AstroChemical Newsletter #106

October 2024

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Abstracts

Multi-line study of the radial extent of SiO, CS, and SiS in AGB envelopes

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The spatial distribution of molecules in AGB circumstellar envelopes is regulated by different processes. In the outer layers all molecules are destroyed due to the interaction with interstellar ultraviolet photons. Here we aim to characterize in a coherent and uniform way the radial extent of three molecules (SiO, CS, and SiS) in envelopes around AGB stars of O- and C-rich character, and to study their dependence with mass loss rate. To that purpose, we used the Yebes 40m and IRAM 30m telescopes to observe 7 M-type and 7 C-type AGB envelopes covering a wide range of mass loss rates (1e-7 - 1e-5 Msun/yr) in lines of SiO, CS, and SiS spanning a range of upper level energies of 2-130 K. We carried out excitation and radiative transfer calculations over a wide parameter space to characterize the molecular abundance and radial extent. A chi2 analysis indicates that the abundance is well constrained while the radial extent is more difficult to constrain. The radial extent increases with increasing envelope density, in agreement with previous observational findings. At high envelope densities, Mdot/vexp > 1e-6 (Msun/yr)/(km/s), the radial extent of SiO, CS, and SiS are similar, while at low envelope densities, Mdot/vexp < 1e-7 (Msun/yr)/(km/s), the radial extent differ among the three molecules, in agreement with theoretical expectations based on destruction due to photodissociation. At low envelope densities we find a sequence of increasing radial extent, SiS -> CS -> SiO. We also find a tentative dependence of the radial extent with the chemical type (O- or C-rich) of the star for SiO and CS. Interferometric observations and further investigation of the photodissociation of SiO, CS, and SiS should allow to clarify the situation on the relative photodissociation radius of SiO, CS, and SiS in AGB envelopes and the dependence with envelope density and C/O ratio.

A&A, 2024, vol 688, A16
DOI: 10.1051/0004-6361/202450188
Full-text URL: https://arxiv.org/abs/2405.19922

The rich interstellar reservoir of dinitriles: Detection of malononitrile and maleonitrile in TMC-1

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While the nitrile group is by far the most prevalent one among interstellar molecules, the existence of interstellar dinitriles (molecules containing two -CN groups) has recently been proven. Here we report the discovery of two new dinitriles in the cold dense cloud TMC-1. These newly identified species are malononitrile, CH2(CN)2, and maleonitrile, the Z isomer of NC-CH=CH-CN, which can be seen as the result of substituting two H atoms with two -CN groups in methane and ethylene, respectively. These two molecules were detected using data from the ongoing QUIJOTE line survey of TMC-1 that is being carried out with the Yebes 40m telescope. We derive column densities of 1.8e11 cm-2 and 5.1e10 cm-2 for malononitrile and maleonitrile, respectively. This means that they are eight and three times less abundant than HCC-CH2-CN and (E)-HCC-CH=CH-CN, respectively, which are analog molecules detected in TMC-1 in which one -CN group is converted into a -CCH group. This is in line with previous findings in which -CCH derivatives are more abundant than the -CN counterparts in TMC-1. We examined the potential chemical pathways to these two dinitriles, and we find that while maleonitrile can be efficiently formed through the reaction of CN with CH2CHCN, the formation of malononitrile is not clear because the neutral-neutral reactions that could potentially form it are not feasible under the physical conditions of TMC-1.

A&A, 2024, vol 688, L31
DOI: 10.1051/0004-6361/202451525
Full-text URL: https://arxiv.org/abs/2408.02843

Excitation and spatial study of a prestellar cluster towards G+0.693-0.027 in the Galactic centre

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Star formation in the central molecular zone (CMZ) is suppressed with respect to that of the Galactic disk, and this is likely related to its high turbulent environment. This turbulence impedes the potential detection of prestellar cores. We present the temperature, density, and spatial structure of the CMZ molecular cloud G+0.693-0.027, which has been proposed to host a prestellar cluster in the Sgr B2 region. We analysed multiple HC3N rotational transitions that were observed with the IRAM 30m, APEX, Yebes 40m, and GBT radio telescopes, together with SMA+APEX spatially resolved maps. The spectral shape of HC3N lines shows three velocity components: a broad component with a line width of 23 km s-1 (C1), and two narrow components with line widths of 7.2 and 8.8 km s-1 (C2 and C3). This suggests that a fraction of the molecular gas in this cloud is undergoing turbulence dissipation. From a non-local thermodynamic equilibrium analysis we have found H2 densities of 2e4 cm-3, 5e4 cm-3, and 4e5 cm-3 and kinetic temperatures of 140 K, 30 K, and 80 K for C1, C2, and C3, respectively. The spatially resolved maps confirm that the colder and high-density condensations C2 and C3, which peak in the 70-85 km s-1 velocity range, are embedded in a more diffuse and warmer gas (C1). The larger-scale structure of the Sgr B2 region shows a hole at 40-50 km s−1 that is likely due to a small cloud that shocked the Sgr B2 region and is spatially related with a massive cloud at 60-80 km s-1. We propose that the impacting small cloud sequentially triggered the formation of Sgr B2(M), (N), and (S) and the condensations in G+0.693-0.027 during its passage. Based on the analysis of the masses of the two condensations and on the virial parameters, C2 might expand, while C3 might further fragment or collapse.

Accepted for publication in A&A
DOI: 10.1051/0004-6361/202451382
Full-text URL: https://arxiv.org/abs/2408.17141

A Thermodynamic Landscape of Hydrogen Cyanide-Derived Molecules and Polymers

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Hydrogen cyanide (HCN)-derived molecules and polymers are featured in several hypotheses on the origin of life. Over half a century of investigations into HCN self-reactions have led to many suggestions regarding the structural nature of the products and an even greater number of proposed polymerization pathways. A comprehensive overview of possible reactions and structures is missing. In this work, we use quantum chemical calculations to map the relative Gibbs free energy of most HCN-derived molecules and polymers that have been discussed in the literature. Our computed free energies indicate that several previously considered polymerization pathways are not spontaneous and should be discarded from future consideration. Among the most thermodynamically favored products are polyaminoimidazole and adenine.

ACS Earth Space Chem. 2024, 8, 6, 1272–1280
DOI: 10.1021/acsearthspacechem.4c00088
Full-text URL: https://chemrxiv.org/engage/chemrxiv/article-details/660e839491aefa6ce1c336ae

Unraveling the Interface Chemistry between HCN and Cosmic Silicates by the Interplay of Infrared Spectroscopy and Quantum Chemical Modeling

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Understanding the interaction between hydrogen cyanide (HCN) and silicate surfaces is crucial for elucidating the prebiotic processes occurring on interstellar grain cores as well as in cometary and meteoritic matrices. In this study, we characterized the adsorption features of HCN on crystalline forsterite (Mg2SiO4) surfaces, one of the most abundant cosmic silicates, by combining experimental infrared spectra at low temperatures (100–150 K) with periodic DFT simulations. Results showed the coexistence of both molecular and dissociative HCN adsorption complexes as a function of the considered forsterite crystalline face. Molecular adsorptions dominate on the most stable surfaces, while dissociative adsorptions occur predominantly on surfaces of lower stability, catalyzed by the enhanced Lewis acid–base behavior of surface-exposed Mg2+–O2– ion pairs. On the whole set of adsorption cases, harmonic frequency calculations were carried out and compared with the experimental infrared bands. To disentangle each vibrational mode contributing to the experimental broad bands, we run the best nonlinear fit between the predicted set of frequencies and the experimental bands. The outcome of this procedure allowed us to (i) deconvolute the experimental IR spectrum by assigning computed normal modes of vibrations to the main features of each band and (ii) reveal which crystal faces are responsible for the largest contribution to the adsorbate vibrational bands, giving information about the morphology of the samples. The present straightforward procedure is quite general and of broad interest in the fine characterization of the infrared spectra of adsorbates on complex inorganic material surfaces.

The Journal of Physical Chemistry C 2024 128 (36), 15171-15178
DOI: 10.1021/acs.jpcc.4c03454
Full-text URL: https://arxiv.org/abs/2409.08074

Ice Chemistry Modeling of Active Phase Comets: Hale-Bopp

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We present a chemical kinetics model of the solid-phase chemical evolution of a comet, beginning with a long period of cold-storage in the Oort Cloud, followed by five orbits that bring the comet close to the Sun. The chemical model is based on an earlier treatment that considered only the cold-storage phase, and which was based on the interstellar ice chemical kinetics model MAGICKAL. The comet is treated as 25 chemically distinct layers. Updates to the previous model includes: (i) Time- and depth-dependent temperature profiles according to heliocentric distance; (ii) a rigorous treatment of back-diffusion for species capable of diffusing through the bulk-ice layers; (iii) adoption of recent improvements in the kinetic treatment of nondiffusive chemical reaction rates. Starting from an initially simple ice composition, interstellar UV photons drive a rapid chemistry in the upper micron of material, but diminished by absorption of the UV by the dust component. Galactic cosmic rays (GCRs) drive a much slower chemistry in the deeper ices over the long cold-storage period down to 10 m. The first solar approach drives off the upper layers of ice material via thermal desorption and/or dissociation, bringing closer to the surface the deeper material that previously underwent long-term processing by GCRs. Subsequent orbits are more uniform in their chemical behavior. Loss of molecular material leads to concentration of the dust in the upper layers.

Substantial quantities of complex organic molecules are formed in the upper 10 m during the cold storage phase, with some of this material released during solar approach; however, their abundances with respect to water appear too low to account for the observed gas-phase values for comet Hale-Bopp, indicating that the majority of complex molecular material observed, at least in comet Hale-Bopp, is an inheritance of primordial material.

Icarus vol.416 (2024) pg.22
DOI: [10.1016/j.icarus.2024.116097](https://doi.org/10.1016/j.icarus.2024.116097)
Full-text URL: https://arxiv.org/abs/2408.15509

Assessing realistic binding energies of some essential interstellar radicals with amorphous solid water. A fully quantum chemical approach

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In the absence of laboratory data, state-of-the-art quantum chemical approaches can provide estimates of the binding energy (BE) of interstellar species with grains. Without BE values, contemporary astrochemical models are compelled to utilize wild guesses, often delivering misleading information. Here, we employed a fully quantum chemical approach to estimate the BE of seven diatomic radicals - CH, NH, OH, SH, CN, NS, and NO - that play a crucial role in shaping the interstellar chemical composition, using a suitable amorphous solid water model as a substrate since water is the principal constituent of interstellar ice in dense and shielded regions. While the BEs are compatible with physisorption, the binding of CH in some sites shows chemisorption, in which a chemical bond to an oxygen atom of a water molecule is formed. While no structural change has been observed for the CN radical, it is believed that the formation of a hemibonded system between the outer layer of the water cluster and the radical is the reason for the unusually large BE in one of the binding sites considered in our study. A significantly lower BE for NO, consistent with recent calculations, is obtained, which helps explain the recently observed HONO/NH2OH and HONO/HNO ratios in the low-mass hot corino IRAS 16293-2422 B with chemical models.

Accepted for publication in Astronomy & Astrophysics (A&A) Journal
DOI: 10.1051/0004-6361/202451642
Full-text URL: https://arxiv.org/abs/2408.14660

Methane Formation Efficiency on Icy Grains: Role of Adsorption States

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Methane (CH4) is one of the major components of the icy mantle of cosmic dust prevalent in cold, dense regions of interstellar media, playing an important role in the synthesis of complex organic molecules and prebiotic molecules. Solid CH4 is considered to be formed via the successive hydrogenation of C atoms accreting onto dust: C + 4H → CH4. However, most astrochemical models assume this reaction on the ice mantles of dust to be barrierless and efficient, without considering the states of adsorption. Recently, we found that C atoms exist in either the physisorbed or chemisorbed state on compact amorphous solid water, which is analogous to an interstellar ice mantle. These distinct adsorption states considerably affect the hydrogenation reactivity of the C atom. Herein, we elucidate the reactivities of physisorbed and chemisorbed C atoms with H atoms via sequential deposition and codeposition processes. The results indicate that only physisorbed C atoms can produce CH4 on ice. Combining this finding with a previous estimate for the fraction of physisorbed C atoms on ice, we determined the upper limit for the conversion of C atoms into CH4 to be 30%.

2024 ApJ 973 80
DOI: 10.3847/1538-4357/ad656a
Full-text URL: https://arxiv.org/abs/2407.13057