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Abstracts

Deuterium chemistry and D/H ratios in Class 0/I proto-brown dwarfs

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We have conducted the first extensive observational survey of several deuterated species in 16 Class 0/I proto-brown dwarfs (proto-BDs) and 4 Class Flat/Class II brown dwarfs. Observations were obtained with the IRAM 30m telescope in the DCO+ (3-2), DCN (3-2), DNC (3-2), and N2D+ (3-2) lines. The DCO+/H13CO+, DCN/H13CN, and DNC/HN13C ratios are comparatively higher and show a narrower range than the DCO+/HCO+, DCN/HCN, and DNC/HNC ratios, respectively. The mean D/H ratios for the proto-BDs derived from these molecules are in the range of 0.02-3. Both low-temperature gas-phase ion-molecule deuteron transfer and grain surface reactions are required to explain the enhanced deuterium fractionation. The very dense and cold (nH2 >= 1e6 cm-3, T <= 10 K) interior of the proto-BDs provide the suitable conditions for efficient deuterium fractionation in these cores. There is no correlation between the D/H ratios and the CO depletion factor, with the exception of the DCN/HCN ratios that show a strong anti-correlation possibly due to the difference in the peak emitting regions of the DCN and HCN molecules. Over a wide range in the bolometric luminosities spanning ~0.002--40 Lsun, we find a trend of higher DCO+/HCO+ (r = -0.7) and DCN/HCN (r = -0.6) ratios, nearly constant DNC/HNC (r = -0.4) and DNC/HN13C (r = -0.1) ratios, lower N2D+/N2H+ ratios (r = 0.6) in the proto-BDs compared to protostars. Only one Class II brown dwarf shows emission in the DCO+ (3-2) line. No correlation is seen between the D/H ratios and the evolutionary stage.

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A spectral survey of CH3CCH in the Hot Molecular Core G331.512-0.103

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A spectral survey of methyl acetylene (CH3CCH) was conducted toward the hot molecular core/outflow G331.512-0.103. Our APEX observations allowed the detection of 41 uncontaminated rotational lines of CH3CCH in the frequency range between 172-356 GHz. Through an analysis under the local thermodynamic equilibrium assumption, by means of rotational diagrams, we determined Texc = 50 ± 1 K, N(CH3CCH) = (7.5 ± 0.4) x 1e15 cm-2, X[CH3CCH/H2] ~ (0.8-2.8) x 1e-8 and X[CH3CCH/CH3OH] ~ 0.42 ± 0.05 for an extended emitting region (~10 arcsec). The relative intensities of the K=2 and K=3 lines within a given K-ladder are strongly negatively correlated to the transitions' upper J quantum-number (r=-0.84). Pure rotational spectra of CH3CCH were simulated at different temperatures, in order to interpret this observation. The results indicate that the emission is characterized by a non-negligible temperature gradient with upper and lower limits of ~45 and ~60 K, respectively. Moreover, the line widths and peak velocities show an overall strong correlation with their rest frequencies, suggesting that the warmer gas is also associated with stronger turbulence effects. The K=0 transitions present a slightly different kinematic signature than the remaining lines, indicating that they might be tracing a different gas component. We speculate that this component is characterized by lower temperatures, and therefore larger sizes. Moreover, we predict and discuss the temporal evolution of the CH3CCH abundance using a two-stage zero-dimensional model of the source constructed with the three-phase Nautilus gas-grain code.

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First CH3D detection in Class 0/I proto-brown dwarfs: constraints on CH4 abundances

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We report the first detection in the JK = 1_0 - 0_0 rotational transition line of CH3D towards three Class 0/I proto-brown dwarfs (proto-BDs) from IRAM 30 m observations. Assuming a rotational temperature of 25 K, the CH3D abundances (relative to H2) are in the range of (2.3 – 14.5) × 1e−7. The CH4 abundances derived from the CH3D abundances and assuming the DCO+/HCO+ ratios are in the range of (0.05 – 4.8) ×1e−5. The gas-phase formation of CH3D via CH2D+ is enhanced at high densities of 1e8 – 1e10 cm^−3 and our observations are likely probing the innermost dense and warm regions in proto-BDs. Thermal and/or non-thermal desorption can return the CH3D and CH4 molecules formed at an early stage on grain surfaces to the gas-phase. The gas phase abundances are indicative of warm carbon-chain chemistry in proto-BDs where carbon-chain molecules are synthesized in a lukewarm (∼20-30 K) region close to the central source.

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Discovery of ammonia (9,6) masers in two high-mass star-forming regions

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Molecular maser lines are signposts of high-mass star formation, probing excitation and kinematics of very compact regions in the close environment of young stellar objects and providing useful targets for trigonometric parallax measurements. Only a few NH 3 (9,6) masers were known so far, and their origin is still poorly understood. Here we aim to find new NH 3 (9,6) masers to provide a better observational basis to study their role in high-mass star-forming regions. We carried out NH 3 (9,6) observations toward Cepheus A and G34.26 + 0.15 with the Effelsberg-100 m telescope and the Karl G. Jansky Very Large Array. We discovered new NH 3 (9,6) masers in Cep A and G34.26 + 0.25, which increases the number of high-mass star-forming regions hosting NH 3 (9,6) masers from five to seven. Long term monitoring (20 months) at Effelsberg shows that the intensity of the (9,6) maser in G34.26 + 0.25 is decreasing, while the Cep A maser remains stable. Compared to the Effelsberg data and assuming linear variations between the epochs of observation, the JVLA data indicate no missing flux. This suggests that the NH 3 (9,6) emission arises from single compact emission regions that are not resolved by the interferometric measurements. As JVLA imaging shows, the NH 3 (9,6) emission in Cep A originates from a sub-arcsecond sized region, slightly to the west of the peak position of the 1.36cm continuum object, HW2. In G34.26 + 0.25, three NH 3 (9,6) maser spots are observed: one is close to the head of the cometary ultracompact HII region C and the other two are emitted from a compact region to the west of the hypercompact HII region A. The newly found (9,6) masers appear to be related to outflows. Higher angular resolution of JVLA and VLBI observations are needed to provide more accurate positions and constraints for pumping scenarios.

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Organic chemistry in the protosolar analogue HOPS-108: Environment matters

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Hot corinos are compact regions around solar-mass protostellar objects that are very rich in interstellar complex organic molecules (iCOMs). They are believed to represent the very early phases of our Solar System's birth, which was very likely also characterized by rich organic chemistry. While most of the studied hot corinos are either isolated or born in a loose protocluster, our Sun was born in a densely packed star cluster, near massive stars whose ultraviolet radiation must have contributed to shaping the evolution of the surrounding environment. In addition, internal irradiation from energetic particles (>10 Mev), whose imprint is seen today in the products of short-lived radionuclides in meteoritic material, is also known to have occurred during the Solar System formation. How did all these conditions affect the chemistry of the proto-Sun and its surroundings is still an open question. To answer this question, we studied HOPS-108, the hot corino located in the protosolar analogue OMC-2 FIR4. The study was carried out with ALMA at 1.3mm with an angular resolution of ∼100 AU. We detected 11 iCOMs such as CH3OH HCOOCH3 and CH3OCH3. Our results can be summarized as follows: (1) an enhancement of HCOOCH3 with respect to other hot corinos, (2) a [CH3OCH3]/[HCOOCH3] abundance ratio of ∼0.2 marginally deviating from the usual trend seen in other sources ([CH3OCH3]/[HCOOCH3] ∼1), (3) a [CH2DOH]/[CH3OH] ratio of 2.5% which is lower than what is seen in Perseus and Ophiuchus hot corinos (∼7%-9%) and similar to that seen in HH212 another source located in Orion. This might result from different physical conditions in the Orion molecular complex compared to other regions.

L. Chahine, A. López-Sepulcre, R. Neri, C. Ceccarelli, S. Mercimek, C. Codella, M. Bouvier, E. Bianchi, C. Favre, L. Podio et al.2022, A&A, 657, A78
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Quantum mechanical simulations of the radical-radical chemistry on icy surfaces

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The formation of the interstellar complex organic molecules (iCOMs) is a hot topic in astrochemistry. One of the main paradigms trying to reproduce the observations postulates that iCOMs are formed on the ice mantles covering the interstellar dust grains as a result of radical--radical coupling reactions. We investigate iCOMs formation on the icy surfaces by means of computational quantum mechanical methods. In particular, we study the coupling and direct hydrogen abstraction reactions involving the HCO/CH3 + X systems, where X = NH2, CH3, HCO, CH3O, CH2OH, plus the CH2OH + CH2OH and CH3O + CH3O systems. We computed the activation energy barriers of these reactions as well as the binding energies of all the studied radicals, by means of density functional theory (DFT) calculations on two ice water models, made of 33 and 18 water molecules. Then, we estimated the efficiency of each reaction using the reaction activation, desorption and diffusion energies and derived kinetics with the Eyring equations. We find that radical--radical chemistry on surfaces is not as straightforward as usually assumed. In some cases, direct H abstraction reactions can compete with radical--radical couplings, while in others they may contain large activation energies. Specifically, we found that (i) ethane, methylamine and ethylene glycol are the only possible products of the relevant radical--radical reactions; (ii) glyoxal, methyl formate,

glycolaldehyde, formamide, dimethyl ether and ethanol formation is likely in competition with the respective H-abstraction products, and (iii) acetaldehyde and dimethyl peroxide do not seem a likely grain surface products.

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The impact of cosmic-ray attenuation on the carbon cycle emission in molecular clouds

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Observations of the emission of the carbon cycle species (C, C+ CO) are commonly used to diagnose gas properties in the interstellar medium but are significantly sensitive to the cosmic-ray ionization rate. The carbon-cycle chemistry is known to be quite sensitive to the cosmic-ray ionization rate, ζ, controlled by the flux of low-energy cosmic rays which get attenuated through molecular clouds. However, astrochemical models commonly assume a constant cosmic-ray ionization rate in the clouds. We investigate the effect of cosmic-ray attenuation on the emission of carbon cycle species from molecular clouds, in particular the [CII] 158 μm, [CI] 609 μm and CO (J = 1 - 0) 115.27 GHz lines. We use a post-processed chemical model of diffuse and dense simulated molecular clouds and quantify the variation in both column densities and velocity integrated line emission of the carbon cycle with different cosmic-ray ionization rate models. We find that the abundances and column densities of carbon cycle species is significantly impacted by the chosen cosmic-ray ionization rate model: no single constant ionization rate can reproduce the abundances modelled with an attenuated cosmic-ray model. Further, we show that constant ionization rate models fail to simultaneously reproduce the integrated emission of the lines we consider, and their deviations from a physically derived cosmic-ray attenuation model is too complex to be simply corrected. We demonstrate that the two clouds we model exhibit a similar average AVeff - n_H relationship, resulting in an average relation between the cosmic-ray ionization rate and density ζ(n_H). We conclude by providing a number of implementation recommendations for CRs in astrochemical models, but emphasize the necessity for column-dependent cosmic-ray ionization rate prescriptions.

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A train of shocks at 3000 au scale? Exploring the clash of an expanding bubble into the NGC 1333 IRAS 4 region. SOLIS XVI

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There is evidence that the star formation process is linked to the intricate net of filaments in molecular clouds, which may be also due to gas compression from external triggers. We studied the southern region of the Perseus NGC 1333 molecular cloud, known to be heavily shaped by similar external triggers, to shed light on the process that perturbed the filament where the Class 0 IRAS4 protostars lie. We use new IRAM-NOEMA observations of SiO and CH3OH, both known to trace violent events as shocks, toward IRAS 4A as part of the Large Program Seeds Of Life in Space (SOLIS). We detected three parallel elongated (>6000 au) structures, called fingers, with narrow line profiles (~1.5 km s−1) peaked at the cloud systemic velocity, tracing gas with high density (5-20 10^5 cm−3) and high temperature (80-160 K). They are chemically different, with the northern finger traced by both SiO and CH3OH ([CH3OH]/[SiO]~160-300), while the other two only by SiO ([CH3OH]/[SiO]< 40). Among various possibilities, a train of three shocks, distanced by >5000 yr, would be consistent with the observations if a substantial fraction of silicon, frozen onto the grain mantles, is released by the shocks.We suggest that the shock train is due to an expanding gas bubble, coming behind NGC 1333 from the southwest and clashing against the filament, where IRAS 4A lies. Finally, we propose a solution to the two-decades long debate on the nature and origin of the widespread narrow SiO emission observed in the south part of NGC 1333, namely that it is due to unresolved trains of shocks.

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Mapping Physical Parameters in Orion KL at High Spatial Resolution

O. H. Wilkins, P. B. Carroll, and G. A. Blake

The Orion Kleinmann-Low nebula (Orion KL) is notoriously complex and exhibits a range of physical and chemical components. We conducted high-angular-resolution (subarcsecond) observations of 13CH3OH ν = 0 (∼0.3" and 0.7") and CH3CN ν8 = 1 (∼0.2" and ∼0.9") line emission with the Atacama Large Millimeter/submillimeter Array (ALMA) to investigate Orion KL's structure on small spatial scales (≤350 au). Gas kinematics, excitation temperatures, and column densities were derived from the molecular emission via a pixel-by-pixel spectral line fitting of the image cubes, enabling us to examine the small-scale variation of these parameters. Subregions of the Hot Core have a higher excitation temperature in a 0.2" beam than in a 0.9" beam, indicative of possible internal sources of heating. Furthermore, the velocity field includes a bipolar ∼7–8 km s−1 feature with a southeast-northwest orientation against the surrounding ∼4–5 km s−1 velocity field, which may be due to an outflow. We also find evidence of a possible source of internal heating toward the Northwest Clump, since the excitation temperature there is higher in a smaller beam versus a larger beam. Finally, the region southwest of the Hot Core (Hot Core-SW) presents itself as a particularly heterogeneous region bridging the Hot Core and Compact Ridge. Additional studies to identify the (hidden) sources of luminosity and heating within Orion KL are necessary to better understand the nebula and its chemistry.

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Detection of HC18O+ in a protoplanetary disk: exploring oxygen isotope fractionation of CO

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The oxygen isotope fractionation scenario, which has been developed to explain the oxygen isotope anomaly in the solar system materials, predicts that CO gas is depleted in 18O in protoplanetary disks, where segregation between solids and gas inside disks had already occurred. Based on ALMA observations, we report the first detection of HC18O+(4-3) in a Class II protoplanetary disk (TW Hya). This detection allows us to explore the oxygen isotope fractionation of CO in the TW Hya disk from optically thin HCO+ isotopologues as a proxy of optically thicker CO isotopologues. Using the H13CO+(4-3) data previously obtained with SMA, we find that the H13CO+/HC18O+ ratio in the central <100 au regions of the disk is 10.3 ± 3.2. We construct a chemical model of the TW Hya disk with carbon and oxygen isotope fractionation chemistry, and estimate the conversion factor from H13CO+/HC18O+ to 13CO/C18O. With the conversion factor (= 0.8), the 13CO/C18O ratio is estimated to be 8.3 ± 2.6, which is consistent with the elemental abundance ratio in the local ISM (8.1 ± 0.8) within error margin. Then there is no clear evidence of 18O depletion in CO gas of the disk, although we could not draw any robust conclusion due to large uncertainties. In conclusion, optically thin lines of HCO+ isotopologues are useful tracers of CO isotopic ratios, which are hardly constrained directly from optically thick lines of CO isotopologues. Future higher sensitivity observations of H13CO+ and HC18O+ would be able to allow us to better constrain the oxygen fractionation in the disk.

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