AstroChemical Newsletter #33

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Abstracts

Hydrogen transfer reactions of interstellar Complex Organic Molecules

S. Álvarez-Barcia, P. Russ, J. Kästner, T. Lamberts

Radical recombination has been proposed to lead to the formation of complex organic molecules (COMs) in CO-rich ices in the early stages of star formation. These COMs can then undergo hydrogen addition and abstraction reactions leading to a higher or lower degree of saturation. Here, we have studied 14 hydrogen transfer reactions for the molecules glyoxal, glycoaldehyde, ethylene glycol, and methylformate and an additional three reactions where CH_nO fragments are involved. Over-the-barrier reactions are possible only if tunneling is invoked in the description at low temperature. Therefore the rate constants for the studied reactions are calculated using instanton theory that takes quantum effects into account inherently. The reactions were characterized in the gas phase, but this is expected to yield meaningful results for CO-rich ices due to the minimal alteration of reaction landscapes by the CO molecules. We found that rate constants should not be extrapolated based on the height of the barrier alone, since the shape of the barrier plays an increasingly larger role at decreasing temperature. It is neither possible to predict rate constants based only on considering the type of reaction, the specific reactants and functional groups play a crucial role. Within a single molecule, though, hydrogen abstraction from an aldehyde group seems to be always faster than hydrogen addition to the same carbon atom. Reactions that involve heavy-atom tunneling, e.g., breaking or forming a C–C or C–O bond, have rate constants that are much lower than those where H transfer is involved.

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Kinematics of dense gas in the L1495 filament

A. Punanova, P. Caselli, J. E. Pineda, A. Pon, M. Tafalla, A. Hacar, L. Bizzocchi

We study the kinematics of the dense gas of starless and protostellar cores traced by the N2D+(2-1), N2H+(1-0), DCO+(2-1), and H13CO+(1-0) transitions along the L1495 filament and the kinematic links between the cores and the surrounding molecular cloud. We measure velocity dispersions, local and total velocity gradients and estimate the specific angular momenta of 13 dense cores in the four transitions using the on-the-fly observations with the IRAM 30 m antenna. To study a possible connection to the filament gas, we use the fit results of the C18O(1-0) survey performed by Hacar et al. (2013). All cores show similar properties along the 10 pc-long filament. N2D+(2-1) shows the most centrally concentrated structure, followed by N2H+(1-0) and DCO+(2-

1), which show similar spatial extent, and H13CO+(1-0). The non-thermal contribution to the velocity dispersion increases from higher to lower density tracers. The change of magnitude and direction of the total velocity gradients depending on the tracer used indicates that internal motions change at different depths within the cloud. N2D+ and N2H+ show smaller gradients than the lower density tracers DCO+ and H13CO+, implying a loss of specific angular momentum at small scales. At the level of cloud-core transition, the core's external envelope traced by DCO+ and H13CO+ is spinning up, consistent with conservation of angular momentum during core contraction. C18O traces the more extended cloud material whose kinematics is not affected by the presence of dense cores. The decrease in specific angular momentum towards the centres of the cores shows the importance of local magnetic fields to the small scale dynamics of the cores. The random distributions of angles between the total velocity gradient and large scale magnetic field suggests that the magnetic fields may become important only in the high density gas within dense cores.

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Dissociative recombination of the CH+ molecular ion at low energy

K Chakrabarti, J Zs Mezei, O Motapon, A Faure, O Dulieu, K Hassouni, I F Schneider

The reactive collision of the CH+ molecular ion with an electron is studied in the framework of the multichannel quantum defect theory, taking into account the contribution of the core-excited Rydberg states. In addition to the X1Σ+ ground state of the ion, we also consider the contribution to the dynamics of the a3Π and A1Π excited states of CH+. Our results—in the case of the dissociative recombination in good agreement with the storage ring measurements—rely on decisive improvements—complete account of the ionisation channels and accurate evaluation of the reaction matrix—of a previously used model.

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Solid deuterated water in space: detection constraints from laboratory experiments

R. G. Urso, M. E. Palumbo, G. A. Baratta, C. Scirè, G. Strazzulla

The comparison between astronomical spectra and laboratory experiments is fundamental to spread light on the structure and composition of ices found in interstellar dense molecular clouds and in Solar System bodies. Water is among the most abundant solid-phase species observed in these environments, and several attempts have been made to investigate the presence of its solid-phase isotopologues. In particular, the detection of the O-D stretching mode band at 4.1 μm due to both D2O and HDO within icy grain mantles is still under debate, and no detection have been reported about the presence of these species within icy bodies in the Solar System yet. In the near future, an important contribution could derive from the data acquired in the O-D stretching mode spectral range by the sensitive instruments on board the James Webb Space Telescope. With this in mind, we performed several laboratory experiments to study the O-D stretching mode band in solid mixtures containing water

and deuterated water deposited in the temperature range between 17 and 155 K, in order to simulate astrophysical relevant conditions. Furthermore, samples have been studied at various temperature and irradiated with energetic ions (200 keV H+) in order to study the effects induced by both thermal and energetic processing. Our results provide some constraints on the detection of the 4.1 μm band in astronomical environments.

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Sulphur chemistry in the L1544 pre-stellar core

Charlotte Vastel, D. Quénard, R. Le Gal, V. Wakelam, A. Andrianasolo, P. Caselli, T. Vidal, C. Ceccarelli, B. Lefloch, and R. Bachiller

The L1544 pre-stellar core has been observed as part of the ASAI IRAM 30m Large Program as well as follow-up programs. These observations have revealed the chemical richness of the earliest phases of low-mass star-forming regions. In this paper we focus on the twenty-one sulphur bearing species (ions, isotopomers and deuteration) that have been detected in this spectral-survey through fifty one transitions: CS, CCS, C3S, SO, SO2, H2CS, OCS, HSCN, NS, HCS+, NS+ and H2S. We also report the tentative detection (4 σ level) for methyl mercaptan (CH3SH). LTE and non-LTE radiative transfer modelling have been performed and we used the nautilus chemical code updated with the most recent chemical network for sulphur to explain our observations. From the chemical modelling we expect a strong radial variation for the abundances of these species, which mostly are emitted in the external layer where non thermal desorption of other species has previously been observed. We show that the chemical study cannot be compared to what has been done for the TMC-1 dark cloud, where the abundance is supposed constant along the line of sight, and conclude that a strong sulphur depletion is necessary to fully reproduce our observations of the prototypical pre-stellar core L1544.

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Chemistry in disks XI. Sulfur-bearing species as tracers of protoplanetary disk physics and chemistry: the DM Tau case

D. Semenov, C. Favre, D. Fedele, S. Guilloteau, R. Teague, Th. Henning, A. Dutrey, E. Chapillon, F. Hersant, and V. Piétu

Context. Several sulfur-bearing molecules are observed in the interstellar medium and in comets, in strong contrast to protoplanetary disks where only CS, H2CS and SO have been detected so far. Aims. We combine observations and chemical models to constrain the sulfur abundances and their sensitivity to physical and chemical conditions in the DM Tau protoplanetary disk. Methods. We obtained 0.5′′ ALMA observations of DM Tau in Bands 4 and 6 in lines of CS, SO, SO2, OCS, CCS, H2CS and H2S, achieving a ~ 5 mJy sensitivity. Using the non-LTE radiative transfer code RADEX and the forward-modeling tool DiskFit, disk-averaged CS column densities and upper limits for the other species were derived. Results. Only CS was detected with a derived column density of ~ 2 − 6 × 10^12 cm−2. We report a first tentative detection of SO2 in DM Tau. The upper limits range between ~ 10^11 and 10^14 cm−2 for the other S-

bearing species. The best-fit chemical model matching these values requires a gas-phase C/O ratio of >1 at r~50−100 au. With chemical modeling we demonstrate that sulfur-bearing species could be robust tracers of the gas-phase C/O ratio, surface reaction rates, grain size and UV intensities. Conclusions. The lack of detections of a variety of sulfur-bearing molecules in DM Tau other than CS implies a dearth of reactive sulfur in the gas phase, either through efficient freeze-out or because most of the elemental sulfur is in other large species, as found in comets. The inferred high CS/SO and CS/SO2 ratios require a non-solar C/O gas-phase ratio of > 1, consistent with the recent observations of hydrocarbon rings in DM Tau. The stronger depletion of oxygen-bearing S-species compared to CS is likely linked to the low observed abundances of gaseous water in DM Tau and points to a removal mechanism of oxygen from the gas.

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Water and interstellar complex organics associated with the HH 212 protostellar disc - On disc atmospheres, disc winds, and accretion shocks

C. Codella, E. Bianchi, B. Tabone, C.-F. Lee, S. Cabrit, C. Ceccarelli, L. Podio, F. Bacciotti, R. Bachiller, E. Chapillon, F. Gueth, A. Gusdorf, B. Lefloch, S. Leurini, G. Pineau des Forets, K.L.J. Rygl, M. Tafalla

Context: The unprecedented combination of high-sensitivity and high-angular resolution provided by the ALMA interferometer allows us to shed light on the processes leading to the formation of the jet-disc system associated with a Sun-like mass protostar. Aims: We investigate the physical and chemical properties of the gas associated with water and interstellar complex organic molecules around a protostar on solar system scales. Methods: The HH 212 protostellar system, in Orion B, has been mapped thanks to ALMA-Band 7 Cycle 1 and Cycle 4 observations of dueterated water (HDO) and acetaldehyde (CH3CHO) emission with an angular resolution down to 0.15" (60 au). Results: Many emission lines due to 14 CH3CHO and 1 HDO transitions at high excitation (Eu between 163 K and 335 K) have been imaged in the inner 70 au region. The local thermal equilibrium analysis of the CH3CHO emission leads to a temperature of 78(14) K and a column density of 7.6(3.2) 10^15 cm^-2, which, when N(H2) of 10^24 cm^-2 is assumed, leads to an abundance of X(CH3CHO) = 8 10^-9. The large velocity gradient analysis of the HDO emission also places severe constraints on the volume density, n(H2) > 10^8 cm^-3. The line profiles are 5--7 km/s wide, and CH3CHO and HDO both show a +- 2 km s/s velocity gradient over a size of 70 au (blue-shifted emission towards the north-west and red-shifted emission towards the south-east) along the disc equatorial plane, in agreement with what was found so far using other molecular tracers. Conclusions: The kinematics of CH3CHO and HDO are consistent with the occurrence of a centrifugal barrier, that is, the infalling envelope-rotating disc ring, which is chemically enriched through low-velocity accretion shocks. The emission radius is 60 au, in good agreement with what was found before for another interstellar complex organic molecule such as NH2CHO. We support a vertical structure for the centrifugal barrier, suggesting the occurrence of two outflowing, expanding, and rotating rings above and below (of about 40-45 au) the optically thick equatorial disc plane. It is tempting to speculate that these rings could probe the basis of a wind launched from this region.

A&A, in press
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Radiative Charge Transfer between the Helium Ion and Argon

James F Babb and Brendan M McLaughlin

The rate coefficient for radiative charge transfer between the helium ion and an argon atom is calculated. The rate coefficient is about 10^-14 cm^3 s-1 at 300 K in agreement with earlier experimental data.

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Announcements

From First Stars to Life: Science with the OST

https://www.ost-meeting.com 4 -7 September, 2018 Univ. of Oxford Second Announcement Scientific Rationale: The infrared is the key wavelength regime for understanding the formation and early evolution of galaxies, stars and planetary systems. These wavelengths probe the obscured Universe from Cosmic Dawn to proto-planetary disks tracing both the dust and the dominant atomic, ionic and molecular cooling lines. When studied together, dust continuum and lines allow us to trace the chemical enrichment of the gas in the Universe and the physical processes which determine the evolution from the primordial gas to habitable exoplanets. In particular, the infrared is host to a series of molecular bio-markers that can be used to characterize the atmospheres of exoplanets. Only in the IR can we follow the water trail in the Universe, from distant galaxies down to the solar system. Building on the success of the previous far-IR missions (IRAS, ISO, Spitzer, Herschel and Planck) and their importance for the European astronomical community, the goal of this workshop is to bring together the community in order to home in on the most pressing questions a next-generation far-IR facility (such as the Origins Space Telescope) would be able to tackle. The Workshop will focus on the following themes: • The rise of metals and dust • Cosmic Dawn and the adolescent Universe • The Starburst-AGN connection: finding the hidden supermassive black holes • Stars and ISM: the baryonic cycle • Astrochemistry • The Solar System & protoplanetary disks • Characterization of Exoplanets The Origins Space Telescope (OST) is one of four NASA 2020 Decadal survey missions currently under study. OST will carry a suite of instruments covering the 6 to 600 microns and with its cooled telescope (down to 4K) will deliver superb imaging and spectroscopic capabilities including far infrared polarimetry. The aim of the Workshop is to bring together -primarily but not exclusively- European scientists interested in the OST to discuss potential science projects. The format: The Workshop will consist of invited talks from the OST team introducing the capabilities of the instruments and the main OST science areas, as well as, contributed talks from the community. We ask interested participants to consult the OST webpages (accessible through the Workshop page) and come prepared to discuss their science projects, posters are also welcome. The audience is limited to 100 people. Invited Speakers: Almudena Alonso Herrero, Cara Battersby, Matt Bradford, Asantha Cooray, Elvire de Beck, Leslie Hunt, David Leisawitz, Stephanie Milam, Klaus Pontoppidan, Itsuki Sakon, Kevin Stevenson, Joaquin Viera, Serena Viti, Martina Wiedner Place of the Workshop: it will be held in the Physics Department, University of Oxford, UK, during September 4-7, 2018. There will be a small registration fee (~80 GBP) to cover coffee breaks and lunches. Registration is now open: https://www.ost-meeting.com/registration Abstract submission: https://www.ost-meeting.com/abstract Abstracts will be accepted until

August 1st 2018 Organizers D. Rigopoulou (Univ. of Oxford, co-Chair), S. Aalto (Chalmers Univ. Of Technology, co-Chair), A. Cooray (UC Irvine), E. De Beck (Chalmers Univ. of Technology), M. Gerin (Paris Observatory), M. Griffin (Univ. of Cardiff), F. Helmich (SRON), M. Meixner (Space Telescope Science Institute), M. Wiedner (Paris Observatory), P. Hartogh (Max-Planck for Solar System Research) Contact: oxford_ost@physics.ox.ac.uk

SOFIA Cycle 7 Call for Proposals Released

The SOFIA project has released two calls for proposals (CfP) for observing time in the Cycle 7 period. The regular call solicits proposals of any size and combination of instruments. A total of 400 hours of observing time and approximately $4 million of funding is available to support these programs. There is a separate call for those affiliated with German institutions administered by the German SOFIA Institute (Deutsches SOFIA Institut; DSI) on behalf of the German Aerospace Center (Deutsches Zentrum für Luft und Raumfahrt; DLR) that will offer an additional approximately 70 hours of observing time. A complementary call for proposals for "SOFIA Legacy Programs" (SLP) has also been released, soliciting large coherent programs aimed at high-impact science that also have a significant promise of valuable archival data sets. Programs up to 100 hours of observing time are solicited in this category. In addition to observing time, these programs are invited to deliver higher level data products (including supporting data, software and theory). Nominally, two SLP programs are expected to be selected per cycle, with observations carried out over two cycles, and a third year included for completion of the higher-level data processing and analysis. Up to $1 million per cycle is available for support of the SLPs. The main parts of the Cycle 7 calendar are: CfP release: June 1, 2018 CfP update: July 16, 2018 Proposal Deadline: September 7, 2018 (9 p.m. PDT) Selections announced: November 2018 Cycle 7: April 27, 2019 - April 27, 2020 The Call for Proposals documents can be found at https://www.sofia.usra.edu/sites/default/files/Other/Documents/SOFIA_Cy7_CfP.pdf and https://www.sofia.usra.edu/sites/default/files/Other/Documents/SOFIA_Cy7_SLP_CfP.pdf Any questions about the Cycle 7 Calls for Proposals can be directed to sofia_help@sofia.usra.edu

PhD position in Experimental Molecular Astrophysics - PhD programme in Physics, University of Trento

The Molecular Astrophysics Laboratory at the University of Trento is seeking for expressions of interest to apply for a position within the PhD Programme in Physics. The PhD position is on ion-molecule reactions for the synthesis and destructions of complex organic molecules in the interstellar space and planetary ionosphere. For a detailed description see the attached document or follow the link www.science.unitn.it/labfm/pmwiki/pmwiki.php?n=Events.PhDInMolecularAstrophysics Call for applicants for the 2018 PhD Programme in Physics and details on how to apply are available at www.unitn.it/en/ateneo/1940/announcement-of-selection Deadline for application is 30th August 2018, 4.00pm. The salary of the PhD student, being fixed in Italy by national rules, is complemented locally by supports and benefits (www.unitn.it/en/servizi/1646/opportunities-for-phd-students). Trento is a small alpine town with a very high quality of life. For more info: www.unitn.it/en/servizi/1647/accommodation. For further information on the activities of the Molecular Astrophysics Lab and on the PhD position please contact Daniela Ascenzi (PhD supervisor) daniela.ascenzi@unitn.it Thanks for your help and apologies for cross-posting Daniela Ascenzi APOLOGIES FOR CROSS POSTING