AstroChemical Newsletter #7

May 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

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.

The (impossible?) formation of acetaldehyde on the grain surfaces: insights from quantum chemical calculations

J. Enrique-Romero, A. Rimola, C. Ceccarelli, N. Balucani

Complex Organic Molecules (COMs) have been detected in the interstellar medium (ISM). However, it is not clear whether their synthesis occurs on the icy surfaces of interstellar grains or via a series of gas-phase reactions. As a test case of the COMs synthesis in the ISM, we present new quantum chemical calculations on the formation of acetaldehyde (CH_3CHO) from the coupling of the HCO and CH_3 radicals, both in gas phase and on water ice surfaces. The binding energies of HCO and CH_3 on the amorphous water ice were also computed (2333 and 734 K, respectively). Results indicate that, in gas phase, the products could be either CH_3CHO, CH_4 + CO, or CH_3OCH, depending on the relative orientation of the two radicals. However, on the amorphous water ice, only the CH_4 + CO product is possible due to the geometrical constraints imposed by the water ice surface. Therefore, acetaldehyde cannot be synthesized by the CH_3 + HCO coupling on the icy grains. We discuss the implications of these results and other cases, such as ethylene glycol and dimethyl ether, in which similar situations can occur, suggesting that formation of these molecules on the grain surfaces might be unlikely.

N2H+ and N15NH+ towards the prestellar core 16293E in L1689N

F. Daniel, A. Faure, L. Pagani, F. Lique, M. Gerin, D.C. Lis, P. Hily-Blant, A. Bacmann, E. Roueff

Understanding the processes that could lead to enrichment of molecules in 15N atoms is of particular interest in order to shed light on the relatively large variations observed in the 14N/15N ratio in various solar system environments. Currently, the sample of molecular clouds where 14N/15N ratios have been measured is small and has to be enlarged in order to allow statistically significant studies. In particular, the N2H+ molecule currently shows the largest spread of 14N/15N ratios in high-mass star forming regions. However, the 14N/15N ratio in N2H was obtained in only two low-mass star forming regions (L1544 and B1b). The current work extends this sample to a third dark cloud. We targeted the 16293E prestellar core, where the N15NH+ J=1-0 line was detected. Using a model previously developed for the physical structure of the source, we solved the molecular excitation with a non-local radiative transfer code. For that purpose, we computed specific collisional rate coefficients for the N15NH+-H2 collisional system. As a first step of the analysis, the N2H+ abundance profile was constrained by reproducing the N2H+ J=1-0 and 3-2 maps. A scaling factor was then applied to this profile to match the N15NH+ J=1-0 spectrum. We derive a column density ratio N2H+ / N15NH+ = 330(+170,-100). The current estimate ~330 agrees with the value typical of the elemental isotopic ratio in the local ISM. It is however lower than in some other cores, where values as high as 1300 have been reported.

Revisiting the OH-CH correlation in diffuse clouds

Bhaswati Mookerjea Tata Institute of Fundamental Research, Mumbai, India

Based on the analysis of available published data and archival data along 24 sightlines (5 of which are new) we derive more accurate estimates of the column densities of OH and CH towards diffuse/translucent clouds and revisit the typically observed correlation between the abundances of these species. The increase in the sample size was possible because of the equivalence of the column densities of CH derived from a combination of the transitions at 3137 & 3143 Angstrom, and a combination of transitions at 3886 & 3890 Angstrom, which we have demonstrated here. We find that with the exception of four diffuse clouds, the entire source sample shows a clear correlation between the column densities of OH and CH similar to previous observations. The analysis presented also verifies the theoretically predicted oscillator strengths of the OH A--X (3078 & 3082Angstrom), CH B--X (3886 & 3890Angstrom) and C--X (3137 & 3143 Angstrom) transitions. We estimate N(H) and N(H2) from the observed E(B-V) and N(CH) respectively. The N(OH)/N(CH) ratio is not correlated with the molecular fraction of hydrogen in the diffuse/translucent clouds. We show that with the exception of HD 34078 for all the clouds the observed column density ratios of CH and OH can be reproduced by simple chemical models which include gas-grain interaction and gas-phase chemistry. The enhanced N(OH)/N(CH) ratio seen towards the 3 new sightlines can be reproduced primarily by considering different cosmic ray ionization rates.

Detection of extragalactic CF+ toward PKS1830-211 -- Chemical differentiation in the absorbing gas

S. Muller, K. Kawaguchi, J. H. Black, & T. Amano

We report the first extragalactic detection of CF+, the fluoromethylidynium ion, in the z=0.89 absorber toward PKS1830-211. We estimate an abundance of ~3E-10 relative to H2 and that ~1% of fluorine is captured in CF+. The absorption line profile of CF+ is found to be markedly different from that of other species observed within the same tuning, and is notably anti-correlated with CH3OH. On the other hand, the CF+ profile resembles that of [C I]. Our results are consistent with expected fluorine chemistry and point to chemical differentiation in the column of absorbing gas.

High spatial resolution imaging of SO and H2CO in AB Auriga: The first SO image in a transitional disk.

S. Pacheco-Vázquez, A. Fuente, C. Baruteau, O. Berné, M. Agúndez, R. Neri, J. R. Goicoechea, J. Cernicharo and R. Bachiller

Context: Transitional disks are structures of dust and gas around young stars with large inner cavities in which planet formation may occur. Lopsided dust distributions are observed in the dust continuum emission at millimeter wavelengths. These asymmetrical structures can be explained as being the result of an enhanced gas density vortex where the dust is trapped, potentially promoting the rapid growth to the planetesimal scale. Aims: AB Aur hosts a transitional disk with a clear horseshoe morphology which strongly suggests the presence of a dust trap. Our goal is to investigate its formation and the possible effects on the gas chemistry. Methods: We used the NOrthern Extended Millimeter Array (NOEMA) interferometer to image the 1 mm continuum dust emission and the $13CO \ J = 2 \rightarrow 1$, $C18O \ J = 2 \rightarrow 1$, $SO \ J = 5,6 \rightarrow 4,5$, and $H2CO \ J = 303 \rightarrow 202$ rotational lines. Results: Line integrated intensity ratio images are built to investigate the chemical changes within the disk. The $I(H2CO \ J = 303 \rightarrow 202)/I(C18O \ J = 2 \rightarrow 1)$ ratio is fairly constant along the disk with values of ~0.15 ± 0.05. On the contrary, the $I(SO \ J = 5,6 \rightarrow 4,5)/I(C18O \ J = 2 \rightarrow 1)$ and $I(SO \ J = 5,6 \rightarrow 4,5)/I(H2CO \ J = 303 \rightarrow 202)$ ratios present a clear northeast-southwest gradient (a factor of 3–6) with the minimum towards the dust trap. This gradient cannot be explained by a local change in the excitation conditions but by a decrease in the SO abundance. Gas densities up to ~1e9 cm-3 are expected in the disk midplane and two-three times larger in the high pressure vortex. We have used a single point (n,T) chemical model to investigate the lifetime of gaseous CO, H2CO, and SO in the dust trap. Our model shows that for densities >1e7 cm-3, the SO molecules are depleted (directly frozen, or converted into SO2 and then frozen out) in less than 0.1 Myr. The lower SO abundance towards the dust trap could indicate that a larger fraction of the gas is in a high density environment. Conclusions: Gas dynamics, grain growth and gas chemistry are coupled in the planet formation process. We detect a chemical signature of the presence of a dust trap in a transitional disk. Because of the strong dependence of SO abundance on the gas density, the sulfur chemistry can be used as a chemical diagnostic to detect the birthsites of future planets. However, the large uncertainties inherent to chemical models and the limited knowledge of the disk's physical structure and initial conditions are important drawbacks.

Observations and modelling of CO and [CI] in protoplanetary disks. First detections of [CI] and constraints on the carbon abundance

M. Kama, S. Bruderer, M. Carney, M. Hogerheijde, E.F. van Dishoeck, D. Fedele, et al.

Context. The gas-solid budget of carbon in protoplanetary disks is related to the composition of the cores and atmospheres of the planets forming in them. The principal gas-phase carbon carriers CO, C0, and C+ can now be observed regularly in disks. Aims: The gas-phase carbon abundance in disks has thus far not been well characterized observationally. We obtain new constraints on the [C]/[H] ratio in a large sample of disks, and compile an overview of the strength of [CI] and warm CO emission. Methods: We carried out a survey of the CO 6-5 line and the [CI] 1-0 and 2-1 lines towards 37 disks with the APEX telescope, and supplemented it with [C II] data from the literature. The data are interpreted using a grid of models produced with the DALI disk code. We also investigate how well the gas-phase carbon abundance can be determined in light of parameter uncertainties. Results: The CO 6-5 line is detected in 13 out of 33 sources, [CI] 1-0 in 6 out of 12, and [CI] 2-1 in 1 out of 33. With separate deep integrations, the first unambiguous detections of the [CI] 1-0 line in disks are obtained, in TW Hya and HD 100546. Conclusions: Gas-phase carbon abundance reductions of a factor of 5-10 or more can be identified robustly based on CO and [CI] detections, assuming reasonable constraints on other parameters. The atomic carbon detection towards TW Hya confirms a factor of 100 reduction of [C]/[H]gas in that disk, while the data are consistent with an ISM-like carbon abundance for HD 100546. In addition, BP Tau, T Cha, HD 139614, HD 141569, and HD 100453 are either carbon-depleted or gas-poor disks. The low [CI] 2-1 detection rates in the survey mostly reflect insufficient sensitivity for T Tauri disks. The Herbig Ae/Be disks with CO and [CII] upper limits below the models are debris-disk-like systems. An increase in sensitivity of roughly order of magnitude compared to our survey is required to obtain useful constraints on the gas-phase [C]/[H] ratio in most of the targeted systems.

Gas and grain chemical composition in cold cores as predicted by the Nautilus 3-phase model

M. Ruaud, V. Wakelam, F. Hersant

We present an extended version of the 2-phase gas-grain code NAUTILUS to the 3-phase modelling of gas and grain chemistry of cold cores. In this model, both the mantle and the surface are considered as chemically active. We also take into account the competition among reaction, diffusion and evaporation. The model predictions are confronted to ice observations in the envelope of low-mass and massive young stellar objects as well as toward background stars. Modelled gas-phase abundances are compared to species observed toward TMC-1 (CP) and L134N dark clouds. We find that our model successfully reproduces the observed ice species. It is found that the reaction-diffusion competition strongly enhances reactions with barriers and more specifically reactions with H2, which is abundant on grains. This finding highlights the importance to have a good approach to determine the abundance of H2 on grains. Consequently, it is found that the major N-bearing species on grains go from NH3 to N2 and HCN when the reaction-diffusion competition is accounted. In the gas-phase and before few 1e5 yrs, we find that

the 3-phase model does not have a strong impact on the observed species compared to the 2-phase model. After this time, the computed abundances dramatically decrease due to the strong accretion on dust, which is not counterbalanced by the desorption less efficient than in the 2-phase model. This strongly constrains the chemical-age of cold cores to be of the order of few 1e5 yrs.

A Study of the Region of Massive Star Formation L379IRS1 in Radio Lines of Methanol and Other Molecules

Kalenskii S. V., Shchurov M. A.

The results of spectral observations of the region of massive star formation L379IRS1 (IRAS18265–1517) are presented. The observations were carried out with the 30-m Pico Veleta radio telescope (Spain) at seven frequencies in the 1-mm, 2-mm, and 3-mm wavelength bands. Lines of 24 molecules were detected, from simple diatomic or triatomic species to complex eight- or nine-atom compounds such as CH_3OCHO or CH_3OCH_3. Rotation diagrams constructed from methanol andmethyl cyanide lines were used to determine the temperature of the quiescent gas in this region, which is about 40–50 K. In addition to this warm gas, there is a hot component that is revealed through high-energy lines of methanol and methyl cyanide, molecular lines arising in hot regions, and the presence of H_2O masers and Class II methanol masers at 6.7 GHz, which are also related to hot gas. One of the hot regions is probably a compact hot core, which is located near the southern submillimeter peak and is related to a group of methanol masers at 6.7 GHz. High-excitation lines at other positions may be associated with other hot cores or hot post-shock gas in the lobes of bipolar outflows. The rotation diagrams can be use to determine the column densities and abundances of methanol (1e-9) and methyl cyanide (about 1e-11) in the quiescent gas. The column densities of A- and E-methanol in L379IRS1 are essentally the same. The column densities of other observedmolecules were calculated assuming that the ratios of the molecular level abundances correspond to a temperature of 40 K. The molecular composition of the quiescent gas is close to that in another region of massive star formation, DR21(OH). The only appreciable difference is that the column density of SO_2 in L379IRS1 is at least a factor of 20 lower than the value in DR21(OH). The SO_2/CS and SO_2/OCS abundance ratios, which can be used as chemical clocks, are lower in L379IRS1 than in DR21(OH), suggesting that L379IRS1 is probably younger than DR21(OH).

Photodissociation of HCN and HNC isomers in the 7-10 eV energy range

A. Chenel, O. Roncero, A. Aguado, M. Agúndez, and J. Cernicharo

The ultraviolet photoabsorption spectra of the HCN and HNC isomers have been simulated in the 7-10 eV photon energy range. For this purpose, the three-dimensional adiabatic potential energy surfaces of the 7 lowest electronic states, and the corresponding transition dipole moments, have been calculated, at multireference configuration interaction level. The spectra are calculated with a quantum wave packet method on these adiabatic potential energy surfaces. The spectra for the 3 lower excited states, the dissociative electronic states, correspond

essentially to predissociation peaks, most of them through tunneling on the same adiabatic state. The 3 higher electronic states are bound, hereafter electronic bound states, and their spectra consist of delta lines, in the adiabatic approximation. The radiative lifetime towards the ground electronic states of these bound states has been calculated, being longer than 10 ns in all cases, much longer that the characteristic predissociation lifetimes. The spectra of HCN is compared with the available experimental and previous theoretical simulations, while in the case of HNC there are no previous studies to our knowledge. The spectrum for HNC is considerably more intense than that of HCN in the 7-10 eV photon energy range, which points to a higher photodissociation rate for HNC, compared to HCN, in astrophysical environments illuminated by ultraviolet radiation.

Announcements

Linking Exoplanet and Disk Compositions - Workshop at the Space Telescope Science Institute, Baltimore MD, USA - September 12-14, 2016

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 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 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. Pre-registration and abstract submission are now open: http://www.cvent.com/d/ffqwn1 Contact: exodisks@stsci.edu

KROME School on Computational Astrochemistry

KROME School on Computational Astrochemistry Villa il Gioiello, Arcetri Firenze, Italy, September 19-21, 2016 The aim of the school is to introduce Master, PhD students, and postdocs to a number of current topics in astrochemistry. Morning sessions will be focused on theory while afternoon session will address specific problems solved through hands-on guided exercises based on the KROME computational software (www.kromepackage.org). The topics covered include several important physical processes in the interstellar medium, such as non-equilibrium gas chemistry, dust physics, heating and cooling, and photochemistry. The school will also address observational aspects of astrochemistry with ALMA, and the practical aspects of linking numerical hydro and MHD simulations with chemical codes. Invited lecturers: - Stefano Bovino (Hamburger Sternwarte) - Stephanie Cazaux (Groeningen University) - Cecilia Ceccarelli (IPAG Grenoble) - Andrea Ferrara (SNS, Pisa) - Tommaso Grassi (STARPLAN Copenhagen) - Troels Haugbølle (STARPLAN Copenhagen) - Alvaro Sanchez-Monge (Koeln University) - Daniel Seifried (Koeln University) - Wing-Fai Thi (MPE Garching) - Malcolm Walmsley (DIAS Dublin) The maximum number of participants is 15. Participants will receive support for lodging expenses and lunches. The school is financially supported by the INAF Progetto Premiale iALMA. Deadline for application is July 31, 2016 Please find more information, our poster, and

the application form under http://www.kromepackage.org/bootcamp With kind regards, the SOC

Rayons Cosmique et Milieu Interstellaire [French]

Dates: journées de la SF2A; deux après midi, Jeudi 16 Juin et Vendredi 17 Juin 2016, 14-18h Thématiques: Très Hautes Énergies / Milieu Interstellaire Résumé: Cet atelier a pour but de rapprocher les communautés "Très Hautes Énergies" et "Milieu Interstellaire" autour d'une réflexion sur les utilisations et exploitations concertées des grands moyens d'observation récents ou en développement: HESS/CTA d'une part, ALMA/NOEMA d'autre part, en vue d'une compréhension cohérente du Milieu Interstellaire incluant les effets des rayons cosmiques. Rationale: HESS délivre dès aujourd'hui des résultats inédits sur les rayons cosmiques qui portent l'avénement prochain du projet CTA, en particulier en lien avec le milieu interstellaire. La compréhension de la composition, des processus d'accélération et de diffusion des rayons cosmiques passe par une évaluation soigneuse du contenu interstellaire (densité/masse, champ magnétique, taux d'ionisation, champ de rayonnement…) des régions observées. Réciproquement, comprendre la chimie du milieu interstellaire nécessite de comprendre l'influence des rayons cosmiques sur le gaz et les poussières interstellaires. Progresser dans notre compréhension des liens entre rayons cosmiques et milieu interstellaire passe par l'utilisation complémentaire de HESS/CTA et NOEMA/ALMA. Le moment est idéal pour initier le développement de synergies reposant sur des programmes d'observation concertés. Ceux-ci devront être supportés par un effort équivalent tant du point de vue de l'astrophysique de laboratoire que de la modélisation numérique. Le PN PCMI propose d'y réfléchir pour optimiser le retour scientifique de ces instruments. Présentations invitées - CTA et HESS - M. Renaud, LUPM Montpellier - ALMA/NOEMA - F. Boone, IRAP Toulouse - Études multi-longueur d'onde extragalactiques - P. Guillard, IAP Paris - Rayons cosmiques et chimie du milieu interstellaire - B. Godard, LERMA Paris - Interaction des rayons cosmiques avec la matière interstellaire : expériences en laboratoire- E. Dartois, IAS Orsay - Accélération et diffusion des rayons cosmiques autour des protoétoiles - M. Padovani, LUPM Montpellier - Accélération et diffusion des rayons cosmiques dans les supernova et restes de supernova - J. Ballet, Irfu CEA - Rayons cosmiques et simulations numériques du milieu interstellaire - B. Commercon, CRAL Lyon 8*25 minutes (questions comprises) pour les invités = 3h20 10*20 minutes (questions comprises) pour les contribution = 3h20 => 2 1/2 journées avec une pause de 30 minutes SOC: A.Gusdorf (chair), J. Pety, A. Marcowith Organisateurs associés: Actions Fédératrices de l'Observatoire de Paris: "CTA" et "ALMA-NOEMA-Herschel", Programme National PCMI Lien vers la page associée: http://sf2a.eu/semaine-sf2a/2016/list_presentations.php Date limite pour soumettre un abstract: 15 Mai par mail a antoine.gusdorf at lra.ens.fr

Workshop "Heating and Cooling processes in the ISM" 7.-9. september in Cologne

Studying the main heating and cooling processes in molecular clouds is vitally important for a better comprehension of the physics and chemistry of the interstellar medium, and ultimately of star formation. The objective of this workshop is to summarize our theoretical and observational understanding of the relative importance of the various heating and cooling processes in the ISM.We want to discuss how to best combine observations using different instruments and settings on SOFIA and complementary telescopes to obtain a complete inventory of the main heating and cooling processes in individual regions. We address the Galactic and extra-galactic community as well as theoristst working in this field. Session topics are: Session 1: Interpreting observations, Session 2: Heating and cooling processes, Session 3: Accessing the THz (FIR) wavelength range Session 4: Radiative heating, Session 5: Shocks https://www.astro.uni-koeln.de/hac2016