AstroChemical Newsletter #2

December 2015

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

Probing non-polar interstellar molecules through their protonated form: Detection of protonated cyanogen (NCCNH+)

M. Agúndez, J. Cernicharo, P. de Vicente, N. Marcelino, E. Roueff, A. Fuente, M. Gerin, M. Guélin, C. Albo, A. Barcia, L. Barbas, R. Bolaño, F. Colomer, M. C. Diez, J. D. Gallego, J. Gómez-González, I. López-Fernández, J. A. López-Fernández, J. A. López-Pérez, I. Malo, J. M. Serna, F. Tercero

Cyanogen (NCCN) is the simplest member of the series of dicyanopolyynes. It has been hypothesized that this family of molecules can be important constituents of interstellar and circumstellar media, although the lack of a permanent electric dipole moment prevents its detection through radioastronomical techniques. Here we present the first solid evidence of the presence of cyanogen in interstellar clouds by detection of its protonated form toward the cold dark clouds TMC-1 and L483. Protonated cyanogen (NCCNH+) has been identified through the J = 5−4 and J = 10−9 rotational transitions using the 40 m radiotelescope of Yebes and the IRAM 30 m telescope. We derive beam-averaged column densities for NCCNH+ of (8.6 ± 4.4)e10 cm-2 in TMC-1 and (3.9 ± 1.8)e10 cm-2 in L483, which translate into fairly low fractional abundances relative to H2, in the range (1–10)e-12. The chemistry of protonated molecules in dark clouds is discussed, and it is found that, in general terms, the abundance ratio between the protonated and non-protonated forms of a molecule increases with increasing proton affinity. Our chemical model predicts an abundance ratio NCCNH+/NCCN of 1e-4, which implies that the abundance of cyanogen in dark clouds could be as high as (1–10)e-8 relative to H2, i.e., comparable to that of other abundant nitriles such as HCN, HNC, and HC3N.

Astronomy & Astrophysics, 579, L10 (2015)
DOI: 10.1051/0004-6361/201526650
Full-text URL: http://www.aanda.org/articles/aa/abs/2015/07/aa26650-15/aa26650-15.html

Non-thermal ion desorption from an acetonitrile (CH3CN) astrophysical ice analogue studied by electron stimulated ion desorption

F. de A. Ribeiro, G. C. Almeida, Y. Garcia-Basabe, W. Wolff, H. M. Boechat-Roberty and M. L. M. Rocco

The incidence of high-energy radiation onto icy surfaces constitutes an important route for leading new neutral or ionized molecular species back to the gas phase in interstellar and circumstellar environments, especially where thermal desorption is negligible. In order to simulate such processes, an acetonitrile ice (CH3CN) frozen at 120 K is bombarded by high energy electrons, and the desorbing positive ions are analyzed by time-of-flight mass spectrometry (TOF-MS). Several fragment and cluster ions were identified, including the Hn=1–3+, CHn=0–3 +/NHn=0–1 +; C2Hn=0–3+ /CHn=0–3N+, C2Hn=0–6N+ ion series and the ion clusters (CH3CN)n=1–2+ and (CH3CN)n=1–2H+. The energy dependence on the positive ion desorption yield indicates that ion desorption is initiated by Coulomb explosion following Auger electronic decay. The results presented here suggest that non-thermal desorption processes, such as desorption induced by electronic transitions (DIET) may be responsible for delivering neutral and ionic fragments from simple nitrile-bearing ices to the gas-phase, contributing to the production of more complex molecules. The derived desorption yields per electron impact may contribute to chemical evolution models in different cold astrophysical objects, especially where the abundance of CH3CN is expected to be high.

Phys.Chem.Chem.Phys., 2015, 17, 27473
DOI: 10.1039/c5cp05040e
Full-text URL:
http://pubs.rsc.org/en/Content/ArticleLanding/2015/CP/C5CP05040E#!divAbstract

Effects of turbulent dust grain motion to interstellar chemistry

J.X. Ge, J.H. He and H.R. Yan

Theoretical studies have revealed that dust grains are usually moving fast through the turbulent interstellar gas, which could have significant effects upon molecular cloud chemistry by modifying grain accretion. This effect is investigated in this work on the basis of numerical gas-grain chemical modeling. Major features of the grain motion effect in the typical environment of dark clouds (DC) can be summarised as follows: 1) decrease of gas-phase (both neutral and ionic) abundances and increase of surface abundances by up to 2-3 orders of magnitude; 2) shifts of the existing chemical jumps to earlier evolution ages for gas-phase species and to later ages for surface species by factors of about ten; 3) a few exceptional cases in which some species turn out to be insensitive to this effect and some other species can show opposite behaviors too. These effects usually begin to emerge from a typical DC model age of about 10^5 yr. The grain motion in a typical cold neutral medium (CNM) can help overcome the Coulomb repulsive barrier to enable effective accretion of cations onto positively charged grains. As a result, the grain motion greatly enhances the abundances of some gas-phase and surface species by factors up to 2-6 or more orders of magnitude in the CNM model. The grain motion effect in a typical molecular cloud (MC) is intermediate between that of the DC and CNM models, but with weaker strength. The grain motion is found to be important to consider in chemical simulations of typical interstellar medium.

accepted in MNRAS
Full-text URL: http://arxiv.org/abs/1510.08680

Porosity and band-strength measurements of multi-phase composite ices

J.-B. Bossa, B. Mate, C. Fransen, S. Cazaux, S. Pilling, W. R. M. Rocha, J. Ortigoso, H. Linnartz

We use experimental mid-infrared optical constants and extended effective medium approximations to determine the porosity and the band-strengths of multi- phase composite ices grown at 30 K. Porous and a set of mixed H_2O:CH_4 ices are taken as a prototypical example. As a benchmark and proof of concept, the stoichiometry of the ice constituents are retreive with good accuracy from the refractive indices and the extinction coefficients of the reference binary ice mixtures with known compositions. Accurate band strengths are then calculated from experimental mid-infrared spectra of complex ices. We notice that the presence of pores has only a small effect on the overall band strenghts, whereas a water dilution can considerably alter them. Different levels of porosity are observed depending on the abundance of methane used as a gas contaminent premixed with water prior to background deposition. The absorption profiles are also found to vary with deposition rate. To explain this, we use Monte Carlo simulations and we observe that the deposition rate strongly affects the pore size distribution as well as the ice morphology through reorganisation processes. Extrapolated to genuine interstellar ices, the methodology presented in this paper can be used to evaluate the porosity and to quantify the relative abundances from observational data.

2015, ApJ, 814, 47
DOI: 10.1088/0004-637X/814/1/47
Full-text URL: http://stacks.iop.org/0004-637X/814/47

Deuterium enrichment of the interstellar grain mantle

Ankan Das, Dipen Sahu, Liton Majumdar and Sandip K. Chakrabarti

We carry out Monte Carlo simulation to study deuterium enrichments of interstellar grain mantles under various physical conditions. Based on the physical properties, various types of clouds are considered. We find that in diffuse cloud regions, very strong radiation fields persists and hardly a few layers of surface species are formed. In translucent cloud regions with a moderate radiation field, significant number of layers would be produced and surface coverage is mainly dominated by photo-dissociation products such as, C, CH_3, CH_2D,OH and OD. In the intermediate dense cloud regions (having number density of total hydrogen nuclei in all forms ~2 × 10^4 cm^−3), water and methanol along with their deuterated derivatives are efficiently formed. For much higher density regions (~106 cm−3), water and methanol productions are suppressed but surface coverages of CO, CO_2, O_2 and O_3 are dramatically increased. We find a very high degree of fractionation of water and methanol. Observational results support a high fractionation of methanol but surprisingly water fractionation is found to be low. This is in contradiction with our model results indicating alternative routes for defractionation of water. Effects of various types of energy barriers are also studied. Moreover, we allow grain mantles to interact with various charged particles (such as H^+, Fe^+, S^+ and C^+) to study the stopping power and projected range of these charged particles on various target ices.

2015, MNRAS, 455, 540–551
DOI: 10.1093/mnras/stv2264
Full-text URL: http://mnras.oxfordjournals.org/content/455/1/540

Quantum Calculation of Inelastic CO Collisions with H. III. Rate Coefficients for Ro-vibrational Transitions

L. Song, N. Balakrishnan, K. M. Walker, P. C. Stancil, W. F. Thi, I. Kamp, A. van der Avoird, G. C. Groenenboom

We present calculated rate coefficients for ro-vibrational transitions of CO in collisions with H atoms for a gas temperature range of 10 K-3000 K, based on the recent three-dimensional ab initio H-CO interaction potential of Song et al (2013). Rate coefficients for ro-vibrational v=1, j=0-30 -> v'=0, j' transitions were obtained from scattering cross sections previously computed with the close-coupling method by Song et al (2015). Combining these with the rate coefficients for vibrational v=1-5 -> v' < v quenching obtained with the infinite-order sudden approximation, we propose a new extrapolation scheme that yields the rate coefficients for ro-vibrational v=2-5,j=0-30 -> v',j' de-excitation. Cross sections and rate coefficients for ro-vibrational v=2, j=0-30-> v'=1,j' transitions calculated with the close-coupling method confirm the effectiveness of this extrapolation scheme. Our calculated and extrapolated rates are very different from those that have been adopted in the modeling of many astrophysical environments. The current work provides the most comprehensive and accurate set of ro-vibrational de-excitation rate coefficients for the astrophysical modeling of the H-CO collision system. Application of the previously available and new data sets in astrophysical slab models shows that the line fluxes typically change by 20-70% in high temperature environments (800 K) with an H/H2 ratio of 1; larger changes occur for lower temperatures.

The Astrophysical Journal, 813, 96, (2015)
DOI: doi:10.1088/0004-637X/813/2/96
Full-text URL: http://arxiv.org/abs/1511.06648

Detectability of deuterated water in prestellar cores

D. Quénard, V. Taquet, C. Vastel, P. Caselli, and C. Ceccarelli

Water is an important molecule in the chemical and thermal balance of dense molecular gas, but knowing its history through-out the various stages of the star formation is a fundamental problem. Its molecular deuteration provides us with a crucial clue to its formation history. H2O has recently been detected for the first time towards the prestellar core L1544 with the Herschel Space Observatory with a high spectral resolution (HIFI instrument). Prestellar cores provide the original reservoir of material from which future planetary systems are built, but few observational constraints exist on the formation of water and none on its deuteration before the collapse starts and a protostar forms at the centre. We report on new APEX observations of the ground state 1,0,1-0,0,0 HDO transition at 464 GHz towards the prestellar core L1544. The line is undetected, and we present an extensive study of the conditions for its detectability in cold and dense cloud cores. The water and deuterated water abundances have been estimated using an advanced chemical model simplified for the limited number of reactions or processes that are active in cold regions (< 15 K). We use the LIME radiative transfer code to compute the expected intensity and profile of both H2O and HDO lines and compare them with the observations. We present several ad hoc profiles that best-fit the observations and compare the profiles with results from an astrochemical modelling, coupling gas phase and grain surface chemistry. Our comparison between observations, radiative transfer, and chemical modelling shows the limits of detectability for singly deuterated water, through the ground-state transitions 1,0,1-0,0,0 and 1,1,1-0,0,0 at 464.9 and 893.6 GHz, respectively, with both single-dish telescope and interferometric observations.

Accepted at A&A in November 2015
DOI: 10.1051/0004-6361/201527008
Full-text URL: http://arxiv.org/pdf/1511.03959v1.pdf

The C(3P) + NH3 Reaction in Interstellar Chemistry. II. Low Temperature Rate Constants and Modeling of NH, NH2, and

NH3 Abundances in Dense Interstellar Clouds

K. M. Hickson, J.-C. Loison, J. Bourgalais, M. Capron, S. D. Le Picard, F. Goulay and V. Wakelam

A continuous supersonic flow reactor has been used to measure rate constants for the C(3P) + NH3 reaction over the temperature range 50–296 K. C(3P) atoms were created by the pulsed laser photolysis of CBr4. The kinetics of the title reaction were followed directly by vacuum ultra-violet laser induced fluorescence of C(3P) loss and through H(2S) formation. The experiments show unambiguously that the reaction is rapid at 296 K, becoming faster at lower temperatures, reaching a value of (1.8 ± 0.2) × 10−10 cm3 molecule−1 s−1 at 50 K. As this reaction is not currently included in astrochemical networks, its influence on interstellar nitrogen hydride abundances is tested through a dense cloud model including gas–grain interactions. In particular, the effect of the ortho-to-para ratio of H2, which plays a crucial role in interstellar NH3 synthesis, is examined.

The Astrophysical Journal, 812:107 (8pp), 2015 October 20
DOI: 10.1088/0004-637X/812/2/107

Quantum Calculation of Inelastic CO Collisions with H. III. Rate Coefficients for Ro-vibrational Transitions

L. Song, N. Balakrishnana, K. M. Walker, P. C. Stancil. W. F. Thi, I. Kamp, A. van der Avoird, G. C. Groenenboom

We present calculated rate coefficients for ro-vibrational transitions of CO in collisions with H atoms for a gas temperature range of 10 K- 3000 K, based on the recent three-dimensional ab initio H-CO interaction potential of Song et al. Rate coefficients for ro-vibrational v=1,j=0-30 --> v'=0, j' transitions were obtained from scattering cross sections previously computed with the close-coupling (CC) method by Song et al. Combining these with the rate coefficients for vibrational v=1-5 --> v' < v quenching obtained with the infinite-order sudden approximation, we propose a new extrapolation scheme that yields the rate coefficients for ro-vibrational v=2-5, j=0-30 --> v',j' de-excitation. Cross sections and rate coefficients for ro-vibrational v=2, j=0-30--> v'=1,j' transitions calculated with the CC method confirm the effectiveness of this extrapolation scheme. Our calculated and extrapolated rates are very different from those that have been adopted in the modeling of many astrophysical environments. The current work provides the most comprehensive and accurate set of ro-vibrational de-excitation rate coefficients for the astrophysical modeling of the H-CO collision system. The application of the previously available and new data sets in astrophysical slab models shows that the line fluxes typically change by 20%-70% in high temperature environments (800 K) with an H/H2 ratio of 1; larger changes occur for lower temperatures.

2015 The Astrophysical Journal, 813, 96
DOI: doi:10.1088/0004-637X/813/2/96
Full-text URL: http://stacks.iop.org/0004-637X/813/i=2/a=96

H-atom addition and abstraction reactions in mixed CO, H2CO and CH3OH ices - an extended view on complex organic molecule formation

K.-J. Chuang; G. Fedoseev; S. Ioppolo; E.F. van Dishoeck; H. Linnartz

Complex organic molecules (COMs) have been observed not only in the hot cores surrounding low- and high-mass protostars, but also in cold dark clouds. Therefore, it is interesting to understand how such species can be formed without the presence of embedded energy sources. We present new laboratory experiments on the low-temperature solid state formation of three complex molecules – methyl formate (HC(O)OCH3), glycolaldehyde (HC(O)CH2OH) and ethylene glycol (H2C(OH)CH2OH) – through recombination of free radicals formed via H-atom addition and abstraction reactions at different stages in the CO→H2CO→CH3OH hydrogenation network at 15 K. The experiments extend previous CO hydrogenation studies and aim at resembling the physical–chemical conditions typical of the CO freeze-out stage in dark molecular clouds, when H2CO and CH3OH form by recombination of accreting CO molecules and H-atoms on ice grains. We confirm that H2CO, once formed through CO hydrogenation, not only yields CH3OH through ongoing H-atom addition reactions, but is also subject to H-atom-induced abstraction reactions, yielding CO again. In a similar way, H2CO is also formed in abstraction reactions involving CH3OH. The dominant methanol H-atom abstraction product is expected to be CH2OH, while H-atom additions to H2CO should at least partially proceed through CH3O intermediate radicals. The occurrence of H-atom abstraction reactions in ice mantles leads to more reactive intermediates (HCO, CH3O and CH2OH) than previously thought, when assuming sequential H-atom addition reactions only. This enhances the probability to form COMs through radical-radical recombination without the need of UV photolysis or cosmic rays as external triggers.

Monthly Notices of the Royal Astronomical Society, 2015, 455(2), 1702-1712
DOI: 10.1093/mnras/stv2288
Full-text URL: http://mnras.oxfordjournals.org/cgi/content/full/stv2288?ijkey=dURi0yNoojFmd3n&keytype=ref

Molecule survival in magnetized protostellar disk winds. II. Predicted H2O line profiles versus Herschel/HIFI observations

W. Yvart, S. Cabrit, G. Pineau des Forets, and J. Ferreira

We investigate whether the broad wings of H2O emission identified with Herschel towards low-mass Class 0 and Class 1 protostars may be consistent with an origin in a dusty MHD disk wind, and the constraints it would set on the underlying disk properties. We present synthetic H2O line profiles predictions for a typical MHD disk wind solution with various values of disk accretion rate, stellar mass, extension of the launching area, and view angle. We compare them in terms of line shapes and intensities with the HIFI profiles observed by the WISH Key Program. We find that a dusty MHD disk wind launched from 0.2--0.6 AU AU to 3--25 AU can reproduce to a remarkable degree the observed shapes and intensities of the broad H2O component, both in the fundamental 557 GHz line and in more excited lines. Such a model also readily reproduces the observed correlation of 557 GHz line luminosity with envelope density, if the infall rate at 1000 AU is 1--3 times the disk accretion rate in the wind ejection region. It is also compatible with the typical disk size and bolometric luminosity in the observed targets. However, the narrower line profiles in Class 1 sources suggest that MHD disk winds in these sources, if present, would have to be slower and/or less water rich than in Class 0 sources. In conclusion, MHD disk winds appear as a valid (though not unique) option to consider for the origin of the broad H2O component in low-mass protostars. ALMA appears ideally suited to further test this model by searching for resolved signatures of the warm and slow wide-angle molecular wind that would be predicted.

Accepted by A&A

DOI: http://dx.doi.org/10.1051/0004-6361/201525915
Full-text URL: http://www.aanda.org/articles/aa/pdf/forth/aa25915-15.pdf

Low-temperature chemistry between water and hydroxyl radicals: H/D isotopic effects

T. Lamberts, G. Fedoseev, F. Puletti, S. Ioppolo, H. M. Cuppen, H. Linnartz

Sets of systematic laboratory experiments are presented -- combining Ultra High Vacuum cryogenic and plasma-line deposition techniques -- that allow us to compare H/D isotopic effects in the reaction of H2O (D2O) ice with the hydroxyl radical OD (OH). The latter is known to play a key role as intermediate species in the solid-state formation of water on icy grains in space. The main finding of our work is that the reaction H2O + OD --> OH + HDO occurs and that this may affect the HDO/H2O abundances in space. The opposite reaction D2O + OH --> OD + HDO is much less effective, and also given the lower D2O abundances in space not expected to be of astronomical relevance. The experimental results are extended to the other four possible reactions between hydroxyl and water isotopes and are subsequently used as input for Kinetic Monte Carlo simulations. This way we interpret our findings in an astronomical context, qualitatively testing the influence of the reaction rates.

MNRAS (January 01, 2016) 455 (1): 634-641
DOI: 10.1093/mnras/stv2305
Full-text URL: http://mnras.oxfordjournals.org/content/455/1/634

Segregation of O2 and CO on the surface of dust grains determines the desorption energy of O2

J. A. Noble, S. Diana and F. Dulieu

Selective depletion towards pre-stellar cores is still not understood. The exchange between the solid and gas phases is central to this mystery. The aim of this paper is to show that the thermal desorption of O2 and CO from a submonolayer mixture is greatly affected by the composition of the initial surface population. We have performed thermally programmed desorption (TPD) experiments on various submonolayer mixtures of O2 and CO. Pure O2 and CO exhibit almost the same desorption behaviour, but their desorption differs strongly when mixed. Pure O2 is slightly less volatile than CO, while in mixtures, O2 desorbs earlier than CO. We analyse our data using a desorption law linking competition for binding sites with desorption, based on the assumption that the binding energy distribution of both molecules is the same. We apply Fermi–Dirac statistics in order to calculate the adsorption site population distribution, and derive the desorbing fluxes. Despite its simplicity, the model reproduces the observed desorption profiles, indicating that competition for adsorption sites is the reason for lower temperature O2 desorption. CO molecules push-out or ‘dislodge’ O2 molecules from the most favourable binding sites, ultimately forcing their early desorption. It is crucial to consider the surface coverage of dust grains in any description of desorption. Competition for access to binding sites results in some important discrepancies between similar kinds of molecules, such as CO and O2. This is an important phenomenon to be investigated in order to develop a better understanding of the apparently selective depletion observed in dark molecular clouds.

2015, MNRAS, 454, 2636–2646
DOI: 10.1093/mnras/stv2157
Full-text URL: http://mnras.oxfordjournals.org/content/454/3/2636.abstract

The peculiar distribution of CH3CN in IRC+10216 seen by ALMA

M. Agundez, J. Cernicharo, G. Quintana-Lacaci, L. Velilla Prieto, A. Castro-Carrizo, N. Marcelino, M. Guelin

IRC+10216 is a circumstellar envelope around a carbon-rich evolved star which contains a large variety of molecules. According to interferometric observations, molecules are distributed either concentrated around the central star or as a hollow shell with a radius of 15 arcsec. We present ALMA Cycle 0 band 6 observations of the J=14–13 rotational transition of CH3CN in IRC+10216, obtained with an angular resolution of 0.76x0.61 arcsec. The bulk of the emission is distributed as a hollow shell located at just 2 arcsec from the star, with a void of emission in the central region up to a radius of 1 arcsec. This spatial distribution is markedly different from those found to date in this source for other molecules. Our analysis indicates that methyl cyanide is not formed in either the stellar photosphere or far in the outer envelope, but at radial distances as short as 1-2 arcsec, reaching a maximum abundance of 0.02 molecules cm-3 at 2 arcsec from the star. Standard chemical models of IRC+10216 predict that the bulk of CH3CN molecules should be present at a radius of 15 arcsec where other species such as polyyne radicals and cyanopolyynes are observed, with an additional inner component within 1 arcsec from the star. The non-uniform structure of the circumstellar envelope and grain surface processes are discussed as possible causes of the peculiar distribution of methyl cyanide in IRC+10216.

The Astrophysical Journal, in press. arXiv:1506.06951
Full-text URL: http://arxiv.org/abs/1506.06951

Excited vibrational level rotational constants for SiC2: A sensitive molecular diagnostic for astrophysical conditions

Ryan C. Fortenberry, Timothy J. Lee, Holger S.P. Müller

Silacyclopropynylidene, SiC2, is a known and highly abundant circumstellar molecule. Its spectrum has been established as a major component of lines observed toward the carbon-rich star IRC +10216 (CW Leonis). It has been detected in its low-lying v3=1v3=1 and 2 vibrational states as well as in various isotopic compositions. Increasing sensitivity and spatial resolution will enable many more emission or absorption lines to be detected. In order to detect new molecular species, unassigned lines of known species must be identified. This work uses established ab initio quartic force fields to produce data necessary for this classification of lines related to SiC2. Agreement between the theoretical vibrational frequencies and known rotational and spectroscopic constants is quite good, as good as 5 cm−1−1 and 3 MHz, respectively in some cases. In addition, experimentally unknown vibrational frequencies and rotational constants are provided for the first overtones and combination bands in addition to 3ν3, the second overtone of the low-lying antisymmetric stretch/carbide rotation mode. Frequencies of v3=3v3=3 low-J rotational transitions of the main isotopic species are also estimated from published data for v3 ≤ 2. Further, we determine rotational and centrifugal distortion parameters for which in most cases vibrational effects due to the ν3 mode were reduced to first, and in several cases also to second order. These values may approximate equilibrium values better than the ground state values. The data produced herein will aid in the experimental and observational characterization of this known astromolecule in order to identify some of the unassigned lines for a known entity.

Molecular Astrophysics - Article in Press

DOI: doi:10.1016/j.molap.2015.07.001
Full-text URL: http://www.sciencedirect.com/science/article/pii/S2405675815300038

The C(3P) + NH3 Reaction in Interstellar Chemistry. I. Investigation of the Product Formation Channels

J. Bourgalais, M. Capron, R. K. A. Kailasanathan, D. L. Osborn, K. M. Hickson, J.-C. Loison, V. Wakelam, F. Goulay and S. D. Le Picard

The product formation channels of ground state carbon atoms, C(3P), reacting with ammonia, NH3, have been investigated using two complementary experiments and electronic structure calculations. Reaction products are detected in a gas flow tube experiment (330 K, 4 Torr) using tunable vacuum-ultraviolet (VUV) photoionization coupled with time of flight mass spectrometry. Temporal profiles of the species formed and photoionization spectra are used to identify primary products of the C + NH3 reaction. In addition, H-atom formation is monitored by VUV laser induced fluorescence (LIF) from room temperature to 50 K in a supersonic gas flow generated by the Laval nozzle technique. Electronic structure calculations are performed to derive intermediates, transition states, and complexes formed along the reaction coordinate. The combination of photoionization and LIF experiments supported by theoretical calculations indicate that in the temperature and pressure range investigated, the H + H2CN production channel represents 100% of the product yield for this reaction. Kinetics measurements of the title reaction down to 50 K and the effect of the new rate constants on interstellar nitrogen hydride abundances using a model of dense interstellar clouds are reported in Paper II.

The Astrophysical Journal, 812:106 (12pp), 2015 October 20
DOI: 10.1088/0004-637X/812/2/106

Exploring Molecular Complexity with ALMA (EMoCA): Deuterated complex organic molecules in Sagittarius B2(N2)

A. Belloche (MPIfR Bonn), H. S. P. Müller (Univ. of Cologne), R.~T. Garrod (Univ. of Virginia), K.~M. Menten (MPIfR Bonn)

Deuteration is a powerful tracer of the history of the cold prestellar phase in star forming regions. Apart from methanol, little is known about deuterium fractionation of complex organic molecules in the interstellar medium, especially in high mass star forming regions. We use a spectral line survey performed with ALMA to search for deuterated complex organic molecules toward the hot molecular core Sgr B2(N2). Population diagrams and integrated intensity maps are constructed to fit rotational temperatures and emission sizes for each molecule. Column densities are derived by modelling the full spectrum under the LTE assumption. The results are compared to predictions of two astrochemical models that treat the deuteration process. We report the detection of CH2DCN toward Sgr B2(N2) with a deuteration level of 0.4%, and tentative detections of CH2DOH, CH2DCH2CN, the chiral molecule CH3CHDCN, and DC3N with levels in the range 0.05%-0.12%. A stringent deuteration upper limit is obtained for CH3OD (<0.07%). Upper limits in the range 0.5-1.8% are derived for the three deuterated isotopologues of vinyl cyanide, the four deuterated species of ethanol, and CH2DOCHO. Ethyl cyanide is less deuterated than methyl cyanide by at least a factor five. Except for methyl cyanide, the measured deuteration levels lie at least a factor four below the predictions of current astrochemical models. The deuteration levels in Sgr B2(N2) are also lower than in Orion KL by a factor of a few up to a factor ten. The discrepancy between the deuteration levels of Sgr B2(N2) and the predictions of chemical models, and the difference between Sgr B2(N2) and Orion KL may both be

due to the higher kinetic temperatures that characterize the Galactic Center region compared to nearby clouds. Alternatively, they may result from a lower overall abundance of deuterium itself in the Galactic Center region by up to a factor ten.

accepted for publication in Astronomy & Astrophysics. The abstract has been shortened.
DOI: 10.1051/0004-6361/201527268
Full-text URL: http://xxx.lanl.gov/abs/1511.05721

Chemical features in the circumnuclear disk of the Galactic center

N. Harada, D. Riquelme, S. Viti, I. Jimenez-Serra, M. A. Requena-Torres, K. M. Menten, S. Martin, R. Aladro, J. Martin-Pintado and S. Hochguertel

The circumnuclear disk (CND) of the Galactic Center is exposed to many energetic phenomena coming from the supermassive black hole Sgr A* and stellar activities. These energetic activities can affect the chemical composition in the CND by the interaction with UV-photons, cosmic-rays, X-rays, and shock waves. We aim to constrain the physical conditions present in the CND by chemical modeling of observed molecular species detected towards it. We analyzed a selected set of molecular line data taken toward a position in the southwest lobe of the CND with the IRAM 30m and APEX 12-meter telescopes and derived the column density of each molecule using a large velocity gradient (LVG) analysis. The determined chemical composition is compared with a time-dependent gas-grain chemical model based on the UCL_CHEM code that includes the effects of shock waves with varying physical parameters. Molecules such as CO, HCN, HCO+, HNC, CS, SO, SiO, NO, CN, H2CO, HC3N, N2H+ and H3O+ are detected and their column densities are obtained. Total hydrogen densities obtained from LVG analysis range between 2×10^4 and 1×10^6 cm−3 and most species indicate values around several ×105cm−3, which are lower than values corresponding to the Roche limit, which shows that the CND is tidally unstable. The chemical models show good agreement with the observations in cases where the density is ~10^4 cm−3, the cosmic-ray ionization rate is high, >10−15 s−1, or shocks with velocities >40km s−1 have occurred. Comparison of models and observations favors a scenario where the cosmic-ray ionization rate in the CND is high, but precise effects of other factors such as shocks, density structures, UV-photons and X-rays from the Sgr A* must be examined with higher spatial resolution data.

Accepted for publication in A&A
DOI: 10.1051/0004-6361/201526994
Full-text URL: http://dx.doi.org/10.1051/0004-6361/201526994

Announcements

Cloudy workshop, 2016 June 20-24, Shandong University, Weihai, China

Registration is now open for the 2016 Cloudy workshop. It will be held June 20-24, Shandong University, Weihai, China Cloudy simulates the microphysics of matter exposed to ionizing radiation. It calculates the atomic physics, chemistry, radiation transport, and dynamics problems simultaneously and self consistently, building from a foundation of individual atomic and molecular processes. The result is a prediction of the conditions in the material and its observed spectrum. The workshop will cover observation, theory, and application of Cloudy to a wide variety of astronomical environments. This includes the theory of diffuse non-LTE matter and quantitative spectroscopy, the science of using spectra to make physical measurements. We will use Cloudy to simulate such objects as AGB stars, Active Galactic Nuclei, Starburst galaxies, and the intergalactic medium. The sessions will consist of a mix of textbook study, using Osterbrock & Ferland, Astrophysics of Gaseous Nebulae and Active Galactic Nuclei, application of the spectral-simulation code Cloudy to a variety of astrophysical problems, and projects organized by the participants. No prior experience with Cloudy is assumed. There is no registration fee and financial support is not available. The site http://cloud9.pa.uky.edu/~gary/cloudy/CloudySummerSchool/ about Cloudy and the workshop. Local details and instructions for registration are on http://cloudy2016.csp.escience.cn/dct/page/1 Shandong University (SDU) is a key comprehensive university with a long history, a variety of disciplines, strong academic strength, and distinctive characteristics. Its main body, Shandong Imperial College (Shandong Da Xue Tang) established in 1901, was the second national university in China, only after the Imperial University of Peking. Shandong University at Weihai, as one of seven campuses of SDU, was established in 1984. Weihai (□□) is the easternmost prefecture-level city of Shandong province,China. Weihai is China’s well-known coastal tourist and leisure resorts and the city of natural hot springs.

EXES postdoc

Dr. Matthew Richter of UC Davis is seeking for a postdoc to work with the Echelon-cross-echelle Spectrograph (EXES) on SOFIA. The high spectral resolution at mid-IR wavelengths unavailable from the ground make EXES an exciting new tool for astrochemistry. See the AAS job ad at http://jobregister.aas.org/job_view?JobID=52471 or contact mjrichter@ucdavis.edu for information.

SUMMER SCHOOL, 29/8-9/9 2016 Grenoble (France)
“ASTROCHEMISTRY: FROM SPACE TO EARTH"

AIMS OF THE SCHOOL Astrochemistry is the field that studies how interstellar atoms combine into molecules, in the gas phase and on the surfaces of the interstellar grains. It is the interplay between these two processes that leads to the rich chemistry observed in space, at galactic and extragalactic scales. To extract all the information from the astronomical observations of molecules and exploit them at the best is, however, a truly multidisciplinary endeavor. It requires complementary approaches (observations, modeling, laboratory, theory) to be combined with accurate knowledge in several fields: astrophysics, chemistry, atomic and molecular physics, solid state physics. This implies different communities to work together and to learn to understand each other, whose languages are often very different. The school aims to offer a series of courses on all the above interdisciplinary aspects of Astrochemistry, from the basic concepts to the state-of-the-art research in each of them. The scope is to train PhD students and young researchers of the different communities that make up Astrochemistry and foster the collaboration/networking among them. PRATICAL INFORMATION The school is organized in two weeks of lectures complemented with extensive “hands-on” activities, where students will have the occasion to apply the concepts to real cases. The school will be held at IPAG in Grenoble (France), during the period 29/8-9/9 2016. The participation will be restricted to 30 students. Submission for application will be open at the end of November. A financial support to students is possible. SOC: C.Ceccarelli (chair), G.Nyman (co-chair), N. Balucani, A.Bergeat, S.Jerosimic, D.Talbi, P.Theulé LOC: P.Hily-Blant (chair), B.Bishop, C.Favre, C.Kahane, B.Lefloch, A.Faure The School is co-organized by the Institut de Planétologie de Grenoble (IPAG), the EU COST Action CM1401, and the French National Project PCMI.