AstroChemical Newsletter #18

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Abstracts

ALMA hints at the existence of an unseen reservoir of diffuse molecular gas in the Galactic bulge

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We aim to understand the unexpected presence of mm-wave molecular absorption at -200 km/s < v < -140$ km/s in a direction that is well away from regions of the Galactic bulge where CO emission at such velocities is prominent. We compared 89 GHz Cycle 2 ALMA absorption spectra of HCO+, HCN, and HNC toward the extragalactic continuum source B1741-312 at l=-2.14°, b=-1.00° with existing CO, H I, and dust emission and absorption measurements. We placed the atomic and molecular gas in the bulge and disk using circular and non-circular galactic kinematics, deriving N(H I) from a combination of 21cm emission and absorption and we derive N(H2) from scaling of the HCO+ absorption. We then inverted the variation of near-IR reddening E(J-K) with distance modulus and scale E(J-K) to a total gas column density N(H) that may be compared to N(H I) and N(H2). At galactocentric radii Rgal > 1.5 kpc, conventional measures such as the standard CO-H2 conversion factor and locally observed N(HCO+)/N(H2) ratio separately imply that H I and H2 contribute about equally to N(H), and the gas-derived N(H) values are in broad agreement with those derived from E(J-K). Within the Galactic bulge at Rgal <1.5 kpc, H I contributes less than 10% of the material inferred from E(J-K), so that the molecular absorption detected here is needed to understand the extinction.

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Formation and stabilization of C6- by radiative electron attachment

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Radiative electron attachment (REA) plays an important role in forming molecular anions in various astrophysical environments. In this work, we determined the rate coefficient for the formation of C6- by REA based on a detailed balance approach. C6- ions are stored in an electrostatic ion beam trap and are photoexcited above their adiabatic detachment energy (4.18 eV). Due to fast internal conversion and intramolecular vibrational redistribution, photoexcitation leads to the formation of temporary negative ions (TNIs), the same as those one formed by the electron attachment. Absolute vibrational autodetachment and recurrent (or Poincaré) fluorescence (RF) rate coefficients have already been reported [V. Chandrasekaran et al., J. Phys. Chem. Lett. 5, 4078 (2014)]. Knowing the branching ratios of the various competing rate coefficients is decisive to the understanding of the formation probability of anions via REA. The radiative stabilization rate of C6- , shown to be dominated by RF, was determined to be 5 x10^4 s-1 at the electron detachment energy, i.e., at least a factor of 100 faster than the stabilization by infrared transitions. The RF is found to very effectively stabilize the TNI formed by electron attachment. Using detailed balance to link the measured delayed detachment rate to the rate of electron attachment, we estimate the REA rate leading to the formation of C6- to be 3 x10^-7 cm^3 s^-1 at 300 K in agreement with theory (1.7 x 10^-7 cm^3 s^-1 [R. Terzieva and E. Herbst, Int. J. Mass Spectrom. 201, 135 (2000)]). Such a high rate for REA to C6 indicates that REA may play a prominent role in the formation of anions in the interstellar medium.

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Two-dimensional ice mapping of molecular cores

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We present maps of the column densities of H2O, CO2 and CO ices towards the molecular cores B 35A, DC 274.2-00.4, BHR 59 and DC 300.7-01.0. These ice maps, probing spatial distances in molecular cores as low as 2200 au, challenge the traditional hypothesis that the denser the region observed, the more ice is present, providing evidence that the relationships between solid molecular species are more varied than the generic picture we often adopt to model gas–grain chemical processes and explain feedback between solid phase processes and gas phase abundances. We present the first combined solid–gas maps of a single molecular species, based upon observations of both CO ice and gas phase C18O towards B 35A, a star-forming dense core in Orion. We conclude that molecular species in the solid phase are powerful tracers of 'small-scale' chemical diversity, prior to the onset of star formation. With a component analysis approach, we can probe the solid phase chemistry of a region at a level of detail greater than that provided by statistical analyses or generic conclusions drawn from single pointing line-of-sight observations alone.

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An ALMA Survey of DCN/H13CN and DCO+/H13CO+ in Protoplanetary Disks

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The deuterium enrichment of molecules is sensitive to their formation environment. Constraining patterns of deuterium chemistry in protoplanetary disks is therefore useful for probing how material is inherited or reprocessed throughout the stages of star and planet formation. We present ALMA observations at ~0.6 arcsec resolution of DCO+, H13CO+, DCN, and H13CN in the full disks around T Tauri stars AS 209 and IM Lup, in the transition disks around T Tauri stars V4046 Sgr and LkCa 15, and in the full disks around Herbig Ae stars MWC 480 and HD 163296. We also present ALMA observations of HCN in the IM Lup disk. DCN, DCO+, and H13CO+ are detected in all disks, and H13CN in all but the IM Lup disk. We find efficient deuterium fractionation for the sample, with estimates of disk-averaged DCO+/HCO+ and DCN/HCN abundance ratios ranging from ~0.02–0.06 and ~0.005–0.08, respectively, which is comparable to values reported for other interstellar environments. The relative distributions of DCN and DCO+ vary between disks, suggesting that multiple formation pathways may be needed to explain the diverse emission morphologies. In addition, gaps and rings observed in both H13CO+ and DCO+ emission provide new evidence that DCO+ bears a complex relationship with the location of the midplane CO snowline.

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Production of complex organic molecules: H-atom addition versus UV irradiation

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Complex organic molecules (COMs) have been identified in different environments in star-forming regions. Laboratory studies show that COMs form in the solid state, on icy grains, typically following a ‘non-energetic’ (atom-addition) or ‘energetic’ (UV-photon absorption) trigger. So far, such studies have been largely performed for single processes. Here, we present the first work that quantitatively investigates both the relative importance and the cumulative effect of ‘(non-)energetic’ processing. We focus on astronomically relevant CO:CH3OH = 4:1 ice analogues exposed to doses relevant for the collapse stage of dense clouds. Hydrogenation experiments result in the formation of methyl formate (MF; HC(O)OCH3), glycolaldehyde (GA; HC(O)CH2OH) and ethylene glycol (EG; H2C(OH)CH2OH) at 14 K. The absolute abundances and the abundance fractions are found to be dependent on the H-atom/CO:CH3OH-molecule ratios and on the overall deposition rate. In the case that ices are exposed to UV photons only, several different COMs are found. Typically, the abundance fractions are 0.2 for MF, 0.3 for GA and 0.5 for EG as opposed to the values found in pure hydrogenation experiments without UV in which MF is largely absent: 0.0, 0.2–0.6 and 0.8–0.4, respectively. In experiments where both are applied, overall COM abundances drop to about half of those found in the pure UV irradiation experiments, but the composition fractions are very similar. This implies COM ratios can be used as a diagnostic tool to derive the processing history of an ice. Solid-state branching ratios derived here for GA and EG compare well with observations, while the MF case cannot be explained by solid-state conditions investigated here.

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Qualitative observation of reversible phase change in astrochemical ethanethiol ices using infrared spectroscopy

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Here we report the first evidence for a reversible phase change in an ethanethiol ice prepared under astrochemical conditions. InfraRed (IR) spectroscopy was used to monitor the morphology of the ice using the SH stretching vibration, a characteristic vibration of thiol molecules. The deposited sample was able to switch between amorphous and crystalline phases repeatedly under temperature cycles between 10 K and 130 K with subsequent loss of molecules in every phase change. Such an effect is dependent upon the original thickness of the ice. Further work on quantitative analysis is to be carried out in due course whereas here we are reporting the first results obtained.

Pavithraa, S. et al. Qualitative observation of reversible phase change in astrochemical ethanethiol ices using infrared spectroscopy. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 178, 166-170, (2017)
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Infrared spectra of HSCS+, c-HSCS, and HCS2− produced on electron bombardment of CS2 in

solid para-hydrogen

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We report infrared (IR) spectra of HSCS+, c-HSCS, HCS2−, and other species produced on electron bombardment of a mixture of CS2 and para-hydrogen (p-H2) during deposition at 3.2 K. After maintenance of the deposited matrix in darkness for 12 h, intensities of absorption lines of HSCS+ at 2477.2 (ν1), 1525.6 (ν2), and 919.6 cm−1 (ν3) decreased through neutralization of HSCS+ with trapped electrons. During this period, intensities of lines of HCS2− at 2875.7 (ν1), 1249.9 (ν5), 1003.2 (ν6), and 814.3 cm−1 (ν4) increased due to reaction H + CS2−. The intensities of lines observed at 2312.7 and 889.0 cm−1, which increased after maintenance in darkness and became greatly diminished after irradiation at 373 nm, are assigned to c-HSCS radical. The IR spectra of HSCS+, HCS2−, and c-HSCS are reported for the first time. The IR absorption lines of t-HSCS radical, t-HC(S)SH, and c-HC(S)SH were also identified; their wavenumbers are similar to those reported for these species in an Ar matrix. The corresponding spectra of the 13C, 34S, and D isotopic variants of these species were observed. The assignments were made according to the expected chemical behavior, predicted potential energies of associated reactions, and a comparison of observed and predicted wavenumbers and their 13C , 34S ,and D isotopic ratios. In contrast to the observed significant red shifts of the OH-stretching wavenumber of HOCO+ and HOCS+ in solid p-H2 from those in the gaseous phase due to proton sharing with H2, the wavenumber of the HS-stretching mode of HSCS+ in solid p-H2 (2477.2 cm−1) is similar to the anharmonic wavenumber of HSCS+ (2424 cm−1) predicted with the B3LYP/aug-cc-pVTZ method, indicating that the sharing of a proton between HSCS+ and neighboring H2 molecules is insignificant.

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The anatomy of the Orion B giant molecular cloud: A local template for studies of nearby galaxies

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We aim to develop the Orion B Giant Molecular Cloud (GMC) as a local template for interpreting extra-galactic molecular line observations. We use the wide-band receiver at the IRAM-30m to spatially and spectrally resolve the Orion B GMC. The observations cover almost 1 square degree at 26" resolution with a bandwidth of 32 GHz from 84 to 116 GHz in only two tunings. Among the mapped spectral lines are the 12CO, 13CO, C18O, C17O, HCN, HNC, 12CN, CCH, HCO+, N2H+ (1-0), and 12CS, 32SO, SiO, c-C3H2, CH3OH (2-1) transitions. We introduce the molecular anatomy of the Orion B GMC, including relations between line intensities and gas column density or far-UV radiation fields, and correlations between selected line and line ratios. We also obtain a dust-traced gas mass that is less than about one third the CO-traced mass, using the standard Xco conversion factor. The presence of overluminous CO can be traced back to the dependence of the CO intensity on UV illumination. In fact, while most lines show some dependence on the UV radiation field, CN and CCH are the most sensitive. Moreover dense cloud cores are almost exclusively traced by N2H+. Other traditional high density tracers, such as HCN (1-0), are also easily detected in extended translucent regions at a typical density of about 500 H2 cm-3. In general, we find no straightforward relation between line critical density and the fraction of the line luminosity coming from dense gas regions. Our initial findings demonstrate that the relations between line (ratio) intensities and environment in GMCs are more complicated than often assumed. Sensitivity (i.e., the molecular column density), excitation, and above all chemistry contribute to the observed line intensity distributions. They must be considered together when developing the next generation of extra-galactic molecular line diagnostics of mass, density, temperature and radiation field.

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Single Photon Thermal Ionization of C60

Klavs Hansen, Robert Richter, Michele Alagia, Stefano Stranges, Luca Schio, Peter Salén Vasyl Yatsyna, Raimund Feifel, and Vitali Zhaunerchyk

We report on experiments which show that C60 can ionize in an indirect, quasithermal boiloff process after absorption of a single photon. The process involves a large number of incoherently excited valence electrons and yields electron spectra with a Boltzmann distribution with temperatures exceeding 10 000 K. It is expected to be present for other molecules and clusters with a comparatively large number of valence electrons. The astrophysical consequences are briefly discussed.

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Radiative association of C(3P) and H+: Triplet States

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The radiative association of C(3P) and H+ is investigated by calculating cross sections for photon emission into bound ro-vibrational states of CH+ from the vibrational continua of initial triplet d 3Pi or b 3Sigma- states. Potential energy curves and transition dipole moments are calculated using multi-reference configuration interaction (MRCI) methods with AV6Z basis sets. The cross sections are evaluated using quantum-mechanical methods and rate coefficients are calculated. The rate coefficients are about 100 times larger than those for radiative association of C+(2Po) and H from the A 1Pi state. We also confirm that the formation of CH^+ by radiative association of C+(2Po) and H via the triplet c 3\Sigma+ state is a minor process.

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Stellar energetic particle ionization in protoplanetary disks around T Tauri stars

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Anomalies in the abundance measurements of short lived radionuclides in meteorites indicate that the protosolar nebulae was irradiated by a high amount of energetic particles (E>=10 MeV). The particle flux of the contemporary Sun cannot explain these anomalies. However, similar to T Tauri stars the young Sun was more active and probably produced enough high energy particles to explain those anomalies. We want to study the interaction of stellar energetic particles with the gas component of the disk and identify possible observational tracers of this interaction. We use a 2D radiation thermo-chemical protoplanetary disk code to model a disk representative for T Tauri stars. We use a particle energy distribution derived from solar flare observations and an enhanced stellar particle flux proposed for T Tauri stars. For this particle spectrum we calculate the stellar particle ionization rate throughout the disk with an accurate particle transport model. We study the impact of stellar particles for models with varying X-ray and cosmic-ray ionization rates. We find that stellar particle ionization has a significant impact on the abundances of the common disk ionization tracers HCO+ and N2H+, especially in models with low cosmic-ray ionization rates. In contrast to cosmic rays and X-rays, stellar particles cannot reach the midplane of the disk. Therefore molecular ions residing in the disk surface layers are more affected by stellar particle ionization than molecular ions tracing the cold layers/midplane of the disk. Spatially resolved observations of molecular ions tracing different vertical layers of the disk allow to disentangle the contribution of stellar particle ionization from other competing ionization sources. Modeling such observations with a model like the one presented here allows to constrain the stellar particle flux in disks around T Tauri stars.

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