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Abstracts

A new multi-beam apparatus for the study of surface chemistry routes to formation of complex organic molecules in space

E. Congiu, A. Sow, T. Nguyen, S. Baouche, and F. Dulieu

A multi-beam ultra-high vacuum apparatus is presented. In this article we describe the design and construction of a new laboratory astrophysics experiment -- VErs de NoUvelles Synthèses (VENUS) -- that recreates the solid-state non-energetic formation conditions of complex organic molecules in dark clouds and circumstellar environments. The novel implementation of four operational differentially-pumped beam lines will be used to determine the feasibility and the rates for the various reactions that contribute to formation of molecules containing more than six atoms. Data are collected by means of Fourier transform infrared spectroscopy and quadrupole mass spectrometry. The gold-coated sample holder reaches temperatures between 7 and 400 K. The apparatus was carefully calibrated and the acquisition system was developed to ensure that experimental parameters are recorded as accurately as possible. A great effort has been made to have the beam lines converge towards the sample. Experiments have been developed to check the beam alignment using reacting systems of neutral species (NH3, H2CO). Preliminary original results were obtained for the NO+H system, which shows that chemistry occurs only in the very first outer layer of the deposited species, that is the chemical layer and the physical layer coincide. This article illustrates the characteristics, performance, and future potential of the new apparatus in view of the forthcoming launch of the James Webb Space Telescope. We show that VENUS will have a major impact through its contributions to surface science and astrochemistry.

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Survey of ortho-H2D+ in high-mass star-forming regions

G. Sabatini, S. Bovino, A. Giannetti, F. Wyrowski, M. A. Ordenes, R. Pascale, T. Pillai, M. Wienen, T. Csengeri and K. M. Menten

(Abridged) We present a large sample of o-H2D+ observations in high-mass star-forming regions and discuss possible empirical correlations with relevant physical quantities to assess its role as a chronometer of star-forming regions through different evolutionary stages. APEX observations of the ground-state transition of o-H2D+ were analysed in a sample of massive clumps selected from ATLASGAL at different evolutionary stages. Column densities and beam-averaged abundances of o-H2D+ with

respect to H2, X(o-H2D+), were obtained by modelling the spectra under the assumption of local thermodynamic equilibrium. We detect 16 sources in o-H2D+ and find clear correlations between X(o-H2D+) and the clump bolometric luminosity and the dust temperature, while only a mild correlation is found with the CO-depletion factor. In addition, we see a clear correlation with the luminosity-to-mass ratio, which is known to trace the evolution of the star formation process. This would indicate that the deuterated forms of H3+ are more abundant in the early stages of the star formation process and that deuteration is influenced by the time evolution of the clumps. In this respect, our findings would suggest that the X(o-H2D+) abundance is mainly affected by the thermal changes rather than density changes in the gas. We have employed these findings together with observations of H13CO+, DCO+, and C17O to provide an estimate of the cosmic-ray ionisation rate in a sub-sample of eight clumps based on recent analytical work. Our study presents the largest sample of o-H2D+ in star-forming regions to date. The results confirm that the deuteration process is strongly affected by temperature and suggests that o-H2D+ can be considered a reliable chemical clock during the star formation processes, as proved by its strong temporal dependence.

Sabatini G., et al., 2020, A&A, 644, A34
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Influence of the ice structure on the soft UV photochemistry of PAHs embedded in solid water

J. A. Noble, E. Michoulier, C. Aupetit, J. Mascetti

The UV photoreactivity of polycyclic aromatic hydrocarbons (PAHs) in porous amorphous solid water has long been known to form both oxygenated photoproducts and photofragments. The aim of this study is to examine the influence of ice structure on reactivity under soft UV irradiation conditions. Mixtures of PAHs with amorphous solid water (porous and compact) and crystalline (cubic and hexagonal) ices were prepared in a high vacuum chamber and irradiated using a mercury lamp for up to 2.5 h. The results show that the production of oxygenated PAHs is efficient only in amorphous water ice, while fragmentation can occur in both amorphous and crystalline ices. We conclude that the reactivity is driven by PAH–water interactions in favourable geometries, notably where dangling bonds are available at the surface of pores. These results suggest that the formation of oxygenated PAH molecules is most likely to occur in interstellar environments with porous (or compact) amorphous solid water and that this reactivity could considerably influence the inventory of aromatics in meteorites.

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An Evolutionary Study of Volatile Chemistry in Protoplanetary Disks

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The volatile composition of a planet is determined by the inventory of gas and ice in the parent disk. The volatile chemistry in the disk is expected to evolve over time, though this evolution is poorly constrained observationally. We present Atacama Large

Millimeter/submillimeter Array observations of C18O, C2H, and the isotopologues H13CN, HC15N, and DCN toward five Class 0/I disk candidates. Combined with a sample of 14 Class II disks presented in Bergner et al., this data set offers a view of volatile chemical evolution over the disk lifetime. Our estimates of C18O abundances are consistent with a rapid depletion of CO in the first ~0.5-1 Myr of the disk lifetime. We do not see evidence that C2H and HCN formation are enhanced by CO depletion, possibly because the gas is already quite under-abundant in CO. Further CO depletion may actually hinder their production by limiting the gas-phase carbon supply. The embedded sources show several chemical differences compared to the Class II stage, which seem to arise from shielding of radiation by the envelope (impacting C2H formation and HC15N fractionation) and sublimation of ices from infalling material (impacting HCN and C18O abundances). Such chemical differences between Class 0/I and Class II sources may affect the volatile composition of planet-forming material at different stages in the disk lifetime.

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Gas-phase Elemental abundances in Molecular cloudS (GEMS) III. Unlocking the CS chemistry: the CS+O reaction

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CS is among the most abundant gas-phase S-bearing molecules in cold dark molecular clouds. It is easily observable with several transitions in the millimeter wavelength range, and has been widely used as a tracer of the gas density in the interstellar medium in our Galaxy and external galaxies. Chemical models fail to account for the observed CS abundances when assuming the cosmic value for the elemental abundance of sulfur. The CS + O -> CO + S reaction has been proposed as a relevant CS destruction mechanism at low temperatures, and could explain the discrepancy between models and observations. Its reaction rate has been experimentally measured at temperatures of 150-400 K, but the extrapolation to lower temperatures is doubtful. Here we calculate the CS+O reaction rate at temperatures <150 K which are prevailing in the interstellar medium. We performed ab initio calculations to obtain the three lowest PES of the CS+O system. These PESs are used to study the reaction dynamics, using several methods to eventually calculate the CS+O thermal reaction rates. We compare the results of our theoretical calculations for 150-400 K with those obtained in the laboratory. Our detailed theoretical study on the CS+O reaction, which is in agreement with the experimental data obtained at 150-400 K, demonstrates the reliability of our approach. After a careful analysis at lower temperatures, we find that the rate constant at 10 K is negligible, which is consistent with the extrapolation of experimental data using the Arrhenius expression. We use the updated chemical network to model the sulfur chemistry in TMC1 based on molecular abundances determined from GEMS project observations. In our model, we take into account the expected decrease of the cosmic ray ionization rate along the cloud. The abundance of CS is still overestimated when assuming the cosmic value for the sulfur abundance.

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Carbon Chain Chemistry in Hot-Core Regions around Three Massive Young Stellar Objects Associated with 6.7 GHz Methanol Masers

Kotomi Taniguchi, Eric Herbst, Liton Majumdar, Paola Caselli, Jonathan C. Tan, Zhi-Yun Li, Tomomi Shimoikura, Kazuhito Dobashi, Fumitaka Nakamura, Masao Saito

We have carried out observations of CCH (N = 1-0), CH3CN (J = 5-4), and three 13C isotopologues of HC3N (J = 10-9) toward three massive young stellar objects (MYSOs), G12.89+0.49, G16.86-2.16, and G28.28-0.36, with the Nobeyama 45-m radio telescope. Combined with previous results on HC5N, the column density ratios of N(CCH)/N(HC5N), hereafter the CCH/HC5N ratios, in the MYSOs are derived to be ~15. This value is lower than that in a low-mass warm carbon chain chemistry (WCCC) source by more than one order of magnitude. We compare the observed CCH/HC5N ratios with hot-core model calculations (Taniguchi et al. 2019). The observed ratios in the MYSOs can be best reproduced by models when the gas temperature is ~85 K, which is higher than in L1527, a low-mass WCCC source (~35 K). These results suggest that carbon-chain molecules detected around the MYSOs exist at least partially in higher temperature regions than those in low-mass WCCC sources. There is no significant difference in column density among the three 13C isotopologues of HC3N in G12.89+0.49 and G16.86-2.16, while HCC13CN is more abundant than the others in G28.28-0.36. We discuss carbon-chain chemistry around the three MYSOs based on the CCH/HC5N ratio and the 13C isotopic fractionation of HC3N.

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Announcements

Postdoctoral Position in quantum chemistry and reaction dynamics

One postdoctoral position is available in the group of Toshiyuki Takayanagi at Department of Chemistry, Saitama University in Japan. The group focuses on quantum chemistry and reaction dynamics. A successful candidate is expected to carry out numerical calculations of potential energy surfaces and reaction dynamics of both gas-phase and grain-surface reactions relevant to astrochemistry in collaboration with the grant group “Next Generation Astrochemistry”. The candidates must have fundamental knowledge on quantum chemistry and interests in astrochemistry. The candidates with research experience in potential energy surface development are particularly welcome. The candidate should have finished his/her doctoral thesis before taking up the position. Japanese language skill is not required. The position is initially for one year with the annual extension depending on performance, up until March 31, 2025. The position is open from April 1, 2021, but the exact starting date is flexible. To learn more and apply, see: link

Postdoctoral Position in physical and chemical processes in

star/planet formation

One postdoctoral position is available in the group of Yuri Aikawa at Department of Astronomy, University of Tokyo in Japan. The group focuses on physical and chemical processes in the star/planet formation. A successful candidate is expected to carry out numerical simulations of physical and chemical processes in interstellar clouds, star-forming cores, and protoplanetary disks in collaboration with the grant group “Next Generation Astrochemistry”. The candidates must have fundamental knowledge on star/planet formation and/or astrochemistry. The candidates with research experience in chemical reaction network models, Monte-Carlo simulations of grain surface reactions, radiation hydrodynamics, radiation transfer calculations for synthetic observations are particularly welcome. The candidate should have finished his/her doctoral thesis before taking up the position. Japanese language skill is not required. The position is initially for one year with the annual extension depending on performance, up until March 31, 2025. The position is open from April 1, 2021, but the exact starting date is flexible. To learn more and apply, see: link