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Abstracts

Infrared Detection of Abundant CS in the Hot Core AFGL 2591 at High Spectral Resolution with SOFIA/EXES

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We have performed a 5-8 micron spectral line survey of the hot molecular core associated with the massive protostar AFGL 2591, using the Echelon-Cross-Echelle Spectrograph (EXES) on the Stratospheric Observatory for Infrared Astronomy (SOFIA). We have supplemented these data with a ground based study in the atmospheric M band around 4.5 micron using the iSHELL instrument on the Infrared Telescope Facility (IRTF), and the full N band window from 8-13 micron using the Texas Echelon Cross Echelle Spectrograph (TEXES) on the IRTF. Here we present the first detection of ro-vibrational transitions of CS in this source. The absorption lines are centred on average around -10 kms-1 and the line widths of CS compare well with the hot component of 13CO (around 10 kms-1). Temperatures for CS, hot 13CO and 12CO v=1-2 agree well and are around 700 K. We derive a CS abundance of 8x10^-3 and 2x10^-6 with respect to CO and H2 respectively. This enhanced CS abundance with respect to the surrounding cloud (1x10^-8) may reflect sublimation of H2S ice followed by gas-phase reactions to form CS. Transitions are in LTE and we derive a density of >10^7 cm-3, which corresponds to an absorbing region of < 0.04 arcsec. EXES observations of CS are likely to probe deeply into the hot core, to the base of the outflow. Submillimeter and infrared observations trace different components of the hot core as revealed by the difference in systemic velocities, line widths and temperatures, as well as the CS abundance.

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The census of interstellar complex organic molecules in the Class I hot corino of SVS13-A

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We present the first census of the interstellar Complex Organic Molecules (iCOMs) in the low-mass Class I protostar SVS13-A, obtained by analysing data from the IRAM-30m Large Project ASAI (Astrochemical Surveys At IRAM). They consist of an high-sensitivity unbiased spectral survey at the 1mm, 2mm and 3mm IRAM bands. We detected five iCOMs: acetaldehyde (CH3CHO), methyl formate (HCOOCH3), dimethyl

ether (CH3OCH3), ethanol (CH3CH2OH) and formamide (NH2CHO). In addition we searched for other iCOMs and ketene (H2CCO), formic acid (HCOOH) and methoxy (CH3O), whose only ketene was detected. The numerous detected lines, from 5 to 37 depending on the species, cover a large upper level energy range, between 15 and 254 K. This allowed us to carry out a rotational diagram analysis and derive rotational temperatures between 35 and 110 K, and column densities between 3 x 10^15 and 1 x 10^17 cm^-2 on the 0."3 size previously determined by interferometric observations of glycolaldehyde. These new observations clearly demonstrate the presence of a rich chemistry in the hot corino towards SVS13-A. The measured iCOMs abundances were compared to other Class 0 and I hot corinos, as well as comets, previously published in the literature. We find evidence that (i) SVS13-A is as chemically rich as younger Class 0 protostars, and (ii) the iCOMs relative abundances do not substantially evolve during the protostellar phase.

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First ALMA maps of HCO, an important precursor of complex organic molecules, towards IRAS 16293-2422

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The formyl radical HCO has been proposed as the basic precursor of many complex organic molecules such as methanol (CH3OH) or glycolaldehyde (CH2OHCHO). Using ALMA, we have mapped, for the first time at high angular resolution (~1´´, ~140 au), HCO towards the Solar-type protostellar binary IRAS 16293−2422, where numerous complex organic molecules have been previously detected. We also detected several lines of the chemically related species H2CO, CH3OH and CH2OHCHO. The observations revealed compact HCO emission arising from the two protostars. The line profiles also show redshifted absorption produced by foreground material of the circumbinary envelope that is infalling towards the protostars. Additionally, IRAM 30m single-dish data revealed a more extended HCO component arising from the common circumbinary envelope. The comparison between the observed molecular abundances and our chemical model suggests that whereas the extended HCO from the envelope can be formed via gas-phase reactions during the cold collapse of the natal core, the HCO in the hot corinos surrounding the protostars is predominantly formed by the hydrogenation of CO on the surface of dust grains and subsequent thermal desorption during the protostellar phase. The derived abundance of HCO in the dust grains is high enough to produce efficiently more complex species such as H2CO, CH3OH, and CH2OHCHO by surface chemistry. We found that the main formation route of CH2OHCHO is the reaction between HCO and CH2OH.

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Chemical tracers in proto-brown dwarfs: CO, ortho-H2CO, para-H2CO, HCO+, CS observations

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We present a study of the CO isotopologues and the high-density tracers H2CO, HCO+, and CS in Class 0/I proto-brown dwarfs (proto-BDs). We have used the IRAM

30m telescope to observe the 12CO (2-1), 13CO (2-1), C18O (2-1), C17O (2-1), H2CO (3-2), HCO+ (3-2), and CS (5-4) lines in 7 proto-BDs. The hydrogen column density for the proto-BDs derived from the CO gas emission is ~2-15 times lower than that derived from the dust continuum emission, indicating CO depletion from the gas-phase. The mean H2CO ortho-to-para ratio is ~3 for the proto-BDs and indicates gas-phase formation for H2CO. We have investigated the correlations in the molecular abundances between the proto-BDs and protostars. Proto-BDs on average show a factor of ~2 higher ortho-to-para H2CO ratio than the protostars. Possible explanations include a difference in the H2CO formation mechanism, spin-selective photo-dissociation, self-shielding effects, or different emitting regions for the ortho and para species. There is a tentative trend of a decline in the HCO+ and H2CO abundances with decreasing bolometric luminosity, while the CS and CO abundances show no particular difference between the proto-BDs and protostars. These trends reflect the scaled-down physical structures for the proto-BDs compared to protostars and differences in the peak emitting regions for these species. The C17O isotopologue is detected in all of the proto-BDs as well as the more evolved Class Flat/Class II BDs in our sample, and can probe the quiescent gas at both early and late evolutionary stages.

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UV Photolysis of Pyrazine and the Production of Hydrogen Isocyanide

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Photolysis of the diazine heterocycle, pyrazine, following irradiation at 308, 248, and 193 nm was examined using nanosecond time-resolved Fourier transform infrared emission spectroscopy. The resulting time-resolved IR emission spectra reveal that for 308 and 248 nm vibrationally highly excited pyrazine is produced, but no photolysis products were detected. However, at 193 nm excitation, the measured IR emission spectra consist solely of resonances originating from rovibrationally excited photofragments, including acetylene (HCCH), hydrogen cyanide (HCN), and hydrogen isocyanide (HNC), indicating that photofragmentation proceeds from vibrationally highly excited pyrazine on the ground electronic state. Spectral fit analysis of the time-resolved HCN and HNC IR emission band shapes and intensities allowed an estimate of the nascent product population distributions, from which a lower bound estimate of the HNC/HCN branching ratio was deduced as $\Phi \geq 0.07$. Additionally, ab initio calculations were performed in order to examine the propensity of photoinduced reactions on the ground- and lowest-energy excited-state surfaces. The calculations provide a basis for understanding the wavelength dependence of UV photolysis and the photolytic production of HNC and also explain previous experimental observations in the literature.

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Probing Nonadiabatic Effects in Low-Energy C(3Pj) + H2 Collisions.

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Nonadiabatic effects are of fundamental interest in collision dynamics. In particular, inelastic collisions between open-shell atoms and molecules, such as the collisional excitation of C(3Pj) by H2, are governed by nonadiabatic and spin−orbit couplings that are the sole responsible of collisional energy transfer. Here, we study collisions between carbon in its ground state C(3Pj=0) and molecular hydrogen (H2) at low collision energies that result in spin−orbit excitation to C(3Pj=1) and C(3Pj=2). State-to-state integral cross sections are obtained experimentally from crossed-beam experiments with a source of almost pure beam of C(3Pj=0) and theoretically from highly accurate quantum calculations. We observe very good agreement between experimental and theoretical data that demonstrates our ability to model nonadiabatic dynamics. New rate coefficients at temperatures relevant to astrochemical modeling are also provided. They should lead to an increase of the abundance of atomic C(3P) derived from the observations of interstellar clouds and a decrease of the efficiency of the cooling of the interstellar gas due to carbon atoms.

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Propylene Oxide Formation on a Silica Surface with Peroxo Defects: Implications in Astrochemistry

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The formation of the chiral molecule propylene oxide (CH3CHCH2O) recently detected in the interstellar medium (ISM) is proposed to take place on an amorphous silicate grain surface where peroxo defects are present. A computational analysis conducted at the DFT and MP2-F12 levels of theory on a neat amorphous silica model supports such a hypothesis resulting in (a) strong thermodynamic driving forces and low activation energies allowing the synthesis of CH3CHCH2O at low temperatures, (b) chemical defects on silica surfaces promoting heterogeneous catalysis of the increasing molecular complexity found in interstellar and circumstellar medium, and (c) chemical defects that have implications on understanding how processing phases modify the nature of the reactive groups on a silica surface affecting the surface catalytic activity.

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Ion irradiation of N2O ices and NO2:N2O4 ice mixtures: first steps to understand the evolution of molecules with the N-O bond in space

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Astronomical observations towards star forming regions have revealed the presence of molecules with the N-O bond such as NO, N2O, and HNO. These species are considered potential precursors of prebiotic molecules. Thus understanding nitrogen and oxygen chemistry may help us to better understand the origin and evolution of prebiotic molecules in space. However, species with the N-O bond are poorly studied and laboratory works on the effects induced on them by solar wind and galactic cosmic rays are still scarce. For this, we wanted to study the effects of ion bombardment on molecules with the N-O bond. We focus here on N2O ices and NO2:N2O4 = 1:1 ice

mixtures (at 16 and 50/60 K) irradiated with 200 keV protons. Infrared transmission spectroscopy (8000-500 cm-1; 1.25-20 micron) was used to analyze the samples. Irradiation of N2O ices and NO2:N2O4 ice mixtures produces comparable effects independent of the irradiation temperature, NO being the main product. Moreover, we show that the maximum amount of N2O and N2O4 destroyed by irradiation, at the highest dose reached in our experiments, is equal to about 98 and 70%, respectively. The dose range covered in the experiments has been compared with the astrophysical timescale of surface processing in space, showing that irradiation of N2O and NO2:N2O4 mixtures can produce, within 10^5-10^8 years, amounts of solid NO ice detectable towards star forming regions by the James Webb Space Telescope.

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Combined IR and XPS characterization of organic refractory residues obtained by ion irradiation of simple icy mixtures

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Context. Multi-year laboratory experiments have demonstrated that frozen icy mixtures containing simple organic and inorganic molecules (such as H2O, N2, CH4, CO, CO2, C2H6, etc.), if exposed to a flux of energetic ions or UV photons, give rise to new more complex molecules at low temperatures (10-50 K). A fraction of the new synthesized molecules is volatile while the remaining fraction is refractory and therefore it is preserved after the warm-up of the substrate to room temperature. Moreover, a part of the refractory material is formed during the annealing to room temperature, when molecules and radicals into the processed ice become mobile and react to form non-volatile molecules. By means of similar mechanisms, complex organic materials may be formed on the icy surfaces of some objects in the outer solar system, such as trans-Neptunian objects, comets and some satellites of the giant planets: in fact the interaction with solar wind and solar flares ions, solar photons and galactic cosmic rays could produce more refractory materials, analogous to those produced in the laboratory. In some cases, the materials thus synthesized may contain functional groups considered relevant to the pre-biotic chemistry in the hypothesis that interplanetary dust particles (IDPs), comets and meteoroids contributed to seed the early Earth with the building blocks of life. Aims. The aim of this work is to investigate the chemical similarities and differences between some organic residues left over after ion bombardment (200 keV H+) of different ice mixtures followed by subsequent warm up under vacuum to room temperature. Methods. Seven organic residues have been prepared in our laboratory following a procedure involving the proton irradiation of seven different icy mixtures and their warm-up to room temperature. All the organic samples were characterized by FTIR spectroscopy with measurements performed in situ, in the ultra-high vacuum condition preventing any sample degradation. Three of them were selected to be characterized by XPS spectroscopy as well. Results. Among the organic residues presented in this paper, only those containing nitrogen and carbon exhibit the multi-component band centred at 2200 cm-1. This multi-component band presents interest from the astrobiological point of view due to its attribution to nitriles and isonitriles. Our results demonstrate that this band is present in the IR spectra of organic nitrogen residues regardless the use of oxygen-bearing species in the icy mixture. This finding is of interest since the 2200 cm-1 band has been observed in some extraterrestrial samples (micro-meteorites) collected in the Antarctica.

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High-Resolution SOFIA/EXES Spectroscopy of SO2 Gas in the Massive Young Stellar Object MonR2 IRS3: Implications for the Sulfur Budget

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Sulfur has been observed to be severely depleted in dense clouds leading to uncertainty in the molecules that contain it and the chemistry behind their evolution. Here, we aim to shed light on the sulfur chemistry in young stellar objects (YSOs) by using high-resolution infrared spectroscopy of absorption by the nu_3 rovibrational band of SO2 obtained with the Echelon-Cross-Echelle Spectrograph on the Stratospheric Observatory for Infrared Astronomy. Using local thermodynamic equilibrium models we derive physical parameters for the SO2 as in the massive YSO MonR2 IRS3. This yields a SO2/H abundance lower limit of 5.6+/-0.5x10^-7, or >4% of the cosmic sulfur budget, and an intrinsic line width (Doppler parameter) of b<3.20 km s^-1. The small line widths and high temperature (T_ex=234+/-15 K) locate the gas in a relatively quiescent region near the YSO, presumably in the hot core where ices have evaporated. This sublimation unlocks a volatile sulfur reservoir (e.g., sulfur allotropes as detected abundantly in comet 67P/Churyumov-Gerasimenko), which is followed by SO2 formation by warm, dense gas-phase chemistry. The narrowness of the lines makes formation of SO2 from sulfur sputtered off grains in shocks less likely toward MonR2 IRS3.

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