AstroChemical Newsletter #19

May 2017

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Abstracts

Effects of Grain Growth on Molecular Abundances in Young Stellar Objects

N. Harada, Y. Hasegawa, Y. Aikawa, H. Hirashita, H. B. Liu, N. Hirano

Recent observations suggested that the growth of dust grains may have already occurred in class 0/I young stellar objects (YSOs). Since chemical reactions on dust grain surfaces are important in determining molecular abundances, the dust size growth may affect chemical compositions in YSOs significantly. In this work, we aim to determine how grain growth affects chemical abundances. We use a time-dependent gas-grain chemical model for a star-forming core to calculate the gas-phase and grain-surface chemical abundances with variation of surface areas of grains to imitate grain growth. We also perform parameter studies in which the initial molecular abundances vary. Our results show that a smaller extent of the surface areas caused by grain growth changes the dominant form of sulfur-bearing molecules by decreasing H_2S abundances and increasing SO and/or SO_2 abundances. We also find that complex organic molecules such as CH_3CN decrease in abundances with larger grain sizes, while the abundance of other species such as CH_3OCH_3 is dependent on other parameters such as the initial conditions. Comparisons with observations of a class 0 protostar, IRAS 16293-2422, indicate that the observed abundance ratios between sulfur-bearing molecules H_2S, SO, and SO_2 can be reproduced very well when dust grains grow to a maximum grain size of a max = 10–100 μm.

Exploring molecular complexity with ALMA (EMoCA): Detection of three new hot cores in Sagittarius B2(N)

M. Bonfand, A. Belloche, K. M. Menten, R. T. Garrod, H. S. P. Mueller

The SgrB2 molecular cloud contains several sites forming high-mass stars. SgrB2(N) is one of its main centers of activity. It hosts several compact and UCHII regions, as well as two known hot molecular cores (SgrB2(N1) and SgrB2(N2)), where complex organic molecules are detected. Our goal is to use the high sensitivity of ALMA to characterize the hot core population in SgrB2(N) and shed a new light on the star formation process. We use a complete 3 mm spectral line survey conducted with ALMA to search for faint hot cores in SgrB2(N). We report the discovery of three new hot cores that we call SgrB2(N3), SgrB2(N4), and SgrB2(N5). The three sources are associated with class II methanol masers, well known tracers of high-mass star formation, and SgrB2(N5) also with a UCHII region. The chemical composition of the sources and the column densities are derived by modelling the whole spectra under the assumption of LTE. The H_2 column densities are computed from ALMA and SMA continuum emission maps. The H_2 column densities of these new hot cores are found to be 16 up to 36 times lower than the one of the main hot core Sgr B2(N1). Their spectra have spectral line densities of 11 up to 31 emission lines per GHz, assigned to 22-25 molecules. We derive rotational temperatures around 140-180 K for the three new hot cores and mean source sizes of 0.4 for SgrB2(N3) and 1.0 for SgrB2(N4) and SgrB2(N5). SgrB2(N3) and SgrB2(N5) show high velocity wing emission in typical outflow tracers, with a bipolar morphology in their integrated intensity maps suggesting the presence of an outflow, like in SgrB2(N1). The associations of the hot cores with class II methanol masers, outflows, and/or UCHII regions tentatively suggest the following age sequence: SgrB2(N4), SgrB2(N3), SgrB2(N5), SgrB2(N1). The status of SgrB2(N2) is unclear. It may contain two distinct sources, a UCHII region and a very young hot core.

Dynamics of the O + H2+ → OH+ + H, OH + H+ proton and hydrogen atom transfer reactions on the two lowest potential energy surfaces

R. Martínez, M. Paniagua, J. Mayneris-Perxachs, P. Gamallo, M. González

The dynamics of the title reaction was studied using mainly the quasiclassical trajectory (QCT) method on the ground 12A'' (OH+ channel) and first excited 12A' (OH channel) potential energy surfaces (PESs) employing ab initio analytical representations of the PESs developed by us. Both PESs correspond to exoergic reactions, are barrierless and present a deep minimum along the minimum energy path (MEP). Some extra calculations (cross sections) were also performed with the time dependent quantum real wave packet method at the centrifugal sudden level (RWP-CS method). A broad set of properties as a function of collision energy (Ecol ≤ 0.5 eV) was considered using the QCT method: cross sections, average

fractions of energy, product rovibrational distributions, two- and three-vector properties, and the microscopic mechanisms analyzing their influence on the dynamics. The proton transfer channel dominates the reactivity of the system and significant differences between the two reaction channels are found for the vibrational distributions and microscopic mechanisms. The results were interpreted according to the properties of the ground and excited PESs. Moreover, the QCT and RWP-CS cross sections are in rather good agreement for both reaction channels. We hope that this study will encourage the experimentalists to investigate the dynamics of this interesting but scarcely studied system, whose two lowest PESs include the ground and first excited electronic states of the H2O+ cation.

Hydrogen atom mobility, kinetic isotope effects and tunneling on interstellar ices (Ih and ASW)
Bethmini Senevirathne, Stefan Andersson, Francois Dulieu, Gunnar Nyman

Transitions of a single H atom between local minima on the surfaces of crystalline ice (Ih) and amorphous solid water (ASW) are studied theoretically in the temperature range 4–25 K. Binding energies, barrier heights, transition rate constants and the kinetic isotope effect (KIE) with and without tunneling are calculated. Harmonic transition state theory is used to obtain the transition rate constants and tunneling is treated with the Wigner tunneling correction, Eckart barrier correction and harmonic quantum transition state theory (HQTST). The classical binding energies are smaller on Ih (<47 meV) than on ASW (<89 meV). Also the classical barrier heights are smaller on Ih (<14 meV) than on ASW (<69 meV) and distributed over a range of energies, in line with previous experimental observations. Similarly the vibrationally adiabatic ground state (VAG) barrier heights are smaller on Ih (< 7 meV) than on ASW (<54 meV). The surface morphology strongly influences the well depths. Tunneling increases some of the transition rate constants substantially but has a much smaller effect on others. The average KIE for Ih is higher than for ASW for the same range of barrier heights.

A New Model of the Chemistry of Ionizing Radiation in Solids: CIRIS
Christopher N. Shingledecker, Romane Le Gal, Eric Herbst

The collisions between high-energy ions and solids can result in significant physical and chemical changes to the material. These effects are potentially important for better understanding the chemistry of interstellar and planetary bodies, which are exposed to cosmic radiation and the solar wind, respectively; however, modeling such collisions on a detailed microscopic basis has thus far been largely unsuccessful. To that end, a new model, entitled CIRIS: the Chemistry of Ionizing Radiation in Solids, was created to calculate the physical and chemical effects of the irradiation of solid materials. With the new code, we simulate O2 ice irradiated with 100 keV protons. Our models are able to reproduce the measured ozone abundances of a previous experimental study, as well as independently predict the approximate thickness of the ice used in that work.

On the reservoir of sulphur in dark clouds : chemistry and elemental abundance reconciled
Thomas H. G. Vidal, Jean-Christophe Loison, Adam Yassin Jaziri, Maxime Ruaud, Pierre Gratier and Valentine Wakelam

Sulphur-bearing species are often used to probe the physical structure of star forming regions of the interstellar medium, but the chemistry of sulphur in these regions is still poorly understood. In dark clouds, sulphur is supposed to be depleted under a form which is still unknown despite numerous observations and chemical modeling studies that have been performed. In order to improve the modeling of sulphur chemistry, we propose an enhancement of the sulphur chemical network using experimental and theoretical literature. We test the effect of the updated network on the outputs of a three phases gas-grain chemical model for dark cloud conditions using different elemental sulphur abundances. More particularly, we focus our study on the main sulphur reservoirs as well as on the agreement between model predictions and the abundances observed in the dark cloud TMC-1 (CP). Our results show that depending on the age of the observed cloud, the reservoir of sulphur could either be atomic sulphur in the gas-phase or HS and H2S in icy grain bulks. We also report the first chemical model able to reproduce the abundances of observed S-bearing species in TMC-1 (CP) using as elemental abundance of sulphur its cosmic value.

L1157-B1, a factory of complex organic molecules in a Solar-type star forming region
B. Lefloch, C. Ceccarelli, C. Codella, C. Favre, L. Podio, C. Vastel, S. Viti, R. Bachiller

We report on a systematic search for oxygen-bearing Complex Organic Molecules (COMs) in the Solar-like protostellar shock region L1157-B1, as part of the IRAM Large Program "Astrochemical Surveys At IRAM" (ASAI). Several COMs are unambiguously detected, some for the first time, such as ketene, dimethyl ether and glycolaldehyde, and others firmly confirmed, such as formic acid and ethanol. Thanks to the high sensitivity of the observations and full coverage of the 1, 2 and 3mm wavelength bands, we detected numerous ($\sim$10–125) lines from each of the detected species. Based on a simple rotational diagram analysis, we derive the excitation conditions and the column densities of the detected COMs. Combining our new results with those previously obtained towards other protostellar objects, we found a good correlation between ethanol, methanol and glycolaldehyde. We discuss the implications of these results on the possible formation routes of ethanol and glycolaldehyde.

The ALMA-PILS survey: Detection of CH3NCO toward the low-mass protostar IRAS 16293-2422 and laboratory constraints on its formation

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Methyl isocyanate (CH3NCO) belongs to a select group of interstellar molecules considered to be relevant precursors in the formation of larger organic compounds, including those with peptide bonds. The molecule has only been detected in a couple of high-mass protostars and potentially on comets. A formation route on icy grains has been postulated for this molecule but experimental evidence is lacking. Here we extend the range of environments where methyl isocyanate is found, and unambiguously identify CH3NCO through the detection of 43 unblended transitions in the ALMA Protostellar Interferometric Line Survey (PILS) of the low mass solar-type protostellar binary IRAS 16293-2422. The molecule is detected toward both components of the binary with a ratio HNCO/CH3NCO ~4–12. The isomers CH3CNO and CH3OCN are not identified, resulting in upper abundance ratios of CH3NCO/CH3CNO > 100 and CH3NCO/CH3OCN > 10. The resulting abundance ratios compare well with those found for related N-containing species toward high-mass protostars. To constrain its formation, a set of cryogenic UHV experiments is performed. VUV irradiation of CH4:HNCO mixtures at 20 K strongly indicate that methyl isocyanate can be formed in the solid-state through CH3 and (H)NCO recombinations. Combined with gas-grain models that include this reaction, the solid-state route is found to be a plausible scenario to explain the methyl isocyanate abundances found in IRAS 16293-2422.

Parameterizing the interstellar dust temperature

S. Hocuk, L. Szucs, P. Caselli, S. Cazaux, M. Spaans, G.B. Esplugues

The temperature of interstellar dust particles is of great importance to astronomers. It plays a crucial role in the thermodynamics of interstellar clouds, because of the gas-dust collisional coupling. It is also a key parameter in astrochemical studies that governs the rate at which molecules form on dust. In 3D (magneto)hydrodynamic simulations often a simple expression for the dust temperature is adopted, because of computational constraints, while astrochemical modelers tend to keep the dust temperature constant over a large range of parameter space. Our aim is to provide an easy-to-use parametric expression for the dust temperature as a function of visual extinction (Av) and to shed light on the critical dependencies of the dust temperature on the grain composition. We obtain an expression for the dust temperature by semi-analytically solving the dust thermal balance for different types of grains and compare to a collection of recent observational measurements. We also explore the effect of ices on the dust temperature. Our results show that a mixed carbonaceous-silicate type dust with a high carbon volume fraction matches the observations best. We find that ice formation allows the dust to be warmer by up to 15% at high optical depths (Av > 20 mag) in the interstellar medium. Our parametric expression for the dust temperature is presented as $T_d = 11 + 5.7 \times \tanh[0.61 - \log_{10}(Av)] \, \chi_{uv}^{1/5.9}$, where χ_{uv} is in units of the Draine (1978) UV field.

How hydroxylation affects hydrogen adsorption and formation on nanosilicates

Boutheïna Kerkeni, Marie-Christine Bacchus-Montabonel, Stefan T. Bromley

Silicate dust constitutes one of the primary solid components of the Universe and is thought to be an essential enabler for complex chemistry in a number of astronomical environments. Hydroxylated silicate nanoclusters (MgO)x(SiO2)y(H2O)z, where strongly absorbed water molecules are dissociated on the silicate surface, are likely to be persistent in diffuse clouds. Such precursor species are thus also primary candidates as seeds for the formation and growth of icy dust grains in dense molecular clouds. Using density functional calculations we investigate the reactivity of hydroxylated pyroxene nanoclusters (Mg4Si4O12)(H2O)N (N = 1−4) towards hydrogen physisorption, chemisorption and H2 formation. Our results show that increased hydroxylation leads to a significant reduction in the energy range for the physisorption and chemisorption of single

H atoms, when compared to bare silicate grains and bare bulk silicate surfaces. Subsequent chemisorption of a second H atom is, however, little affected by hydroxylation. The H2 reaction barrier for the recombination of two chemisorbed H atoms tends to follow a linear correlation with respect to the 2Hchem binding energy, suggestive of a general Brønsted–Evans–Polanyi relation for H2 formation on silicate grains, independent of dust grain size, composition and degree of hydroxylation.

Spectrally-resolved UV photodesorption of CH4 in pure and layered ices

R. Dupuy, M. Bertin, G. Féraud, X. Michaut, P. Jeseck, M. Doronin, L. Philippe, C. Romanzin and J.-H. Fillion

Context. Methane is among the main components of the ice mantles of insterstellar dust grains, where it is at the start of a rich solid-phase chemical network. Quantification of the photon-induced desorption yield of these frozen molecules and understanding of the underlying processes is necessary to accurately model the observations and the chemical evolution of various regions of the interstellar medium. Aims. This study aims at experimentally determining absolute photodesorption yields for the CH4 molecule as a function of photon energy. The influence of the ice composition is also investigated. By studying the methane desorption from layered CH4:CO ice, indirect desorption processes triggered by the excitation of the CO molecules is monitored and quantified. Methods. Tunable monochromatic VUV light from the DESIRS beamline of the SOLEIL synchrotron is used in the 7 - 13.6 eV (177 - 91 nm) range to irradiate pure CH4 or layers of CH4 deposited on top of CO ice samples. The release of species in the gas phase is monitored by quadrupole mass spectrometry and absolute photodesorption yields of intact CH4 are deduced. Results. CH4 photodesorbs for photon energies higher than ~9.1 eV (~136 nm). The photodesorption spectrum follows the absorption spectrum of CH4, which confirms a desorption mechanism mediated by electronic transitions in the ice. When it is deposited on top of CO, CH4 desorbs between 8 and 9 eV with a pattern characteristic of CO absorption, indicating desorption induced by energy transfer from CO molecules. Conclusions. The photodesorption of CH4 from the pure ice in various interstellar environments is around 2.0 x 10^-3 molecules per incident photon. Results on CO-induced indirect desorption of CH4 provide useful insights for the generalization of this process to other molecules co-existing with CO in ice mantles.

Spatially resolved images of reactive ions in the Orion Bar

J. R. Goicoechea, S. Cuadrado, J. Pety, E. Bron, J. H. Black, J. Cernicharo, E. Chapillon, A. Fuente, M. Gerin

We report high angular resolution (4.9" x 3.0") images of reactive ions SH+, HOC+, and SO+ toward the Orion Bar photodissociation region (PDR). We used ALMA-ACA to map several rotational lines at 0.8 mm, complemented with multi-line observations obtained with the IRAM 30m telescope. The SH+ and HOC+ emission is restricted to a narrow layer of 2"-to 10"-width (~800 to 4000 AU depending on the assumed PDR geometry) that follows the vibrationally excited H2^* emission. Both ions efficiently form very close to the H/H2 transition zone, at a depth of A_V < 1 mag into the neutral cloud, where abundant C+, S+, and H2^* coexist. SO+ peaks slightly deeper into the cloud. The observed ions have low rotational temperatures (T_rot~10-30 K << T_k}) and narrow line-widths (~2-3 km/s), a factor of ~2 narrower that those of the lighter reactive ion CH+. This is consistent with the higher reactivity and faster radiative pumping rates of CH+ compared to the heavier ions, which are driven relatively faster toward smaller velocity dispersion by elastic collisions and toward lower T_rot by inelastic collisions. We estimate column densities and average physical conditions from an excitation model (n(H2)~10^5-10^6 cm^{-3}}, n(e^-)~10 cm^{-3}, and T_k~200 K). Regardless of the excitation details, SH+ and HOC+ clearly trace the most exposed layers of the UV-irradiated molecular cloud surface, whereas SO+ arises from slightly more shielded layers.

Announcements

Postdoctoral position: The physics and chemistry of interstellar and circumstellar clouds

We seek a candidate with a PhD, preferentially in Astrophysics, for a postdoctoral research position on the study of the physics and chemistry of interstellar and/or circumstellar clouds. The goal of the project is to develop models that include basic physical and chemical processes to confront with astronomical observations obtained with millimeter-to-optical observatories (ALMA, IRAM, SOFIA, JWST, GTC). The ideal candidate should have experience in the development of numerical models studying aspects such as the energy balance, hydrodynamics, shocks, chemical processes on the gas phase and on grain surfaces, radiative transfer, etc. We will also consider candidates with a background in the analysis of data gathered with (sub-)millimeter, infrared, and optical telescopes. The postdoc will take part of the Molecular Astrophysics group of CSIC, based in Madrid (Spain). The selected candidate will be employed for a period of 2 to 3 years (depending of funding and status of the project) with a salary that will depend on research experience. The preferred starting date is September 2017, although it may be adapted to the selected candidate. Application: If you are interested, please send a Curriculum Vitae and a short letter of motivation to the following e-mail address: marcelino.agundez@icmm.csic.es. Applications received before June 2017 will receive full consideration. For further details you can contact: Dr. Marcelino

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