AstroChemical Newsletter #45

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Abstracts

C2O and C3O in low-mass star-forming regions

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C2O and C3O belong to the carbon chain oxides family. Both molecules have been detected in the gas phase towards several star-forming regions, and to explain the observed abundances, ion-molecule gas-phase reactions have been invoked. On the other hand, laboratory experiments have shown that carbon chain oxides are formed after energetic processing of CO-rich solid mixtures. Therefore, it has been proposed that they are formed in the solid phase in dense molecular clouds after cosmic ion irradiation of CO-rich icy grain mantles and released in the gas phase after their desorption. In this work, we contribute to the understanding of the role of both gas-phase reactions and energetic processing in the formation of simple carbon chain oxides that have been searched for in various low-mass star-forming regions. We present observations obtained with the Noto-32m and IRAM-30m telescopes towards star-forming regions. We compare these with the results of a gas-phase model that simulates C2O and C3O formation and destruction, and laboratory experiments in which both molecules are produced after energetic processing (with 200 keV protons) of icy grain mantle analogues. New detections of both molecules towards L1544, L1498, and Elias 18 are reported. The adopted gas phase model is not able to reproduce the observed C2O/C3O ratios, while laboratory experiments show that the ion bombardment of CO-rich mixtures produces C2O/C3O ratios that agree with the observed values. Based on the results obtained here, we conclude that the synthesis of both species is due to the energetic processing of CO-rich icy grain mantles. Their subsequent desorption because of non-thermal processes allows the detection in the gas-phase of young star-forming regions. In more evolved objects, the non-detection of both C2O and C3O is due to their fast destruction in the warm gas.

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Discovery of the first Ca-bearing molecule in space: CaNC

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We report on the detection of calcium isocyanide, CaNC, in the carbon-rich evolved star IRC+10216. We derived a column density for this species of (2.0+/-0.5)E+11 cm^-2. Based on the observed line profiles and the modelling of its emission through the envelope, the molecule has to be produced in the intermediate and outer layers of the circumstellar envelope where other metal-isocyanides have previously been found in this source. The abundance ratio of CaNC relative to MgNC and FeCN is ~1/60 and ~1, respectively. We searched for the species CaF, CaCl, CaC, CaCCH, and CaCH3 for which accurate frequency predictions are available. Only upper limits have been obtained for these molecules.

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Cyanopolyyne Chemistry around Massive Young Stellar Objects

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Recent radio astronomical observations have revealed that HC5N, the second shortest cyanopolyyne (HC2n+1N), is abundant around some massive young stellar objects (MYSOs), which is not predicted by classical carbon-chain chemistry. For example, the observed HC5N abundance toward the G28.28−0.36 MYSO is higher than that in L1527, which is one of the warm carbon chain chemistry (WCCC) sources, by more than one order of magnitude (Taniguchi et al., 2017). In this paper, we present chemical simulations of hot-core models with a warm-up period using the astrochemical code Nautilus. We find that the cyanopolyynes are formed initially in the gas phase and accreted onto the bulk and surface of granular ice mantles during the lukewarm phase, which occurs at 25 < T < 100 K. In slow warm-up period models, the peak abundances occur as the cyanopolyynes desorb from dust grains after the temperature rises above 100 K. The lower limits of the abundances of HC5N, CH3CCH, and CH3OH observed in the G28.28−0.36 MYSO can be reproduced in our hot-core models, after their desorption from dust grains. Moreover, previous observations suggested chemical diversity in envelopes around different MYSOs. We discuss possible interpretations of relationships between stages of the star-formation process and such chemical diversity, such as the different warm-up timescales. This timescale depends not only on the mass of central stars but also on the relationship between the size of warm regions and their infall velocity.

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Hydrogen abstraction/addition tunneling reactions elucidate the interstellar H2NCHO/HNCO ratio and H2 formation

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Formamide (H2NCHO) is the smallest molecule possessing the biologically important amide bond. Recent interstellar observations have shown a strong correlation between the abundance of formamide and isocyanic acid (HNCO), indicating that they are likely to be chemically related, but no experiment or theory explains this correlation satisfactorily. We performed H + H2NCHO reactions in a para-hydrogen quantum-solid matrix host and identified production of H2NCO and HNCO from hydrogen-abstraction reactions. We identified also D2NCO, DNCO, HDNCO, and HDNCHO from the reaction H + D2NCHO, indicating the presence of hydrogen-addition reactions of DNCO and HDNCO. From the observed temporal profiles of H2NCHO, H2NCO, HNCO, and their deuterium isotopologues, we showed that a dual-cycle consisting of hydrogen abstraction and hydrogen addition can satisfactorily explain the quasi-equilibrium between H2NCHO and HNCO and explain other previous experimental results. Furthermore, this mechanism also indicates that the catalytic formation of H2 from H atoms might occur in interstellar ice grains.

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Quantum Behavior of Spin-Orbit Inelastic Scattering of C-Atoms by D2 at Low Energy

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Fine-structure populations and collision–induced energy transfer in atoms are of interest for many fields, from combustion to astrophysics. In particular, neutral carbon atoms are known to play a role in interstellar media, either as probes of physical conditions (ground state 3Pj spin-orbit populations), or as cooling agent (collisional excitation followed by radiative decay). This work aims at investigating the spin-orbit excitation of atomic carbon in its ground electronic state due to collisions with molecular deuterium, an isotopic variant of H2, the most abundant molecule in the interstellar medium. Spin-orbit excitations of C(3Pj) by H2 or D2 are governed by non-adiabatic and spin-orbit couplings, which make the theoretical treatment challenging, since the Born-Oppenheimer approximation no longer holds. Inelastic collisional cross-sections were determined for the C(3P0) + D2 → C(3Pj) + D2 (with j = 1 and 2) excitation process. Experimental data were acquired in a crossed beam experiment at low collision energies, down to the excitation thresholds (at 16.42 and 43.41 cm−1, respectively). C-atoms were produced mainly in their ground spin-orbit state, 3P0, by dissociation of CO in a dielectric discharge through an Even-Lavie pulsed valve. The C-atom beam was crossed with a D2 beam from a second valve. The state-to-state cross-sections were derived from the C(3Pj) (j = 1 or 2) signal measured as a function of the beam crossing angle, i.e., as a function of the collision energy. The results show different quantum behaviors for excitation to C(3P1) or C(3P2) when C(3P0) collides with ortho-D2 or normal-D2. These experimental results are analyzed and discussed in the light of highly accurate quantum calculations. A good agreement between experimental and theoretical results is found. The present data are compared with those obtained for the C-He and C-H2 collisional systems to get new insights into the dynamics of collision induced spin-orbit excitation/relaxation of atomic carbon.

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First-Principles Study of the Reaction Mechanism of CHO + H on Graphene Surface

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We analyzed the reaction of HCO + H on a graphene surface using ab initio molecular dynamics simulations as a case study of the formation and desorption of organic molecules on interstellar dust particles. During the reactions of chemisorbed CHO (chemisorbed at the C atom) with free H, CO was generated and efficiently desorbed from the surface. These results suggest that the reactions, of which the reactant forms a covalent bond with the surface while the product does not, cause efficient desorption of the product upon reaction. In such reactions a repulsive force between the product and the surface would be generated and accelerate translation of the product in a specific direction. In addition, it was also shown that the branching ratio of the reactions between radical species on the surface would be affected by the form of the adsorption on the surface.

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Quantum-state–selective electron recombination studies suggest enhanced abundance of

primordial HeH+

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The epoch of first star formation in the early universe was dominated by simple atomic and molecular species consisting mainly of two elements: hydrogen and helium. Gaining insight into this constitutive era requires thorough understanding of molecular reactivity under primordial conditions. We used a cryogenic ion storage ring combined with a merged electron beam to measure state-specific rate coefficients of dissociative recombination, a process by which electrons destroy molecular ions. We found a dramatic decrease of the electron recombination rates for the lowest rotational states of HeH+, compared to previous measurements at room temperature. The reduced destruction of cold HeH+ translates into an enhanced abundance of this primordial molecule at redshifts of first star and galaxy formation.

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Molecular analysis of a high-mass prestellar core candidate in W43-MM1

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High-mass analogues of low-mass prestellar cores are searched for to constrain the models of high-mass star formation. Several high-mass cores, at various evolutionary stages, have been recently identified towards the massive star-forming region W43-MM1 and amongst them a high-mass prestellar core candidate. We aim to characterise the chemistry in this high-mass prestellar core candidate, referred to as W43-MM1 core #6, and its environment. Using ALMA high-spatial resolution data of W43-MM1, we have studied the molecular content of core #6 and a neighbouring high-mass protostellar core, referred to as #3, which is similar in size and mass to core #6. We first subtracted the continuum emission using a method based on the density distribution of the intensities on each pixel. Then, from the distribution of detected molecules, we identified the molecules centred on the prestellar core candidate (core #6) and those associated to shocks related to outflows and filament formation. Then we constrained the column densities and temperatures of the molecules detected towards the two cores. While core #3 appears to contain a hot core with a temperature of about 190 K, core #6 seems to have a lower temperature in the range from 20 K to 90 K from a rotational diagram analysis. We have considered different source sizes for core #6 and the comparison of the abundances of the detected molecules towards the core with various interstellar sources shows that it is compatible with a core of size 1000 au with T=20−90 K or a core of size 500 au with T∼80 K. Core #6 of W43-MM1 remains one of the best high-mass prestellar core candidates even if we cannot exclude that it is at the very beginning of the protostellar phase of high-mass star formation.

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Surface Science Investigations of Icy Mantle Growth on Interstellar Dust Grains in Cooling Environments

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Experimental measurements on the thermal and non-thermal behaviour of water and other simple molecules, including organic compounds such as methanol and benzene, on model interstellar dust grain surfaces and on solid water surfaces using surface science techniques and methodologies are reviewed. A simple qualitative model of the early stages mantle growth arising from a synthesis of the results of such investigations from our own laboratory and others is presented.

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Laboratory rotational spectroscopy of isotopic acetone, CH3 13C(O)CH3 and 13CH3C(O)CH3, and astronomical search in Sagittarius B2(N2)

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We want to study the rotational spectra of CH3 13C(O)CH3 and 13CH3C(O)CH3 and search for them in Sagittarius B2(N2). We investigated the laboratory rotational spectrum of isotopically enriched CH3 13C(O)CH3 between 40 GHz and 910 GHz and of acetone between 36 GHz and 910 GHz in order to study 13CH3C(O)CH3 in natural isotopic composition. In addition, we searched for emission lines produced by these species in a molecular line survey of Sagittarius B2(N) carried out with ALMA. Discrepancies between predictions of the main isotopic species and the ALMA spectrum prompted us to revisit the rotational spectrum of this isotopolog. We assigned 9711 new transitions of CH3 13C(O)CH3 and 63 new transitions of 13CH3C(O)CH3 in the laboratory spectra. More than 1000 additional lines were assigned for the main isotopic species. We modeled the ground state data of all three isotopologs satisfactorily with the ERHAM program. We find that models of the

torsionally excited states v12=1 and v17=1 of CH3C(O)CH3 improve only marginally. No transition of CH3 13C(O)CH3 is clearly detected toward the hot molecular core Sgr B2(N2). However, we report a tentative detection of 13CH3C(O)CH3 with a 12C/13C isotopic ratio of 27 that is consistent with the ratio previously measured for alcohols in this source. Several dozens of transitions of both torsional states of the main isotopolog are detected as well. Our predictions of CH3 13C(O)CH3 and CH3C(O)CH3 are reliable into the terahertz region. The spectrum of 13CH3C(O)CH3 should be revisited in the laboratory with an enriched sample. Transitions pertaining to the torsionally excited states v12=1 and v17=1 of CH3C(O)CH3 could be identified unambiguously in Sagittarius B2(N2).

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Announcements

Opening of 6 PhD positions for recruitment in astrochemistry

Opening of 6 PhD positions for recruitment starting from September within the ITN AstroChemical Origins https://aco-itn.oapd.inaf.it/job-opportunities

Applications are invited for Postdoctoral Fellow (PDF) positions in the School of Earth and Planetary Sciences, National Institute of Science Education and Research (NISER), Bhubaneswar, India.

Looking for hiring highly motivated and bright postdoctoral candidates interested in different areas of Astrochemistry:
(i) the chemistry during star and planet formation and its effects on planet compositions,
(ii) radio/sub-millimeter/infrared astronomy to study star and planet formation,
(iii) develop scientific research on the fields covered by the SKA cradle of life science consortium and prepare the feasibility of future observations using SKA-India.
The candidate will have access to the ALMA Cycle 6 and 7, SOFIA Cycle 7 data as well as guaranteed time JWST-MIRI observations. The interested candidates are strongly encouraged to contact Dr. Liton Majumdar and send a detailed CV directly to liton@niser.ac.in.
The detail postdoc application information is available on the NISER website from our school:
https://www.niser.ac.in/notices/2019/recruitments/PDF-SEPS.pdf