of research papers using data cite the original experimental and theoretical papers as well as the relevant databases.

Journal of Physics B: Atomic, Molecular and Optical Physics, Volume 49, Number 7
DOI: [10.1088/0953-4075/49/7/074003](https://doi.org/10.1088/0953-4075/49/7/074003)
Full-text URL: <http://iopscience.iop.org/article/10.1088/0953-4075/49/7/074003/pdf>

Announcements

Linking Exoplanet and Disk Compositions - workshop at the Space Telescope Science Institute

This workshop will gather scientists working on the compositional characterization of planets and planet-forming regions in protoplanetary disks. Recent and upcoming advancements make it timely to have a round-table conversation among the several communities involved, to join forces in tackling our most compelling questions on the origins of exoplanet diversity. Do exoplanet compositions retain the imprint of large-scale disk processes? Do disks include compositional trends that imprint on planets? What do we learn in this context from observations of Solar System bodies? And what can we test with observations of disks and exoplanets in the near future? We intend to identify long-lasting and observable links between exoplanet and disk compositions, to help the community in shaping ongoing modeling efforts as well as the essential parameter space to cover with existing and upcoming observatories for exoplanet and disk characterization. Abstract submission will begin on March 26, 2016 through the link provided below. SOC: Daniel Apai (Univ. of Arizona), Andrea Banzatti (STScI, chair), Fred Ciesla (Univ. of Chicago), Jonathan Fortney (UCSC), Sarah Horst (JHU), Inga Kamp (Kapteyn Inst., Groningen), Nikole Lewis (STScI, co-chair), Amaya Moro-Martín (STScI), Karin Oberg (Harvard CfA), Klaus Pontoppidan (STScI), Olivia Venot (Katholieke Univ. Leuven), Marie Ygouf (STScI). Confirmed Invited Speakers: Conel Alexander (Carnegie DTM), Uma Gorti (SETI, NASA Ames), Jonathan Lunine (Cornell Univ.), Christoph Mordasini (Univ. of Bern), Ilaria Pascucci (Univ. of Arizona), Sean Raymond (Univ. of Bordeaux), Leslie Rogers (Univ. of Chicago). Website: <http://www.cvent.com/d/ffqwn1>

Brave New Worlds: Understanding the Planets of Other Stars

May 29-June 03, 2016 – Lake Como School of Advanced Studies. Only nine planets were known before 1995, the ones orbiting our favourite star, the Sun, which then included Pluto. Twenty years later, we have «lost» Pluto but we have gained two thousands planets in orbit around other stars. Current statistical estimates indicate that, on average, every star in our Galaxy hosts at least one planetary companion, i.e. our Milky Way is crowded with one hundred billion planets! The most revolutionary aspect of this young field is the discovery that the Solar System does not appear to be the paradigm in our Galaxy, but rather one of the many possible configurations we are seeing out there. These include planets completing a revolution in less than one day, as well as planets orbiting two stars or moving on trajectories so eccentric as to resemble comets. Some of them are freezing cold, some are so hot that their surface is molten. Finding out why are these new worlds as they are is one of the key challenges of modern astrophysics. The school is directed to Ph.D. students and young researchers who are interested in widening their knowledge in the field exoplanets, through an integrated approach covering observations, data analysis and interpretation. More information is available at: <http://gatr.lakecomoschool.org>

Interstellar shocks: models, observations & experiments

To be held in Toruń, Poland, from the 14th - 16th September 2016. The website of the workshop: <http://shocks2016.faj.org.pl/> Meeting overview and goals ----- Shocks are ubiquitous in the interstellar medium, including protostars, evolved stars, supernovae blast waves as well as spiral arms. On small scales, shocks have a strong impact on the local physical conditions, the gas chemistry and they deeply affect dust grains, through sputtering of their ice mantle or their refractory cores, or even through shattering in the fastest shocks. On larger scales, shocks produced by spiral arms can induce colliding flows, triggering the formation of molecular clouds. The cumulative impact of shocks influence the evolution of molecular clouds by injecting supersonic turbulence, and in turn their star formation efficiency, hence play a major role in regulating the star formation rate of galaxies. Shocks are therefore relevant for many astrophysical and chemical processes and their detailed understanding, which needs a combination of observations, models and laboratory experiments, has a wide range of applications. This meeting will cover all aspects of shocks in the interstellar medium: from microphysics to impact on galaxy scales. The program of the workshop reflects this broad range of topics related to interstellar shocks: - Observations of shocks and related chemistry in protostars, supernovae remnants and evolved stars from UV to sub-mm - Models of shocks, with a special focus on the impact of UV irradiation, the shock geometry, and the role of grains - Laboratory studies of shocks, jets and sputtering phenomenon - Shocks in stellar cluster and at molecular cloud scales The objective of the meeting is to bring together astronomers with diverse observational, experimental, and theoretical backgrounds, to foster new collaborations, and to identify the major open questions relating to interstellar shocks. Invited speakers: - Sybille Anderl (IPAG Grenoble, FR) - Hector Arce (Yale University, USA) - Sylvie Cabrit (Observatoire de Paris, FR) - Andrea Ciardi (Observatoire de Paris, FR) - Antoine Gusdorf (Observatoire de Paris, FR) - Michael Kaufman (San Jose State University, USA) - Ralf Klessen (Heidelberg University, DE) - Lars Kristensen (Center for Astrophysics, Harvard, USA) - David Neufeld (Johns Hopkins University, USA) - John Raymond (Smithsonian Astrophysical Observatory, USA) - Steven Sibener (University of Chicago, USA) - Mario Tafalla (Observatorio Astronómico Nacional, ES) SOC: Sylvie Cabrit Paola Caselli Andrea Ciardi Ewine van Dishoeck Helen Fraser Maryvonne Gerin Vincent Guillet Antoine Gusdorf Michal Hanasz Agata Karska Michael Kaufman Lars Kristensen Alexandre Marcowith David Neufeld Linda Podio

Origins of Habitable Planets - A cross-disciplinary programme on planet formation

From May 2 to June 10, 2016, researchers in the fields of physics, chemistry, astronomy, geology and engineering gather in Gothenburg with one common goal: To advance our understanding of how planets which can harbour life are formed. This unique research programme is led by Dr. Leonardo Testi of the European Southern Observatory. The programme includes scientific workshops focusing on different aspects related to future observational instrumentation and synergies between astrophysical observations, models and lab work, seminars, group discussions, and public lectures. For more information visit <http://www.chalmers.se/en/centres/GoCAS>