AstroChemical Newsletter #10

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Abstracts

Binding Energy of Molecules on Water Ice: Laboratory Measurements and Modeling

J. He, K. Acharyya, G. Vidali

We measured the binding energy of N2, CO, O2, CH4, and CO2 on non-porous (compact) amorphous solid water (np-ASW), of N2 and CO on porous amorphous solid water (p-ASW), and of NH3 on crystalline water ice. We were able to measure binding energies down to a fraction of 1% of a layer, thus making these measurements more appropriate for astrochemistry than the existing values. We found that CO2 forms clusters on np-ASW surface even at very low coverages. The binding energies of N2, CO, O2, and CH4 decrease with coverage in the submonolayer regime. Their values at the low coverage limit are much higher than what is commonly used in gas-grain models. An empirical formula was used to describe the coverage dependence of the binding energies. We used the newly determined binding energy distributions in a simulation of gas-grain chemistry for cold cloud and hot core models. We found that owing to the higher value of desorption energy in the sub-monlayer regime a fraction of all these ices stays much longer and up to higher temperature on the grain surface compared to the single value energies currently used in the astrochemical models.

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The ionization rates of galactic nuclei and disks from Herschel/HIFI observations of water and its associated ions

Floris van der Tak (SRON / U Groningen), Axel Weiss, Lijie Liu, Rolf Guesten (MPIfR Bonn)

(Abridged) We present Herschel/HIFI spectra of the H2O 1113 GHz and H2O+ 1115 GHz lines toward five nearby prototypical starburst/AGN systems, and OH+ 971 GHz spectra toward three of these. The beam size of 20" corresponds to resolutions between 0.35 and 7 kpc. The observed line profiles range from pure absorption (NGC 4945, M82) to P-Cygni indicating outflow (NGC 253, Arp 220) and inverse P-Cygni indicating infall (Cen A). The similarity of the H2O, OH+, and H2O+ profiles to each other and to HI indicates that diffuse and dense gas phases are well mixed. We estimate column densities assuming negligible excitation (for absorption features) and using a non-LTE model (for emission features), adopting calculated collision data for H2O and OH+, and rough estimates for H2O+. Column densities range from ~1e13 to ~1e15 cm-2 for each species, and are similar between absorption and emission components, indicating that the nuclear region does not contribute much to the

emission in these ground-state lines. The N(H2O)/N(H2O+) ratios of 1.4-5.6 indicate an origin of the lines in diffuse gas, and the N(OH+)/N(H2O+) ratios of 1.6-3.1 indicate a low H2 fraction (~11%) in the gas. Adopting recent Galactic values for the average gas density and the ionization efficiency, we find ionization rates for our sample galaxies of ~3e-16 s-1 which are similar to the value for the Galactic disk, but ~10x below that of the Galactic Center and ~100x below estimates for AGN from excited-state H3O+ lines. We conclude that the ground-state lines of water and its associated ions probe primarily non-nuclear gas in the disks of these centrally active galaxies. Our data thus provide evidence for a decrease in ionization rate by a factor of ~10 from the nuclei to the disks of galaxies, as found before for the Milky Way.

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ALMA-resolved salt emission traces the chemical footprint and inner wind morphology of VY CMa

L. Decin, A. M. S. Richards, T. J. Millar, A. Baudry, E. De Beck, W. Homan, N. Smith, M. Van de Sande, and C. Walsh

We aim to study the inner-wind structure (R<250 Rstar) of the well-known red supergiant VY CMa. We analyse high spatial resolution (~0".24x0".13) ALMA Science Verification (SV) data in band 7 in which four thermal emission lines of gaseous sodium chloride (NaCl) are present at high signal-to-noise ratio. For the first time, the NaCl emission in the inner wind region of VY CMa is spatially resolved. The ALMA observations reveal the contribution of up to four different spatial regions. The NaCl emission pattern is different compared to the dust continuum and TiO2 emission already analysed from the ALMA SV data. The emission can be reconciled with an axisymmetric geometry, where the lower density polar/rotation axis has a position angle of ~50 degrees measured from north to east. However, this picture can not capture the full morphological diversity, and discrete mass ejection events need to be invoked to explain localized higher-density regions. The velocity traced by the gaseous NaCl line profiles is significantly lower than the average wind terminal velocity, and much slower than some of the fastest mass ejections, signalling a wide range of characteristic speeds for the mass loss. Gaseous NaCl is detected far beyond the main dust condensation region. Realising the refractory nature of this metal halide, this hints at a chemical process preventing all NaCl from condensing onto dust grains. We show that in the case of the ratio of the surface binding temperature to the grain temperature being ~50, only some 10% of NaCl remains in gaseous form, while for lower values of this ratio thermal desorption efficiently evaporates NaCl. Photodesorption by stellar photons seems not to be a viable explanation for the detection of gaseous NaCl at 220 Rstar from the central star, and instead, we propose shock-induced sputtering driven by localized mass ejection events as alternative.

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Insight into the molecular composition of laboratory organic residues produced from interstellar/pre-cometary ice analogues using very high resolution mass spectrometry

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Experimental simulations in the laboratory may provide important information about the chemical evolution occurring in various astrophysical objects such as extraterrestrial ices. Interstellar or (pre)cometary ice analogues made of H2O, CH3OH, and NH3 at 77 K, when subjected to an energetic process (VUV photons, electrons or ions) and then warmed-up to room temperature, lead, in the laboratory, to the formation of an organic residue. In this paper we expand our previous analysis of the residues in order to obtain a better insight into their molecular content. Data analyses show that three different chemical groups are present in the residue in the negative electrospray ionization (ESI) mode: CHN, CHO and CHNO- whereas only two groups are detected in the positive ESI mode: CHN and CHNO. In both cases, the CHNO group is the most abundant. The application of specific data treatment shows that residue mainly contains aliphatic linear molecules or cyclic structures connected to unsaturated chemical functions such as esters, carboxylic acids, amides or aldehydes. In lower abundances, some molecules do present aromatic structures. The comparison of our residue with organic compounds detected in the Murchison meteorite gives an interesting match, which suggests that laboratory simulation of interstellar ice chemistry is relevant to understand astrophysical organic matter evolution.

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Chemical differentiation in a prestellar core traces non-uniform illumination

Silvia Spezzano, Luca Bizzocchi, Paola Caselli, Jorma Harju and Sandra Bruenken

Dense cloud cores present chemical differentiation due to the different distribution of C-bearing and N-bearing molecules, the latter being less affected by freeze-out onto dust grains. In this letter we show that two C-bearing molecules, CH3OH and c-C3H2, present a strikingly different (complementary) morphology while showing the same kinematics toward the prestellar core L1544. After comparing their distribution with large scale H2 column density N(H2) map from the Herschel satellite, we find that these two molecules trace different environmental conditions in the surrounding of L1544: the c-C3H2 distribution peaks close to the southern part of the core, where the surrounding molecular cloud has a N(H2) sharp edge, while CH3OH mainly traces the northern part of the core, where N(H2) presents a shallower tail. We conclude that this is evidence of chemical differentiation driven by different amount of illumination from the interstellar radiation field: in the South, photochemistry maintains more C atoms in the gas phase allowing carbon chain (such as c-C3H2) production; in the North, C is mainly locked in CO and methanol traces the zone where CO starts to freeze out significantly. During the process of cloud contraction, different gas and ice compositions are thus expected to mix toward the central regions of the core, where a potential Solar-type system will form. An alternative view on carbon-chain chemistry in star-forming regions is also provided.

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Cometary ices in forming protoplanetary disc midplanes

Maria N. Drozdovskaya, Catherine Walsh, Ewine F. van Dishoeck, Kenji Furuya, Ulysse Marboeuf, Amaury Thiabaud, Daniel Harsono and Ruud Visser

Low-mass protostars are the extrasolar analogues of the natal Solar System. Sophisticated physicochemical models are used to simulate the formation of two protoplanetary discs from the initial prestellar phase, one dominated by viscous spreading and the other by pure infall. The results show that the volatile prestellar fingerprint is modified by the chemistry en route into the disc. This holds relatively independent of initial abundances and chemical parameters: physical conditions are more important. The amount of CO2 increases via the grain-surface reaction of OH with CO, which is enhanced by photodissociation of H2O ice. Complex organic molecules are produced during transport through the envelope at the expense of CH3OH ice. Their abundances can be comparable to that of methanol ice (few % of water ice) at large disc radii (R > 30 AU). Current Class II disc models may be underestimating the complex organic content. Planet population synthesis models may underestimate the amount of CO2 and overestimate CH3OH ices in planetesimals by disregarding chemical processing between the cloud and disc phases. The overall C/O and C/N ratios differ between the gas and solid phases. The two ice ratios show little variation beyond the inner 10 AU and both are nearly solar in the case of pure infall, but both are sub-solar when viscous spreading dominates. Chemistry in the protostellar envelope en route to the protoplanetary disc sets the initial volatile and prebiotically-significant content of icy planetesimals and cometary bodies. Comets are thus potentially reflecting the provenances of the midplane ices in the Solar Nebula.

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Modeling the role of electron attachment rates on column density ratios for CnH-/CnH (n=4,6,8) in dense molecular clouds

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(abridged) The fairly recent detection of a variety of anions in the Interstellar Molecular Clouds have underlined the importance of realistically modeling the processes governing their abundance. To this aim, our earlier calculations for the radiative electron attachment (REA) rates for C4H-, C6H-, and C8H- are employed to generate the corresponding column density ratios of anion/neutral (A/N) relative abundances. The latter are then compared with those obtained from observational measurements. The calculations involved the time-dependent solutions of a large network of chemical processes over an extended time interval and included a series of runs in which the values of REA rates were repeatedly scaled. Macroscopic parameters for the clouds' modeling were also varied to cover a broad range of physical environments. It was found that, within the range and quality of the processes included in the present network,and selected from state-of-the-art astrophysical databases, the REA values required to match the observed A/N ratios needed to be reduced by orders of magnitude for C4H- case, while the same rates for C6H- and C8H- only needed to be scaled by much smaller factors. The results suggest that the generally proposed formation of interstellar anions by REA mechanism is overestimated by current models for the C4H- case, for which is likely to be an inefficient path to formation . This path is thus providing a rather marginal contribution to the observed abundances of C4H-, the latter being more likely to originate from other chemical processes in the network, as

we discuss in some detail in the present work.Possible physical reasons for the much smaller differences against observations found instead for the values of the (A/N) ratios in two other, longer members of the series are put forward and analyzed within the evolutionary modeling discussed in the present work.

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Combined infrared and Raman study of solid CO

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

Knowledge about the composition and structure of interstellar ices is mainly based on the comparison between astronomical and laboratory spectra of astrophysical ice analogues. Carbon monoxide is one of the main components of the icy mantles of dust grains in the interstellar medium. Because of its relevance, several authors have studied the spectral properties of solid CO both pure and in mixtures. The aim of this work is to study the profile (shape, width, peak position) of the solid CO band centered at about 2140 cm-1 at low temperature, during warm up, and after ion irradiation to search for a structural variation of the ice sample. We also report on the appearance of the longitudinal optical-transverse optical (LO-TO) splitting in the infrared spectra of CO films to understand if this phenomenon can be related to a phase change. We studied the profile of the 2140 cm-1 band of solid CO by means of infrared and Raman spectroscopy. We used a free web interface that we developed that allows us to calculate the refractive index of the sample to measure the thickness of the film. The profile of the fundamental band of solid CO obtained with infrared and Raman spectroscopy does not show any relevant modification after warm up or ion bombardment in the dose range investigated. We explain that the LO-TO splitting is not connected to a structural variation of the film. Ion irradiation causes the formation of new molecular species. Raman spectroscopy allowed us to detect, among other bands, a band centered at 1817 cm -1 that has been attributed to the infrared inactive species C2 and a band centered at 1767 cm-1 that remains unidentified.

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Announcements

NANOCOSMOS post-doctoral position at the Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC, Madrid, Spain) in the field of laboratory astrophysics and surface science

NANOCOSMOS (“Gas and dust from the stars to the laboratory: exploring the Nanocosmos”) is an ERC-funded project through the IDEAS program (Synergy Grant call) under the FP7. Nanocosmos tries to unveil how dust is formed in the inner part of the atmospheres of Asymptotic Giant Branch stars (AGB stars) by taking advantage of the new observational capabilities provided by the ALMA radiointerferometer and a novel top-level ultra-high vacuum facility, called the Stardust machine, fully designed and developed at the Instituto de Ciencia de Materiales de Madrid. The Stardust machine will simulate the various processes that dust and gas ejected from AGBs undergoes as it travels from the star photosphere into the outer shells of its circumstellar envelope, as well as analyse the dust-formed properties using earthly surface science based techniques. We are seeking a senior post-doctoral researcher to work on: “Simulation

experiments on the Stardust machine". The candidate should have a strong expertise in Laboratory Astrophysics, gas and solid-phase chemistry. The knowledge of surface science characterization techniques and synthesis of nanoparticles is desirable. A good record of publications in peer-reviewed journals is a strong asset. Also the knowledge on physics and chemical modelling will also be an advantage. The selection is primarily based on scientific excellence in the field of Laboratory Astrophysics. If you are interested in this position, please submit your CV together with a motivation letter and a recommendation letter, ALL IN ONE SINGLE PDF FILE, at the latest by the 15th of October, to: Prof. J. Cernicharo / Prof. J. A. Martín Gago jose.cernicharo at csic.es / gago at icmm.csic.es Instituto de Ciencia de Materiales de Madrid (CSIC) Sor Juana Inés de la Cruz 3, 28049 Cantoblanco (Madrid, Spain)

Nature Astronomy is now open for submissions.

Nature Astronomy is a truly multidisciplinary journal launching in January 2017. It will represent — and foster closer interaction between — all of the key astronomy-relevant disciplines. As a Nature Research journal, it will publish the most significant research, review and comment at the cutting edge of astronomy, astrophysics, cosmology and planetary science. Nature Astronomy will offer a range of content types — including original research, Review Articles, Perspectives, Commentaries, News & Views and Research Highlights — to explore topical issues as well as showcasing significant advances in the field. Publication in Nature Astronomy is free of charge, and its publication policy allows the posting of submitted manuscripts on preprint servers, and the self-archiving of the published versions of papers six months after publication. Please visit the Nature Astronomy website for more information and to submit a manuscript: www.nature.com/natastron

IAEA Technical Meeting, 19-21 December 2016 in Vienna, on Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications

The IAEA Atomic and Molecular Data Unit (Division of Physical and Chemical Sciences) is organizing a Technical Meeting on Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications to be held Monday-Wednesday 19-21 December 2016 at IAEA Headquarters in Vienna, Austria. https://www-amdis.iaea.org/meetings/UQ2016/ The deadline for submission of one-page abstracts is Monday 15 August 2016. With all the Christmas markets Vienna should be quite attractive at the time of the meeting. The meeting is intended to bring together leading theoretical and experimental atomic and molecular (A+M) physicists with plasma physics users of A+M data to discuss verification, validation and uncertainty quantification (VVUQ) of computer simulations for A+M processes in plasma. We are interested in benchmark calculations and experiments, uncertainty assessments for calculated data, and calculations of uncertainty propagation from primary A+M calculations through plasma simulations. The meeting is also intended to enhance contacts between the involved communities and to help define priorities for further work on A+M data for fusion and other plasma applications. Our A+M Data Unit has a special interest in encouraging benchmark experiments to support VVUQ for calculated A+M data that is relevant for fusion and other plasma applications. Invited talks and other contributions at the meeting will support discussions in the following areas. • Prioritization of A+M data needs for fusion applications. • Experimental methods and systems to benchmark theoretical A+M data. • Target uncertainties of A+M data for fusion applications. • Uncertainty quantification methods for theoretical A+M data. • Network of A+M physicists doing benchmark experiments and computations. Among other things the meeting will identify the most important data needs for fusion applications, decide what can be done to benchmark those data and

formulate a plan of action among experimental and theoretical A+M physicists to carry out this benchmarking and perform the associated uncertainty assessment. Questions to be addressed include: • How can benchmarking measurements be organized taking into account the most recent developments in the experimental as well as theoretical areas? • How can detailed measurements of the reaction dynamics, as benchmarks for theory, help to improve reliability of theoretical calculations for a given collision system? The discussions should lead to specific proposals for measurements to set new benchmarks for prioritized data. These measurements will obviously be very difficult in some cases, but they will set the standard. Along with the discussions about new benchmark experiments there will be discussions and proposals about suitable theoretical methods to compute these data, and how and by whom this can be done. The calculations should be accompanied by a full discussion of the inherent uncertainties.