AstroChemical Newsletter #12

October 2016

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Abstracts

A primordial origin for molecular oxygen in comets: A chemical kinetics study of the formation and survival of O2 ice from clouds to disks

V. Taquet, K. Furuya, C. Walsh, E. F. van Dishoeck

Molecular oxygen has been confirmed as the fourth most abundant molecule in cometary material O2/H2O ∼4 %) and is thought to have a primordial nature, i.e., coming from the interstellar cloud from which our solar system was formed. However, interstellar O2 gas is notoriously difficult to detect and has only been observed in one potential precursor of a solar-like system. Here, the chemical and physical origin of O2 in comets is investigated using sophisticated astrochemical models. Three origins are considered: i) in dark clouds, ii) during forming protostellar disks, and iii) during luminosity outbursts in disks. The dark cloud models show that reproduction of the observed abundance of O2 and related species in comet 67P/C-G requires a low H/O ratio facilitated by a high total density (≥1e5 cm−3), and a moderate cosmic ray ionisation rate (≤1e−16 s−1) while a temperature of 20 K, slightly higher than the typical temperatures found in dark clouds, also enhances the production of O2. Disk models show that O2 can only be formed in the gas phase in intermediate disk layers, and cannot explain the strong correlation between O2 and H2O in comet 67P/C-G together with the weak correlation between other volatiles and H2O. However, primordial O2 ice can survive transport into the comet-forming regions of disks. Taken together, these models favour a dark cloud (or "primordial") origin for O2 in comets, albeit for dark clouds which are warmer and denser than those usually considered as solar system progenitors.

Accepted for publication in MNRAS
DOI: 10.1093/mnras/stw2176
Full-text URL: http://arxiv.org/abs/1608.07130

The formation of ethylene glycol and other complex organic molecules in star-forming regions

Rivilla, V. M., Beltrán, M. T., Cesaroni, R., Fontani, F., Codella, C., Zhang, Q.

We study the molecular abundance and spatial distribution of the simplest sugar alcohol, ethylene glycol (EG), the simplest sugar glycoladehyde (GA), and other chemically related complex organic species towards the massive star-forming region G31.41+0.31. We have analyzed multiple single dish and interferometric data, and obtained excitation temperatures and column densities using an LTE analysis. We have reported for the first time the presence of EG towards G31.41+0.31, and we have also detected multiple transitions of other complex organic molecules such as GA, methyl formate (MF), dimethyl ether (DME) and ethanol (ET). The high angular resolution images show that the EG emission is very compact, peaking towards the maximum of the continuum. These observations suggest that low abundance complex organic molecules, like EG or GA, are good probes of the gas located closer to the forming stars. Our analysis confirms that EG is more abundant than GA in G31.41+0.31, as previously observed in other interstellar regions. Comparing different star-forming regions we find evidence of an increase of the EG/GA abundance ratio with the luminosity of the source. The DME/MF and EG/ET ratios are nearly constant with luminosity. We have also found that the abundance ratios of pairs of isomers GA/MF and ET/DME decrease with the luminosity of the sources. The most likely explanation for the behavior of the EG/GA ratio is that these molecules are formed by different chemical formation routes not directly linked; although warm-up timescales effects and different formation and destruction efficiencies in the gas phase cannot be ruled out. The most likely formation route of EG is by combination of two CH2OH radicals on dust grains. We also favor that GA is formed via the solid-phase dimerization of the formyl radical HCO, and a chemical link between MF and DME.

Accepted in Astronomy & Astrophysics
Full-text URL: http://arxiv.org/abs/1608.07491

A New Reference Chemical Composition for TMC-1

Gratier, P.; Majumdar, L.; Ohishi, M.; Roueff, E.; Loison, J. C.; Hickson, K. M.; Wakelam, V.

Recent detections of complex organic molecules in dark clouds have rekindled interest in the astrochemical modeling of these environments. Because of its relative closeness and rich molecular complexity, TMC-1 has been extensively observed to study the chemical processes taking place in dark clouds. We use local thermodynamical equilibrium radiative transfer modeling coupled with a Bayesian statistical method which takes into account outliers to analyze the data from the Nobeyama spectral survey of TMC-1 between 8 and 50 GHz. We compute the abundance relative to molecular hydrogen of 57 molecules, including 19 isotopologues in TMC-1 along with their associated uncertainty. The new results are in general agreement with previous abundance determination from Ohishi & Kaifu and the values reported in the review from Agúndez & Wakelam. However, in some cases, large opacity and low signal to noise effects allow only upper or lower limits to be derived, respectively.

The Astrophysical Journal Supplement Series, Volume 225, Issue 2, article id. 25, pp. (2016).
DOI: 10.3847/0067-0049/225/2/25
Full-text URL: http://arxiv.org/abs/1610.00524

Laboratory spectroscopic study and astronomical detection of vibrationally excited n-propyl cyanide

Holger S. P. Müller, Adam Walters, Nadine Wehres, Arnaud Belloche, Olivia H. Wilkins, Delong Liu, Rémi Vicente, Robin T. Garrod, Karl M. Menten, Frank Lewen, Stephan Schlemmer

We performed a spectral line survey called Exploring Molecular Complexity with ALMA (EMoCA) toward Sagittarius~B2(N) between 84.1 and 114.4 GHz with the Atacama Large Millimeter/submillimeter Array (ALMA) in its Cycles 0 and 1. We determined line intensities of n-propyl cyanide in the ground vibrational states of its gauche and anti conformers toward the hot molecular core Sagittarius B2(N2) which suggest that we should also be able to detect transitions pertaining to excited vibrational states. We wanted to determine spectroscopic parameters of low-lying vibrational states of both conformers of n-propyl cyanide to search for them in our ALMA data. We recorded laboratory rotational spectra of n-propyl cyanide in two spectral windows between 36 and 127 GHz. We searched for emission lines produced by these states in the ALMA spectrum of Sagittarius B2(N2). We modeled their emission and the emission of the ground vibrational states assuming local thermodynamic equilibrium (LTE). We have made extensive assignments of a- and b-type transitions of the four lowest vibrational states of the gauche conformer which reach J and Ka quantum numbers of 65 and 20, respectively. We assigned mostly a-type transitions for the anti conformer with J and Ka quantum numbers up to 48 and 24, respectively. Rotational and Fermi perturbations between two anti states allowed us to determine their energy difference. The resulting spectroscopic parameters enabled us to identify transitions of all four vibrational states of each conformer in our ALMA data. The emission features of all states, including the ground vibrational state, are well-reproduced with the same LTE modeling parameters, which gives us confidence in the reliability of the identifications, even for the states with only one clearly detected line.

Astron. Astrophys., accepted
DOI: 10.1051/0004-6361/201629309
Full-text URL: http://de.arxiv.org/abs/1608.08129

Grand challenges in protoplanetary disc modelling

Haworth, Thomas J.; Ilee, John D.; Forgan, Duncan H.; Facchini, Stefano; Price, Daniel J.; Boneberg, Dominika M.; Booth, Richard A.; Clarke, Cathie J.; Gonzalez, Jean-François; Hutchison, Mark A.; Kamp, Inga; Laibe, Guillaume; Lyra, Wladimir; Meru, Farzana; Mohanty, Subhanjoy; Panić, Olja; Rice, Ken; Suzuki, Takeru; Walsh, Catherine; Woitke, Peter

The Protoplanetary Discussions conference --- held in Edinburgh, UK, from 7th-11th March 2016 --- included several open sessions led by participants. This paper reports on the discussions collectively concerned with the multiphysics modelling of protoplanetary discs, including the self-consistent calculation of gas and dust dynamics, radiative transfer and chemistry. After a short introduction to each of these disciplines in isolation, we identify a series of burning questions and grand challenges associated with their continuing development and integration. We then discuss potential pathways towards solving these challenges, grouped by strategical, technical and collaborative developments. This paper is not intended to be a review, but rather to motivate and direct future research and collaboration across typically distinct fields based on community driven input, to encourage further progress in our understanding of circumstellar and protoplanetary discs.

Accepted for publication in PASA
Full-text URL: http://arxiv.org/pdf/1608.01315v2.pdf

Importance of the H2 abundance in protoplanetary disk ices for the molecular layer chemical composition

V. Wakelam, M. Ruaud, F. Hersant, A. Dutrey, D. Semenov, L. Majumdar, S. Guilloteau

Protoplanetary disks are the target of many chemical studies (both observational and theoretical) as they contain the building material for planets. Their large vertical and radial gradients in density and temperature make them challenging objects for chemical models. In the outer part of these disks, the large densities and low temperatures provide a particular environment where the binding of species onto the dust grains can be very efficient and can affect the gas-phase chemical composition. We attempt to quantify to what extent the vertical abundance profiles and the integrated column densities of molecules predicted by a detailed gas-grain code are affected by the treatment of the molecular hydrogen physisorption at the surface of the grains. We performed three different models using the Nautilus gas-grain code. One model uses a H2 binding energy on the surface of water (440 K) and produces strong sticking of H2. Another model uses a small binding energy of 23 K (as if there were already a monolayer of H2), and the sticking of H2 is almost negligible. Finally, the remaining model is an intermediate solution known as the encounter desorption mechanism. We show that the efficiency of molecular hydrogen binding (and thus its abundance at the surface of the grains) can have a quantitative effect on the predicted column densities in the gas phase of major species such as CO, CS, CN, and HCN.

Accepted for publication as a Research Note in A&A
DOI: 10.1051/0004-6361/201628748
Full-text URL: http://lanl.arxiv.org/abs/1609.01471

OH+ and H2O+ absorption toward PKS1830-211

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We report the detection of OH+ and H2O+ in the z=0.89 absorber toward the lensed quasar PKS1830-211. The abundance ratio of OH+ and H2O+ is used to quantify the molecular hydrogen fraction (fH2) and the cosmic-ray ionization rate of atomic hydrogen (zH) along two lines of sight, located at ~2 kpc and ~4 kpc to either side of the absorber's center. The molecular fraction decreases outwards, from ~0.04 to ~0.02, comparable to values measured in the Milky Way at similar galactocentric radii. For zH, we find values of ~2e-14 s^-1 and ~3e-15 s^-1, respectively, which are slightly higher than in the Milky Way at comparable galactocentric radii, possibly due to a higher average star formation activity in the z=0.89 absorber. The ALMA observations of OH+, H2O+, and other hydrides toward PKS1830-211 reveal the multi-phase composition of the absorbing gas. Taking the column density ratios along the southwest and northeast lines of sight as a proxy of molecular fraction, we classify the species ArH+, OH+, H2Cl+, H2O+, CH, and HF as tracing gases increasingly more molecular. Incidentally, our data allow us to improve the accuracy of H2O+ rest frequencies and thus refine the spectroscopic parameters.

Accepted for publication in A&A
DOI: 10.1051/0004-6361/201629073
Full-text URL: https://arxiv.org/abs/1609.01060

Photo-fragmentation behavior of methyl- and methoxy-substituted derivatives of hexa-peri-hexabenzocoronene (HBC) cations

Junfeng Zhen, Pablo Castellanos, Harold Linnartz, Alexander G.G.M. Tielens

A systematic study, using ion trap time-of-flight mass spectrometry, is presented for the photo-fragmentation of methyl- and methoxy-substituted derivatives of HBC cations, (OCH3)6HBC+ and (CH3)4(OCH3)2HBC+. Both substituted HBC cations fragment through sequential loss of CH3CO units upon laser (595nm) irradiation, resulting in a PAH-like derivative C36H12+ and a methyl-substituted PAH derivative C44H24+, respectively. Upon ongoing irradiation, these species further fragment. For lower laser energy C44H24+ dehydrogenates and photo-fragments through CH3 and CHCH2 unit losses; for higher laser energy isomerization takes place, yielding a regular PAH-like configuration, and both stepwise dehydrogenation and C2/C2H2 loss pathways are found. C36H12+ follows largely this latter fragmentation scheme upon irradiation. It is concluded that the photo-dissociation mechanism of the substituted PAH cations studied here is site selective in the substituted subunit. This work also shows experimental evidence that photo-fragmentation of substituted PAHs may contribute to the formation in space of smaller species that are normally considered to form by merging atoms and molecules.

Molecular Astrophysics, Volume 5, November 2016, Pages 1–8
DOI: 10.1016/j.molap.2016.08.001
Full-text URL: http://www.sciencedirect.com/science/article/pii/S240567581630001X

Prediction of the Spectroscopic Parameters of new Iron Compounds: Hydride of Iron Cyanide/Isocyanide, HFeCN/HFeNC

P. Redondo, A. Largo, C. Barrientos

Iron is the most abundant transition metal in space, its abundance is similar to that of magnesium, and until today only FeO and FeCN are detected. However, magnesium bearing compounds such as MgCN, MgNC, and HMgNC are found in IRC+10216. It seems that hydrides of iron cyanide/isocyanide could be good candidates to be present in space. In the present work we carried out a characterization of the different minima on the quintet and triplet [C, Fe, H, N] potential energy surfaces employing several theoretical approaches. The most stable isomers are predicted to be hydride of iron cyanide HFeCN, and isocyanide HFeNC in their 5□ states. Both isomers are found to be quasi-isoenergetics. The HFeNC isomer is predicted to lie about 0.5 kcal/mol below HFeCN. The barrier for the interconversion process is estimated to be around 6.0 kcal/mol, making this process unfeasible under low temperature conditions, such as those in the interstellar medium. Therefore, both, HFeCN and HFeNC, could be candidates for their detection. We report geometrical parameters, vibrational frequencies and rotational constants that could help in their experimental characterization.

2016, ApJ, 828:45
DOI: 10.3847/0004-637X/828/1/45
Full-text URL: http://iopscience.iop.org/article/10.3847/0004-637X/828/1/45/meta

The ortho-to-para ratio of interstellar NH2: Quasi-classical trajectory calculations and new simulations

R. Le Gal, E. Herbst, C. Xie, A. Li, H. Guo

Based on recent Herschel results, the ortho-to-para ratio (OPR) of NH2 has been measured towards the following high-mass star-forming regions: W31C (G10.6-0.4), W49N (G43.2-0.1), W51 (G49.5-0.4), and G34.3+0.1. The OPR at thermal equilibrium ranges from the statistical limit of three at high temperatures to infinity as the temperature tends toward zero, unlike the case of H2. Depending on the position observed along the lines-of-sight, the OPR was found to lie either slightly below the high temperature limit of three (in the range 2.2-2.9) or above this limit (~3.5, > 4.2, and > 5.0). In low temperature interstellar gas, where the H2 is para-enriched, our nearly pure gas-phase astrochemical models with nuclear-spin chemistry can account for anomalously low observed NH2-OPR values. We have tentatively explained OPR values larger than three by assuming that spin thermalization of NH2 can proceed at least partially by H-atom exchange collisions with atomic hydrogen, thus increasing the OPR with decreasing temperature. In this paper, we present quasi-classical trajectory calculations of the H-exchange reaction NH2 + H, which show the reaction to proceed without a barrier, confirming that the H-exchange will be efficient in the temperature range of interest. With the inclusion of this process, our models suggest both that OPR values below three arise in regions with temperatures higher than ~20-25 K, depending on time, and values above three but lower than the thermal limit arise at still lower temperatures.

Accepted for publication in A&A
DOI: 10.1051/0004-6361/201629107
Full-text URL: http://arxiv.org/pdf/1609.02485v1.pdf

Photochemical-dynamical models of externally FUV irradiated protoplanetary discs

Haworth, Thomas J.; Boubert, Douglas; Facchini, Stefano; Bisbas, Thomas G.; Clarke, Cathie J.

There is growing theoretical and observational evidence that protoplanetary disc evolution may be significantly affected by the canonical levels of far ultraviolet (FUV) radiation found in a star forming environment, leading to substantial stripping of material from the disc outer edge even in the absence of nearby massive stars. In this paper we perform the first full radiation hydrodynamic simulations of the flow from the outer rim of protoplanetary discs externally irradiated by such intermediate strength FUV fields, including direct modelling of the photon dominated region (PDR) which is required to accurately compute the thermal properties. We find excellent agreement between our models and the semi-analytic models of Facchini et al. (2016) for the profile of the flow itself, as well as the mass loss rate and location of their "critical radius". This both validates their results (which differed significantly from prior semi-analytic estimates) and our new numerical method, the latter of which can now be applied to elements of the problem that the semi--analytic approaches are incapable of modelling. We also obtain the composition of the flow, but given the simple geometry of our models we can only hint at some diagnostics for future observations of externally irradiated discs at this stage. We also discuss the potential for these models as benchmarks for future photochemical-dynamical codes.

Accepted for publication in MNRAS
DOI: 10.1093/mnras/stw2280
Full-text URL: https://arxiv.org/abs/1609.02153

ExoMol line lists XVIII. The high temperature spectrum of VO.

Laura K. McKemmish, Sergei N. Yurchenko and Jonathan Tennyson

An accurate line list, VOMYT, of spectroscopic transitions is presented for hot VO. The 13 lowest electronic states are considered. Curves and couplings are based on initial ab initio electronic structure calculations and then tuned using available experimental data. Dipole moment curves, used to obtain transition intensities, are computed using high levels of theory (e.g. MRCI/aug-cc-pVQZ using state-specific or minimal-state CAS for dipole moments). This line list contains over 277 million transitions between almost 640,000 energy levels. It covers the wavelengths longer than 0.29 μm and includes all transitions from energy levels within the lowest nine electronic states which have energies less than 20,000 cm−1 to upper states within the lowest 13 electronic states which have energies below 50,000 cm−1. The line lists give significantly increased absorption at infrared wavelengths compared to currently available VO line lists. The full line lists is made available in electronic form via the CDS database and at www.exomol.com.

MNRAS (November 21, 2016) 463 (1): 771-793.
DOI: 10.1093/mnras/stw1969
Full-text URL: http://mnras.oxfordjournals.org/content/463/1/771.full

Photo and thermochemical evolution of astrophysical ice analogs as a source for soluble and insoluble organic materials in solar system minor bodies

P. de Marcellus, A. Fresneau, R. Brunetto, G. Danger, F. Duvernay, C. Meinert, U. J. Meierhenrich, Ferenc Borondics, T. Chiavassa, and L. Le Sergeant d'Hendecourt

Soluble and Insoluble Organic Matter is a key feature of primitive carbonaceous chondrites. We observe the formation of organic materials in the photo-thermochemical treatment of astrophysical ices in the laboratory. Starting from a low vacuum ultraviolet (VUV) irradiation dose on templates of astrophysical ices at 77 K, we obtain first a totally soluble form of organic matter at room temperature. Once this organic residue is formed, irradiating it further in vacuum results in the production of a thin altered dark crust on top of the initial soluble one. The whole residue is studied here by non-destructive methods inducing no alteration of samples, visible microscopy and mid-infrared (micro)-spectroscopy. After water extraction of the soluble part, an insoluble fraction remains on the sample holder which provides a largely different infrared spectrum when compared to the one of the soluble sample. Therefore, from the same VUV and thermal processing of initial simple ices, we produce first a soluble material from which a much larger irradiation dose leads to an insoluble one. Interestingly, this insoluble fraction shows some spectral similarities with natural samples of Insoluble Organic Matter (IOM) extracted from two meteorites (Tagish Lake and Murchison), selected as examples of primitive materials. It suggests that the organic molecular diversity observed in meteorites may partly originate from the photo and thermal processing of interstellar/circumstellar ices at the final stages of molecular cloud evolution toward the build-up of our solar system.

Accepted in Monthly Notices of the Royal Astronomical Society
DOI: 10.1093/mnras/stw2292
Full-text URL: http://mnras.oxfordjournals.org/content/early/2016/09/12/mnras.stw2292.full.pdf?keytype=ref&ijkey=ZBbVDomZwcO6Op4

Formation of silicon monoxide by radiative association: the impact of resonances

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

Detailed quantum chemistry calculations within the multireference configuration interaction approximation with the Davidson correction are presented using an aug-cc-pV6Z basis set, for the potential energy curves and transition dipole moments between low lying molecular states of singlet spin symmetry for the SiO molecule. The high quality molecular data are used to obtain radiative association cross sections and rate coefficients for collisions between ground state Si and O atoms. Quantal calculations are compared with semiclassical results. Using a quantum kinetic theory of radiative association in which quasibound levels are assumed to be in local thermodynamic equilibrium, we find that resonances play an important role in enhancing the rate coefficients at low temperatures by several orders of magnitude from that predicted by standard quantum scattering formulations. These new molecular formation rates may have important implications for applications in astrophysics.

J. Phys. B: At. Mol. Opt. Phys. 49 (2016) 184002
DOI: [10.1088/0953-4075/49/18/184002](10.1088/0953-4075/49/18/184002)
Full-text URL: https://arxiv.org/abs/1605.09640

The ExoMol database: Molecular line lists for exoplanet and other hot atmospheres

Jonathan Tennyson, Sergei N. Yurchenko, Ahmed F. Al-Refaie, Emma J. Barton, Katy L. Chubb, Phillip A. Coles, S. Diamantopoulou, Maire N. Gorman, Christian Hill, Aden Z. Lam, Lorenzo Lodi, Laura K. McKemmish, Yueqi Na, Alec Owens, Oleg L. Polyansky, Tom Rivlin, Clara Sousa-Silva, Daniel S. Underwood, Andrey Yachmenev, Emil Zak

The ExoMol database (www.exomol.com) provides extensive line lists of molecular transitions which are valid over extended temperature ranges. The status of the current release of the database is reviewed and a new data structure is specified. This structure augments the provision of energy levels (and hence transition frequencies) and Einstein A coefficients with other key properties, including lifetimes of individual states, temperature-dependent cooling functions, Landé g-factors, partition functions, cross sections, k-coefficients and transition dipoles with phase relations. Particular attention is paid to the treatment of pressure broadening parameters. The new data structure includes a definition file which provides the necessary information for utilities accessing ExoMol through its application programming interface (API). Prospects for the inclusion of new species into the database are discussed.

JMS, Volume 327, September 2016, Pages 73–94
DOI: [10.1016/j.jms.2016.05.002](10.1016/j.jms.2016.05.002)
Full-text URL: http://www.sciencedirect.com/science/article/pii/S0022285216300807

Kinetics and mechanisms of the acid-base reaction between NH3 and HCOOH in interstellar ice analogs

J. B. Bergner, K. I. Oberg, M. Rajappan, E. C. Fayolle

Interstellar complex organic molecules (COMs) are commonly observed during star formation, and are proposed to form through radical chemistry in icy grain mantles. Reactions between ions and neutral molecules in ices may provide an alternative cold channel to complexity, as ion-neutral reactions are thought to have low or even no energy barriers. Here we present a study of a the kinetics and mechanisms of a potential ion-generating acid-base reaction between NH3 and HCOOH to form the salt NH4+HCOO−. We observe salt growth at temperatures as low as 15K, indicating that this reaction is feasible in cold environments. The kinetics of salt growth are best fit by a two-step model involving a slow "pre-reaction" step followed by a fast reaction step. The reaction energy barrier is determined to be 70 ± 30K with a pre-exponential factor 1.4 ± 0.4 x 1e-3 s^−1. The pre-reaction rate varies under different experimental conditions and likely represents a combination of diffusion and orientation of reactant molecules. For a diffusion-limited case, the pre-reaction barrier is 770 ± 110K with a pre-exponential factor of ∼7.6 x 1e−3 s^−1. Acid-base chemistry of common ice constituents is thus a potential cold pathway to generating ions in interstellar ices.

Accepted for publication in ApJ
DOI: [10.3847/0004-637X/829/2/85](10.3847/0004-637X/829/2/85)
Full-text URL: http://arxiv.org/abs/1608.00010

On the Inference of the Cosmic Ray Ionization Rate ζ from the HCO+-to-DCO+ Abundance Ratio:

The Effect of Nuclear Spin

Christopher N. Shingledecker, Jennifer B. Bergner, Romane Le Gal, Karin I. Oberg, Ugo Hincelin, Eric Herbst

The chemistry of dense interstellar regions was analyzed using a time-dependent gas-grain astrochemical simulation and a new chemical network that incorporates deuterated chemistry taking into account nuclear spin-states for the hydrogen chemistry and its deuterated isotopologues. With this new network, the utility of the [HCO+]/[DCO+] abundance ratio as a probe of the cosmic ray ionization rate has been reexamined, with special attention paid to the effect of the initial value of the molecular hydrogen ortho-to-para ratio (OPR). After discussing the use of the probe for cold cores, we then compare our results with previous theoretical and observational results for a molecular cloud close to the supernova remnant W51C, which is thought to have an enhanced cosmic ray ionization rate ζ caused by the nearby γ-ray source. In addition, we attempt to use our approach to estimate the cosmic ray ionization rate for L1174, a dense core with an embedded star. Beyond the previously known sensitivity of [HCO+]/[DCO+] to ζ, we demonstrate its additional dependence on the initial OPR and, secondarily, on the age of the source, its temperature, and its density. We conclude that the usefulness of the [HCO+]/[DCO+] abundance ratio to constrain the cosmic ray ionization rate in dense regions increases with source age and ionization rate as the ratio becomes far less sensitive to the initial value of the OPR.

ApJ (accepted)
Full-text URL: http://arxiv.org/abs/1609.04728

High-molecular-weight organic matter in the particles of comet 67P/Churyumov–Gerasimenko

Nicolas Fray, Anaïs Bardyn, Hervé Cottin, Kathrin Altwegg, Donia Baklouti, Christelle Briois, Luigi Colangeli, Cécile Engrand, Henning Fischer, Albrecht Glasmachers, Eberhard Grün, Gerhard Haerendel, Hartmut Henkel, Herwig Höfner, Klaus Hornung, Elmar K. Jessberger, Andreas Koch, Harald Krüger, Yves Langevin, Harry Lehto, Kirsi Lehto, Léna Le Roy, Sihane Merouane, Paola Modica, François-Régis Orthous-Daunay, John Paquette, François Raulin, Jouni Rynö, Rita Schulz, Johan Silén, Sandra Siljeström, Wolfgang Steiger, Oliver Stenzel, Thomas Stephan, Laurent Thirkell, Roger Thomas, Klaus Torkar, Kurt Varmuza, Karl-Peter Wanczek, Boris Zaprudin, Jochen Kissel & Martin Hilchenbach

The presence of solid carbonaceous matter in cometary dust was established by the detection of elements such as carbon, hydrogen, oxygen and nitrogen in particles from comet 1P/Halley. Such matter is generally thought to have originated in the interstellar medium, but it might have formed in the solar nebula—the cloud of gas and dust that was left over after the Sun formed. This solid carbonaceous material cannot be observed from Earth, so it has eluded unambiguous characterization. Many gaseous organic molecules, however, have been observed; they come mostly from the sublimation of ices at the surface or in the subsurface of cometary nuclei. These ices could have been formed from material inherited from the interstellar medium that suffered little processing in the solar nebula. Here we report the in situ detection of solid organic matter in the dust particles emitted by comet 67P/Churyumov–Gerasimenko; the carbon in this organic material is bound in very large macromolecular compounds, analogous to the insoluble organic matter found in the carbonaceous chondrite meteorites. The organic matter in meteorites might have formed in the interstellar medium and/or the solar nebula, but was almost certainly modified in the meteorites' parent bodies. We conclude that the observed cometary carbonaceous solid matter could have the same origin as the meteoritic insoluble organic matter, but suffered less modification before and/or after being incorporated into the comet.

Nature, Advance Online Publication
DOI: 10.1038/nature19320
Full-text URL: http://www.nature.com/nature/journal/vaop/ncurrent/full/nature19320.html

Design and Testing of Temperature Tunable de Laval Nozzles for Applications in Gas-Phase Reaction Kinetics

A. Canosa, A.J. Ocaña, M. Antiñolo, B. Ballesteros, E. Jiménez, and J. Albaladejo.

A series of three de Laval nozzles initially designed to generate uniform supersonic flows in helium at 23 and 36 K and in argon at 50 K have been used with either pure nitrogen or mixtures of nitrogen with helium or argon in order to make a sequence of pulsed supersonic flows working at different temperatures. For this, a computer homemade program has been used to design de Laval nozzles contours for gas mixtures in order to determine the theoretical pressure P and temperature T in these supersonic flows. Spatial evolution of T along the flow axis downstream of the nozzle exit has been characterized with a fast response Pitot tube instrument newly developed. Twenty-eight different gas mixture conditions have been tested, indicating a very good agreement with the corresponding calculated flow conditions. The length of uniformity ΔL of the supersonic flows have been found to be >30 cm in more than 80 % of the situations and >50 cm for more than 50 % of the tested conditions. Fine temperature tunability was achieved in the range 22–107 K with very small fluctuations of the mean temperature along ΔL. Advantages and limits of these new developments for studies of gas-phase reaction kinetics are discussed.

Experiments in Fluids, 57[9], 152 (2016)
DOI: 10.1007/s00348-016-2238-1
Full-text URL: http://link.springer.com/article/10.1007/s00348-016-2238-1/fulltext.html

The millimeter IRAM-30m line survey toward IK Tau

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We carried out a millimeter wavelength line survey between 79 and 356 GHz with the IRAM-30m telescope to investigate the physical and chemical properties of the molecular envelope of the oxygen-rich AGB star IK Tau. We analysed the molecular lines detected using the population diagram technique to derive rotational temperatures and column densities. Additionally, we conducted a radiative transfer analysis of the SO2 lines detected. For the first time in this source we detected rotational lines in the ground vibrational state of HCO+, NS, NO, and H2CO, as well as several isotopologues of molecules previously identified. We also detected several rotational lines in vibrationally excited states of SiS and SiO isotopologues, and rotational lines of H2O (v2=2). We have also increased the number of rotational lines detected of molecules that were previously identified, enabling a detailed study of the molecular abundances and excitation temperatures. IK Tau displays a rich chemistry for an oxygen-rich circumstellar envelope. We highlight the detection of NS and H2CO with fractional abundances of f(NS)∼1e−8 and f(H2CO)∼[1e−7 – 1e−8]. Most of the molecules display rotational temperatures between 15 and 40 K. NaCl and SiS isotopologues display rotational temperatures higher than the average (~65 K). In the case of SO2 a warm component with Trot∼290 K is also detected. This SO2 warm component is probably arising from the inner regions of the envelope (at ∼8R∗) where SO2 has a fractional abundance of f(SO2)∼1e−6. This result should be considered for future investigation of the main formation channels of this, and other, parent species in the inner winds of O-rich AGB stars, which at present are not well reproduced by current chemistry models.

Accepted in Astronomy and Astrophysics
DOI: 10.1051/0004-6361/201628776
Full-text URL: https://arxiv.org/abs/1609.01904

Spatial distribution of FIR rotationally excited CH+ and OH emission lines in the Orion Bar PDR

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The abundance of CH+ and OH and excitation are predicted to be enhanced by the presence of vibrationally excited H2 or hot gas (~500-1000 K) in PDRs with high incident FUV radiation field. The excitation may also originate in dense gas (>10^5 cm-3) followed by nonreactive collisions. Previous observations suggest that the CH+ and OH correlate with dense and warm gas, and formation pumping contributes to CH+ excitation. We examine the spatial distribution of the CH+ and OH emission in the Orion Bar to establish their physical origin and main formation and excitation mechanisms. We present spatially sampled maps of the CH+ J=3-2 transition at 119.8 µm and the OH Λ-doublet at 84 µm in the Orion Bar over an area of 110"x110" with Herschel (PACS). We compare the spatial distribution of these molecules with those of their chemical precursors, C+, O and H2, and tracers of warm and dense gas. We assess the spatial variation of CH+ J=2-1 velocity-resolved line profile observed with Herschel (HIFI). The OH and CH+ lines correlate well with the high-J CO emission and delineate the warm and dense molecular region. While similar, the differences in the CH+ and OH morphologies indicate that CH+ formation and excitation are related to the observed vibrationally excited H2. This indicates that formation pumping contributes to the excitation of CH+. Interestingly, the peak of the rotationally excited OH 84 µm emission coincides with a bright young object, proplyd 244-440, which shows that OH can be an excellent tracer of UV-irradiated dense gas. The spatial distribution of CH+ and OH revealed in our maps is consistent with previous modeling studies. Both formation pumping and nonreactive collisions in a UV-irradiated dense gas are important CH+ J=3-2 excitation processes. The excitation of the OH Λ-doublet at 84 µm is mainly sensitive to the temperature and density.

Accepted to A&A
Full-text URL: http://arxiv.org/pdf/1609.04359v1.pdf

Announcements

International conference on the Hydride Toolbox, 12-15 Dec. 2016, Paris - Registration and Payment Deadline: 10 October 2016

Dear colleagues, Registration and payment deadline is coming very soon: 10 October 2016 Please visit our website for all useful information at http://hydride-toolbox.sciencesconf.org 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 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

Joint ICTP-IAEA School on Atomic Processes in Plasmas, 27 Feb - 3 Mar 2017 at ICTP in Trieste, Italy; applications are due Thu 20 Oct 2016

The Abdus Salam International Centre for Theoretical Physics (ICTP) and the International Atomic Energy Agency (IAEA) will jointly organize the 2017 Joint ICTP-IAEA School on Atomic Processes in Plasmas to be held at ICTP in Miramare, Trieste, Italy, from 27 February to 3 March 2017. The event will provide advanced training in theoretical and computational methods for atomic processes in plasmas. The schedule will feature lectures by international experts, exposure to some important codes, invited and contributed research talks, posters and discussion sessions, with good time available for personal interaction. We wish to attract advanced Ph.D. students, post-docs, early career faculty and other young researchers from around the world. https://www-amdis.iaea.org/Workshops/ICTP2017/ The school is concerned with theoretical and computational methods for the study of collisional and radiative atomic processes in plasmas including the following: atomic processes in low-density plasmas (e.g. astrophysical, fusion and laboratory); atomic processes in warm and hot dense matter and X-ray sources; computational methods for atomic structure and collisions; principles of spectroscopic diagnostics of plasma; collisional-radiative modelling and calculation of plasma spectra; simulations of non-Maxwellian and highly transient plasmas; opacity (radiation transport) effects on plasma properties and plasma diagnostics; methods for analysis of spectral line shapes and profiles; online codes for calculation of ionization distributions and spectra. The expected lecturers are Connor Ballance, Queen's University Belfast, UK, Hyun-Kyung Chung, International Atomic Energy Agency, Austria, Stephan Fritzsche, Helmholtz-Institut Jena, Germany, Hans-Joachim Kunze, Ruhr University Bochum,, Germany, Yuri Ralchenko, National Institute of Standards and Technology, USA, Howard A. Scott, Lawrence Livermore National Laboratory, USA, John Seely, Artep, Inc., USA, Evgeny Stambulchik, Weizmann Institute of Science, Israel. The event will feature lectures during the mornings. During the afternoons there will be computer classes to provide exposure to some widely used codes, poster sessions for participants to present their work, additional lectures, research talks and discussion sessions. The desired participants by application are advanced Ph.D. students, post-docs and other young researchers working in atomic or plasma physics with a special interest in collisional and radiative processes of atomic ions in fusion, astrophysical and industrial plasma or warm and hot dense matter. Please see the meeting web page linked earlier for instructions about applying. A one-page free-format abstract of a scientific contribution (expected to be presented as a poster) is requested as a part of the applications procedure. The school does not have a registration fee and accommodation at ICTP is available at low cost. A limited number of grants are available to support the travel and living expenses of selected participants, with priority given to participants working in a developing country and who are at the early stages of their career. Directors: Bas Braams (IAEA), Hyun-Kyung Chung (IAEA), Yuri Ralchenko (NIST). Local organizer: Joe Niemela (ICTP). Bas Braams