AstroChemical Newsletter #9

July 2016

You can access the full abstracts by clicking the paper titles. Submit your abstracts before the 25th of each month for inclusion in the following newsletter.

Abstracts

Determining protoplanetary disk gas masses from CO isotopologues line observations

A. Miotello, E. F. van Dishoeck, M. Kama, S. Bruderer

Despite intensive studies of protoplanetary disks, there is still no reliable way to determine their total mass and their surface density distribution, quantities that are crucial for describing both the structure and the evolution of disks up to the formation of planets. The goal of this work is to use less abundant CO isotopologues, whose detection is routine for ALMA, to infer the gas mass of disks. Isotope-selective effects need to be taken into account in the analysis, because they can significantly modify CO isotopologues line intensities. CO isotope-selective photodissociation has been implemented in the physical-chemical code DALI and 800 disk models have been run for a range of disk and stellar parameters. Dust and gas temperature structures have been computed self-consistently, together with a chemical calculation of the main species. Both disk structure and stellar parameters have been investigated. Total fluxes have been ray-traced for different CO isotopologues and for various transitions for different inclinations. A combination of 13CO and C18O total intensities allows inference of the total disk mass, although with non-negligible uncertainties. These can be overcome by employing spatially resolved observations, i.e. the disk's radial extent and inclination. Comparison with parametric models shows differences at the factor of a few level, especially for extremely low and high disk masses. Finally, total line intensities for different CO isotopologue and for various low-J transitions are provided and are fitted to simple formulae. The effects of a lower gas-phase carbon abundance and different gas/dust ratios are investigated as well, and comparison with other tracers is made. Disk masses can be determined within a factor of a few by comparing CO isotopologue lines observations with the simulated line fluxes, modulo the uncertainties in the volatile elemental abundances.

Accepted in Astronomy & Astrophysics
Full-text URL: http://arxiv.org/abs/1605.07780

Discovery of the interstellar chiral molecule propylene oxide (CH3CHCH2O)

Brett A. McGuire & P. Brandon Carroll, Ryan A. Loomis, Ian A. Finneran, Philip R. Jewel, Anthony J. Remijan, and Geoffrey A. Blake

Life on Earth relies on chiral molecules—that is, species not superimposable on their mirror images. This manifests itself in the selection of a single molecular handedness, or homochirality, across the biosphere. We present the astronomical detection of a chiral molecule, propylene

oxide (CH3CHCH2O), in absorption toward the Galactic center. Propylene oxide is detected in the gas phase in a cold, extended molecular shell around the embedded, massive protostellar clusters in the Sagittarius B2 star-forming region. This material is representative of the earliest stage of solar system evolution in which a chiral molecule has been found.

Science (2016)
DOI: 10.1126/science.aae0328
Full-text URL: http://science.sciencemag.org/content/early/2016/06/15/science.aae0328

Ion processing of ices and the origin of SO2 and O3 on the icy surfaces of the icy jovian satellites

P. Boduch , R. Brunetto, J.J. Ding, A. Domaracka, Z. Kánuchová, M.E. Palumbo, H. Rothard, G. Strazzulla

We present new experimental results relative to 144 keV S9+ or Ar9+ ion implantation in targets made of oxygen rich frozen gases (O2 , CO2) and mixtures with water ice. Spectra in the UV (200–400 nm) range have been obtained before and after implantation. The targets have been selected because they can be representative of the parent molecules from which SO2 and O3, observed to be present on the surfaces of Jupiter's icy Moons, could be formed due to radiolysis induced by the abundant magnetospheric ions. The results indicate that sulfur dioxide is not detectable after sulfur implantation in oxygen bearing species. Ozone is formed after argon and sulfur ion implantation. Sulfur implantation in O2 and CO2 targets also induces the formation of a band centered at about 255 nm (that we tentatively attribute to SO3– radicals). In the mixtures with water the band appears initially at the same wavelength and shifts to about 247 nm at higher ion fluences possibly indicating the formation of sulfite (HSO3–) ions. An absorption band observed on Ganymede is well fitted by using three components: ozone, sulfite ions and a not identified component having an absorption band centered at 298 nm. In all of the studied cases ion implantation produces a spectral reddening over the investigated spectral range (200–400 nm) that well mimics the observed spectral slopes of Jupiter's icy satellites.

Icarus 277 (2016) 424–432
DOI: doi:10.1016/j.icarus.2016.05.026
Full-text URL: http://www.sciencedirect.com/science/article/pii/S0019103516302214

Temperature spectra of interstellar dust grains heated by cosmic-rays I: translucent clouds

Juris Kalvāns

Heating of whole interstellar dust grains by cosmic-ray (CR) particles affects the gas-grain chemistry in molecular clouds by promoting molecule desorption, diffusion, and chemical reactions on grain surfaces. The frequency of such heating f(T), s^-1, determines how often a certain temperature T(CR), K, is reached for grains hit by CR particles. This study aims to provide astrochemists with comprehensive and updated dataset on the CR-induced whole-grain heating. We present calculations of f(T) and T(CR) spectra for bare olivine grains with radius a of 0.05; 0.1; 0.2 um, and such grains covered with ice mantles of thickness 0.1a and 0.3a. Grain shape and structure effects are considered, as well as 30 CR elemental constituents with an updated energy spectrum corresponding to a translucent cloud with A(V)=2 mag. Energy deposition by CRs in grain material was calculated with the SRIM program. We report full T(CR) spectra for all nine grain types and consider initial grain temperatures of 10 K and 20 K. We also provide frequencies for a range of minimum T(CR) values. The calculated dataset can be simply and

flexibly implemented in astrochemical models. The results show that, in the case of translucent clouds, the currently adopted rate for heating of whole grains to temperatures in excess of 70 K is underestimated by approximately two orders of magnitude in astrochemical numerical simulations. Additionally, grains are heated by CRs to modest temperatures (20--30 K) with intervals of a few years, which reduces the possibility of ice chemical explosions.

2016 ApJS 224 42
DOI: 10.3847/0067-0049/224/2/42
Full-text URL: http://arxiv.org/abs/1605.09120

Understanding the C3H2 cyclic-to-linear ratio in L1544

O. Sipilä, S. Spezzano, and P. Caselli

Aims. We aim to understand the high cyclic-to-linear C3H2 ratio (32 ± 4) that has been observed toward L1544. Methods. We combined a gas-grain chemical model with a physical model for L1544 to simulate the column densities of cyclic and linear C3H2 observed toward L1544. The most important reactions for the formation and destruction of both forms of C3H2 were identified, and their relative rate coefficients were varied to find the best match to the observations. Results. We find that the ratio of the rate coefficients of C3H3+ + e- --> C3H2 + H for cyclic and linear C3H2 must be ∼20 to reproduce the observations, depending on the branching ratios assumed for the C3H3+ + e- --> C3H + H2 reaction. In current astrochemical networks it is assumed that cyclic and linear C3H2 are formed in a 1:1 ratio in the aforementioned reactions. Laboratory studies and/or theoretical calculations are needed to confirm the results of our chemical modeling, which is based on observational constraints.

2016, A&A 591, L1
DOI: 10.1051/0004-6361/201628689
Full-text URL: https://arxiv.org/pdf/1605.07379.pdf

First Detection of Gas-phase Methanol in a Protoplanetary Disk

Catherine Walsh, Ryan A. Loomis, Karin I. Öberg, Mihkel Kama, Merel van't Hoff, Tom J Millar, Yuri Aikawa, Eric Herbst, Susanna Widicus Weaver, Hideko Nomura

The first detection of gas-phase methanol in a protoplanetary disk (TW Hya) is presented. In addition to being one of the largest molecules detected in disks to date, methanol is also the first disk organic molecule with an unambiguous ice chemistry origin. The stacked methanol emission, as observed with the Atacama Large Millimeter/submillimeter Array, is spectrally resolved and detected across six velocity channels (> 3σ), reaching a peak signal-to-noise of 5.5σ , with the kinematic pattern expected for TW Hya. Using an appropriate disk model, a fractional abundance of 3e-12–4e-11 (with respect to H2) reproduces the stacked line profile and channel maps, with the favored abundance dependent upon the assumed vertical location (midplane versus molecular layer). The peak emission is offset from the source position, suggesting that the methanol emission has a ring-like morphology: the analysis here suggests it peaks at ≈ 30 {{au}}, reaching a column density ≈ 3e12–6e12 cm-2. In the case of TW Hya, the larger (up to millimeter-sized) grains, residing in the inner 50 au, may thus host the bulk of the disk ice reservoir. The successful detection of cold gas-phase methanol in a protoplanetary disk implies that the products of ice chemistry can be explored in disks, opening a window into studying complex organic chemistry during planetary system formation.

2016, ApJL, 823, L10

DOI: 10.3847/2041-8205/823/1/L10
Full-text URL: http://cdsads.u-strasbg.fr/abs/2016ApJ...823L..10W

Hot and dense water in the inner 25 AU of SVS13-A

C. Codella, C. Ceccarelli, E. Bianchi, R. Bachiller, B. Lefloch, F. Fontani, V. Taquet, L. Testi

In the context of the ASAI (Astrochemical Surveys At IRAM) project, we carried out an unbiased spectral survey in the millimeter window towards the well known low-mass Class I source SVS13-A. The high sensitivity reached (3-12 mK) allowed us to detect at least 6 HDO broad (FWHM ~ 4-5 km/s) emission lines with upper level energies up to Eu = 837 K. A non-LTE LVG analysis implies the presence of very hot (150-260 K) and dense (> 3e7 cm-3) gas inside a small radius (25 AU) around the star, supporting, for the first time, the occurrence of a hot corino around a Class I protostar. The temperature is higher than expected for water molecules are sublimated from the icy dust mantles (~ 100 K). Although we cannot exclude we are observing the effects of shocks and/or winds at such small scales, this could imply that the observed HDO emission is tracing the water abundance jump expected at temperatures ~ 220-250 K, when the activation barrier of the gas phase reactions leading to the formation of water can be overcome. We derive X(HDO) ~ 3e-6, and a H2O deuteration > 1.5e-2, suggesting that water deuteration does not decrease as the protostar evolves from the Class 0 to the Class I stage.

MNRAS Letters, in press
DOI: 10.1093/mnrasl/slw127
Full-text URL: http://arxiv.org/abs/1606.06847

Announcements

International conference on the Hydride Toolbox, 12-15 Dec. 2016 - Paris

Dear colleagues, We are pleased to announce that the Hydride Toolbox, an international conference on the interest of hydrides for interstellar astrophysics, will be held on 12-15 December 2016, at the University Pierre et Marie-Curie, in Paris, France. For more information, please visit the conference website: http://hydride-toolbox.sciencesconf.org The goal of the event is to bring together experts in molecular physics (gas phase & solid phase ; theory & experiments), theoretical and numerical modelling, and astronomical observations, in order to review our current knowledge of interstellar hydrides, benchmark their diagnostic capabilities, and expand the validation domain from the local universe to distant systems. The sessions will be organized with introductory review talks, and ample time for contributed talks and poster presentations. Main topics Molecular physics and chemistry of hydrides Diffuse ISM, turbulence, and shocks Cosmic rays and magnetic field Extragalactic and AGN activity Solid phase processes and chemistry Stars and planet formation, exoplanets ISM life cycle Future projects Important dates Registration and Abstract submission are now open, please see the conference website: http://hydride-toolbox.sciencesconf.org Registration June 1st - October 10th Abstract submission June 1st - September 15th Payment June 15th - October 10th Subvention requests June 1st - September 15th The LOC has secured a small budget for travel grants to subsidize student participation in the conference. To apply for these grants, please send us a CV and a funding justification letter before September the 15th 2016. Scientific Organizing Committee Y. Aikawa E. Bergin J. Black P. Caselli M. Gerin (chair) J. Goicoechea (chair) E. Gonzalez-Alfonso D. Li X. Michaut D. Neufeld (chair) K. Öberg E. van Dishoeck Invited speakers S. Aalto M. Agundez J. Black P. Caselli I. Cleeves E. Dartois A. Faure S. Federman D. Galli B. Godard E. Gonzalez-Alfonso T. Hama N. Indriolo M. Kaufman H. Kreckel K. Menten K. Öberg A. Omont V.

Ossenkopf K. Pontoppidan E. Roueff J. Tennyson G. Tinetti W. Ubachs E. van Dishoeck We are looking forward to seeing you in Paris! The local organizing committee

PhD position in Experimental Astrochemistry - Doctoral programme in Physics, University of Trento ITALY

The PhD Programme in Physics of the University of Trento (Italy) has opened the new call for applications (XXXII cycle), with deadline 31 August 2016. 16 positions are available starting from 1 November 2016. The call is open to those who are interested to work in a dynamic environment which covers state-of-the-art topics in physics. Research topics are described in the web page of the Department of Physics. The activity in Experimental Astrochemistry is within the group of Prof. Daniela Ascenzi and Prof. Paolo Tosi and further information can be obtained by mail at daniela.ascenzi@unitn.it The salary of the PhD student, being fixed in Italy by national rules, is complemented locally by supports and benefits. Moreover, Trento is a small town with a very high quality of life. If you want more info, please visit http://www.unitn.it/en/servizi/1647/accommodation. For more information about the PhD program please contact the secretariat at phd.physics@unitn.it Daniela Ascenzi

iCOMET 2017 in Innsbruck

Dear colleagues, we are pleased to announce the next International Conference on Molecular Energy Transfer in Complex Systems iCOMET 2017. It will take place in Innsbruck, Austria from January 15 to 20, 2017, after being hosted in Chengdu (2015, China), Ventura (2013, USA), and Oxford (2011, UK). This conference brings together researchers who strive towards understanding complex dynamical problems such as reaction dynamics, molecular interactions at surfaces and in the condensed phase, biological molecules and technology applications. In this way the conference aims to support obtaining an atomic scale understanding of dynamical events controlling complex physico-chemical phenomena. The field is characterized by advanced experimental tools and has demonstrated a close connection with highly sophisticated theoretical analysis. Specific topics of iCOMET include: Chemical Reaction Dynamics Advances in Theoretical Chemistry Photo-fragmentation Dynamics Dynamics at Surfaces Cold Collisions and Clusters Non-covalent bonding including in biological systems Ultrafast Dynamics Electronically Nonadiabatic Phenomena Energy Conversion Processes Elementary process in heterogeneous catalysis Registration is now open. The deadline for early-bird registration and abstract submission is September 1st, 2016. Please mark your calendars. Approximately 10-15 abstract submissions will be selected for hot topic talks. We welcome in particular the participation of young researchers and students. For up-to-date information please visit: http://www.icasec.uni-goettingen.de/icomet-2017/ We looking forward to seeing you next year in Tyrol! With best regards Roland Wester and Alec Wodtke University of Innsbruck and Max Planck Institut for Biophysical Chemistry Göttingen iCOMET 2017 Organizing Committee