AstroChemical Newsletter #116

September 2025

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Abstracts

Discovery of interstellar phenalene (c-C13H10): A new piece for the chemical puzzle of PAHs in space

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We present the discovery of the unsubstituted polycyclic aromatic hydrocarbon (PAH) phenalene (C13H10) in TMC-1 as part of the QUIJOTE line survey. In spite of the low dipole moment of this three-ring PAH we have found a total of 267 rotational transitions with quantum numbers J and Ka up to 34 and 14, respectively, corresponding to 100 independent frequencies. The identification of this new PAH from our survey was based on the agreement between the rotational parameters derived from the analysis of the lines and those obtained by quantum chemical calculations. Subsequent chemical synthesis of this PAH and the investigation of its laboratory microwave spectrum unequivocally support our identification. The column density of phenalene in TMC-1 is (2.8+/-1.6)e13 cm-2.

Accepted as a Letter to the Editor in Astronomy & Astrophysics
DOI: 10.1051/0004-6361/202556687
Full-text URL: http://arxiv.org/abs/2508.13857

Low D/H ratio for benzonitrile in TMC-1: Implication for the origin of polycyclic aromatic hydrocarbons in cold dark clouds

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Radioastronomical observations have recently discovered PAHs of moderate size (up to 24 carbon atoms) in cold dark clouds, although it is currently unknown whether they are formed in situ through a bottom-up mechanism or from larger PAHs (20-100 carbon atoms) inherited from a previous diffuse stage in a top-down scenario. Infrared observations have recently shown that large PAHs present in UV-illuminated regions are strongly enriched in deuterium. In order to shed light on the origin of PAHs in cold clouds, we have searched for deuterated benzonitrile in the cold dark cloud TMC-1. To that purpose we have synthesized the three isomers (ortho, meta, and para) of monodeuterated benzonitrile, measured their rotational spectra across the 2-18 GHz and 75-110 GHz frequency ranges in the laboratory, and searched for them in TMC-1 using data from the QUIJOTE line survey. We did not detect any of the three species and have derived a 3sigma upper limit on the column density of each of them of 3.0e10 cm-2, meaning a fractional abundance relative to H2 of <3e-12. We derived a D/H ratio (which we define as the total number of D atoms with respect to the total number of H atoms present in benzonitrile) of <1.2 %. This value is in line with the range of D/H ratios observed for other molecules in TMC-1 (0.06-3.3 %), where deuterium enrichment is explained in terms of isotopic fractionation at low temperature. It is however below the range of D/H ratios derived for large unspecific PAHs from JWST observations of the galactic PDRs Orion Bar and M17 and the galaxies M51 and NGC3256-S (between 1% and <17%). Although it is not straightforward to compare the deuteration of PAHs in dark and UV-irradiated clouds, our results suggest that the population of PAHs detected in cold dark clouds does not result from the fragmentation of larger PAHs inherited from the previous diffuse stage in a top-down scenario.

A&A, 700, A281 (2025)
DOI: 10.1051/0004-6361/202555552
Full-text URL: https://arxiv.org/abs/2507.16552

A D/H Ratio Consistent with Earth's Water in Halley-type Comet 12P from ALMA HDO Mapping

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Isotopic measurements of Solar System bodies provide a primary paradigm within which to understand the origins and histories of planetary materials. The D/H ratio in particular, helps reveal the relationship between (and heritage of) different H2O reservoirs within the Solar System. Here we present interferometric maps of water (H2O) and semiheavy water (HDO) in the gas-phase coma of a comet (Halley-type comet 12P/Pons-Brooks), obtained using the Atacama Large Millimeter/submillimeter Array (ALMA). The maps are consistent with outgassing of both H2O and HDO directly from the nucleus, and imply a coma D/H ratio (for water) of (1.71±0.44)×1e−4. This is at the lower end of the range of previously-observed values in comets, and is consistent with D/H in Earth's ocean water. Our results suggest a possible common heritage between a component of the Oort cloud's water ice reservoir, and the water that was delivered to the young Earth during the early history of the Solar System.

Published in Nature Astronomy, August 2025
DOI: 10.1038/s41550-025-02614-7
Full-text URL: https://arxiv.org/abs/2508.05925

Gas-Phase Vibrational Spectra of [C2H5O2]+ Isomers: Protonated Glycolaldehyde, Acetic Acid, and Methyl Formate

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Methyl formate, acetic acid, and glycolaldehyde comprise an isomeric family that is abundant in the interstellar medium. Their astronomically observed relative abundances are commonly used to gain insights into the potential formation pathways of these complex organic molecules (iCOMs). Several of the proposed synthesis routes involve their protonated analogs. However, to date, only limited spectroscopic data are available on any of the protonated isomers, hampering their astronomical detection that might shed light on specific formation pathways. Here, we present the first broadband vibrational study of protonated methyl formate, acetic acid, and glycolaldehyde (m/z 61, [C2H5O2]+). The protonated species were formed in a storage ion source by electron impact ionization of the respective vapors (the dimer in the case of glycolaldehyde) and subsequent (self-)protonation reactions. The vibrational spectra of the mass-selected ions were recorded in the range of 640–1800 cm–1 using Ne-tagging infrared predissociation spectroscopy in a cryogenic 22-pole ion trap instrument coupled to the infrared free-electron lasers at the FELIX Laboratory. The experimental spectra are compared to calculated vibrational frequencies obtained at the B2PLYP-D3 level of theory using different basis sets and methods, and the influence of anharmonicity on the spectra is discussed. Protonated forms of both structural conformers of methyl formate (syn and anti) were observed and assigned, with protonation on the carbonyl oxygen in the trans (lowest-energy conformer) and cis orientation, respectively. Dominantly, the lowest-energy conformer EZ of carbonyl-protonated acetic acid was observed when using acetic acid as precursor. When using the glycolaldehyde dimer as a precursor, the lowest-energy conformers of both protonated glycolaldehyde and acetic acid were observed.

ACS Earth Space Chem. 2025, 9, 7, 1724–1736
DOI: 10.1021/acsearthspacechem.4c00395
Full-text URL: https://doi.org/10.1021/acsearthspacechem.4c00395

Solid and Gaseous Methane in IRAS 23385+6053 as Seen with Open JWST Data

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We present a new description of the 7.7 μm region towards the high-mass star-forming region IRAS 23385+6053 taken from open James Webb Space Telescope Mid-Infrared Instrument Medium Resolution Spectrometer (JWST MIRI/MRS) data. This area is commonly attributed to the ν4 deformation mode of methane ice. For the first time gaseous and solid methane were analyzed simultaneously in IRAS 23385+6053. The band at 7.58–7.8 μm (1320–1280 cm-1) is interpreted as a wide solid absorption methane feature overlapped by the sharp features of the methane emission. We report the detection of gaseous methane and estimate its emitting area radius R, temperature T and column density N as R=2940 au, T=103(−11;+13) K, and N=0.78(−0.64;+6.18)e17 cm-2, correspondingly. The ice content was analyzed with the laboratory spectra dataset of methane in different molecular environments obtained on the Ice Spectroscopy Experimental Aggregate (ISEAge). We were able to describe the wide feature of solid methane with the following laboratory spectra: CH4 : CO2 = 1 : 5 (at 27.4(−10.8;+6.0) K) and CH4 : H2O = 1 : 10 (at 8.4(−1.7;+16.4) K) deposited at 6.7 K and warmed up at a rate of 0.5 K per minute. The derived column densities are N_CH4(CO2) = 2.97(−0.57;+0.37)e17 cm-2 and N_CH4(H2O) = 1.02(−0.27;+0.46)e17 cm-2. According to the best fit solid methane is mostly surrounded by CO2 rather than H2O. The residuals analysis reveals the unassigned region at 1283–1297 cm-1 (7.71–7.79 μm) which is tentatively assigned to nitrous oxide (N2O) in various environments.

ApJL (2025) 978, L46
DOI: 10.3847/2041-8213/ada290
Full-text URL: https://arxiv.org/abs/2412.17028

JWST reveals cosmic ray dominated chemistry in the local ULIRG IRAS 07251−0248

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We analyze the ro-vibrational absorption bands of various molecular cations (HCO+, HCNH+, and N2H+) and neutral species (HCN, HNC, and HC3N) detected in the JWST/MIRI MRS spectrum (4.9–27.9 μm) of the local ultra luminous infrared galaxy (ULIRG) IRAS 07251−0248. We find that the molecular absorptions are blueshifted by 160 km/s relative to the systemic velocity of the target. Using local thermal equilibrium (LTE) excitation models, we derive rotational temperatures (T_rot) from 42 to 185 K for these absorption bands. This range of measured T_rot can be explained by infrared (IR) radiative pumping as a byproduct of the strength, effective critical density, and opacity of each molecular band. Thus, these results suggest that these absorptions originate in a warm expanding gas shell (Ṁ~90–330 M_sun/yr), which might be the base of the larger scale cold molecular outflow detected in this source. Finally, the elevated abundance of molecular cations can be explained by a high cosmic ray ionization rate, with log(zeta_H2 / n_H [cm3/s]) in the range of −18.2 (from H3+) to −19.1 (inferred from HCO+ and N2H+, which are likely tracing denser gas), consistent with a cosmic ray

dominated chemistry as predicted by chemical models.

Accepted for publication in MNRAS
DOI: 10.1093/mnrasl/slaf079
Full-text URL: https://arxiv.org/abs/2506.17390

First detection of HS2 in a cold dark cloud

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We report the first detection of HS2 towards the cold dark cloud TMC-1. This is the first observation of a chemical species containing more than one sulphur atom in this type of sources. The astronomical observations are part of QUIJOTE, a line survey of TMC-1 in the Q band (31–50 GHz) with the Yebes-40m telescope. The detection is confirmed by the observation of the fine and hyperfine components of two rotational transitions (2(0, 2)–1(0, 1) and 3(0, 3)–2(0, 2)). Assuming a rotational temperature of 7 K, we derived an HS2 column density of 5.7e11 cm-2, using a local thermodynamic equilibrium model that reproduces the observed spectra. The abundance of HS2 relative to H2 is 5.7e-11, which means that it is about seven times more abundant than its oxygenated counterpart HSO. We also explored the main formation and destruction mechanisms of HS2 using a chemical model, which reproduces the observed abundance of HS2 and indicates that dissociative recombination reactions from the ions H2S2+ and H3S2+ play a major role in forming HS2.

Astronomy & Astrophysics Letters, Volume 699, id.L2, 5
DOI: 10.1051/0004-6361/202555384
Full-text URL: https://arxiv.org/abs/2506.12974

Discovery of propenethial (CH2CHCHS) in TMC-1: The sulphur analogue of acrolein

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We present the detection of propenethial (CH2CHCHS), the sulphur analogue of interstellar acrolein (CH2CHCHO), towards TMC-1. The detection of this new sulphur molecule in TMC-1 is based on the data derived from rotational spectroscopy laboratory experiments, including new data in the millimetre wave domain, which are also presented in this work. Propenethial was observed in the cold dark cloud TMC-1 using data from the ongoing QUIJOTE line survey, which is being carried out with the Yebes 40m telescope. A total of nine rotational transitions with J = 6 up to 9 and Ka = 0 and 1 were detected in the 31.0–50.4 GHz range. We derive a total column density for propenethial of (4.4+/-0.4) e10 cm-2, which is 2, 6.8, and 27 times smaller than those for CH3CHS, HCCHS, and NCCHS, which are the other thioaldehyde derivatives detected in TMC-1. The abundance ratio found in TMC-1 between the aldehyde counterpart, acrolein, and propenethial is 4.7, which is also different from those found for other pairs of aldehydes-thioaldehydes in this source. Our investigation of possible chemical formation pathways suggests that CH2CHCHS likely results from a combination of gas- and surface-phase reactions.

Astronomy & Astrophysics, 698, L24 (2025)
DOI: 10.1051/0004-6361/202554670
Full-text URL: https://doi.org/10.1051/0004-6361/202554670

Rotational spectroscopy and astronomical search of the HCCSO radical

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The number of sulphur-bearing species detected to date in the interstellar medium (ISM) is small compared to oxygen- and nitrogen-bearing species. In fact, the chemistry of sulphur-bearing molecules is strongly dependent on the depletion of sulphur. One of the main inputs to understand the chemistry of sulphur in the ISM is to unveil new molecules containing this element as well as to understand their formation paths. For this purpose, we investigate the rotational spectrum of the HCCSO radical, which seems to be a potential candidate for observation in the molecular clouds where the simpler analogue, HSO, has already been detected. The HCCSO radical has been produced by an electric discharge of thionyl chloride (Cl2SO) and acetylene (HCCH) in argon, and its rotational spectrum between 11 and 40 GHz has been characterized using a Balle–Flygare narrow band-type Fourier-transform microwave spectrometer. Accurate spectroscopic parameters were derived from the spectral analysis and employed to obtain reliable frequency predictions for astronomical searches in different sources. We searched for HCCSO in several molecular clouds where HSO has been observed, B1-b, L183, L483, and TMC-1, but did not detect it. The upper limits to its abundance in these sources were derived.

MNRAS 539, 3257–3262 (2025)
DOI: 10.1093/mnras/staf701
Full-text URL: https://doi.org/10.1093/mnras/staf701

Exploring circumstellar chemistry in X-ray emitting AGB stars

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Aims. Our goal is to characterise the chemistry and physical conditions of the circumstellar envelopes (CSEs) of Asymptotic Giant Branch (AGB) binary candidate stars with UV-excess and X-ray emission. In particular, our aim is to identify the effects of the internal X-ray emission in the abundance of certain key molecules. Methods. We observed the 86.0–94.0 and 260.0–272.5 GHz spectral ranges and searched for rotational transitions of the X-ray sensitive molecule HCO+ in four AGB stars. Two detected in both UV and X-ray emission, and the other two detected only in UV. We derived the CSEs's physical parameters from previous CO observations and determined the molecular abundances of the detected species using radiative transfer models. We developed chemical kinetics models that account for the effects of internal X-ray emission (as well as UV radiation) and compared our predictions with observations. Results. We report the detection of HCO+ in the X-ray emitting C-rich AGB T Dra, while it remains undetected in the spectra of the other three sources. In T Dra we also detected SiO, HCN, HNC, HC3N, SiC2, C2H, and SiS. For the other targets, only HCN and SiO were detected. The high fractional abundance of HCO+ derived for T Dra ([1.5–3.0]×10^{-8}) is in good agreement with the predictions from our chemical kinetics models including the effects of internal X-ray emission, and one order of magnitude higher than the values expected for C-rich AGB stars. Additionally, we identified abundance enhancements for HNC and HC3N alongside a depletion of CO in the innermost regions of T Dra's envelope. Conclusions. An internal X-ray source can significantly alter molecular abundances in AGB CSEs, and enhance HCO+, N2H+, HNC, and HC3N while depleting parent species like CO. The UV radiation has a weaker effect unless the envelope is optically thin or porous.

2025 A&A, 698, A319
DOI: 10.1051/0004-6361/202553819
Full-text URL: https://arxiv.org/abs/2504.19616

The mutual influence of disequilibrium composition and temperature in exoplanet atmospheres

Marcelino Agundez

We have developed a 1D planetary atmosphere model that solves in a self-consistent manner the evolution of temperature and disequilibrium chemistry in the vertical direction. Thermochemical kinetics is based on a reaction network built from scratch that includes 164 gaseous species composed of H, C, N, O, S, Si, P, Ti, He, and Ar, connected by 2352 forward reactions. The model is applied to the well-known gas giant exoplanets WASP-33b, HD209458b, HD189733b, GJ436b, and GJ1214b, and to secondary atmospheres that exoplanets characterized in the future may plausibly have. For irradiated gas giants with solar or supersolar metallicity, the corrections to the temperature due to disequilibrium chemistry are relatively small, on the order of 100 K at most, in agreement with previous studies. Although the atmospheric composition of some of these planets deviates significantly from chemical equilibrium, the impact on the temperature is moderate because the abundances of the main atmospheric species that provide opacity, such as H2O, CO2, CO, and/or CH4, are not seriously modified by disequilibrium chemistry. An impact on the temperature greater than 100 K appears in hot Jupiters due to TiO, which is predicted to be seriously depleted by UV photons in the upper layers. However, the extent of this depletion, and thus of its impact on the temperature, is uncertain due to the lack of knowledge about TiO photodestruction. In secondary atmospheres, the impact of disequilibrium chemistry on the temperature depends on the composition. In atmospheres dominated by H2O and/or CO2 the temperature is not affected to an important extent. However, reducing atmospheres dominated by CH4 and oxidizing atmospheres dominated by O2 see their temperature being seriously affected due to the important processing of the atmospheric composition induced by disequilibrium chemistry.

2025, A&A, 699, A306
DOI: 10.1051/0004-6361/202554732
Full-text URL: https://arxiv.org/abs/2506.11658

Metallic species in interstellar medium: Astrochemical modeling

Ankan Das, Milan Sil, and Paola Caselli

Metal-bearing species in diffuse or molecular clouds are often overlooked in astrochemical modeling except for the charge exchange process. However, catalytic cycles involving these metals can affect the abundance of other compounds. We prepared a comprehensive chemical network for Na, Mg, Al, Fe, K, and Si-containing species. Assuming water as the major constituent of interstellar ice in dark clouds, quantum chemical calculations were carried out to estimate the binding energy of important metallic species, considering amorphous solid water as substrate. Significantly lower binding energies (approximately 5 to 6 times) were observed for Na and Mg, while the value for Fe was roughly 4 times higher than what was used previously. Here, wecalculated binding energy values for Al and K, for which no prior guesses were available. The total dipole moments and enthalpies of formation for several newly included species are unknown. Furthermore, the assessment of reaction enthalpies is necessary to evaluate the feasibility of the new reactions under interstellar conditions. These parameters were estimated and subsequently integrated into models. Some additional species that were not included in the UMIST/KIDA database have been introduced. The addition of these new species, along with their corresponding reactions, appears to significantly affect the abundances of related species. Some key reactions that significantly influence general metal-related chemistry include: M^+ + H_2 -> MH_2^+ + h nu, MH + O -> MO + H (M = Fe, Na, Mg, Al, K), and M_1^+ + M_2H -> M_1H + M_2^+ (where M_1 not equal to M_2, M_1, M_2 = Na, Mg, Al, K, Fe). Significant changes were observed in magnesium and sodium-bearing cyanides, isocyanides, and aluminum fluoride when additional reaction pathways were considered.

Accepted for publication in Astronomy and Astrophysics
DOI: 10.1051/0004-6361/202452044
Full-text URL: http://arxiv.org/abs/2506.19463

Announcements

Announcements

Conference (Save the date): ECLA 2026, “Exploring the cold universe”

The next European Conference on Laboratory Astrophysics (ECLA) will be held from September 21st, 2026 to September 25th, 2026 at the Max Planck Institute for Nuclear Physics (MPIK) in Heidelberg, Germany. The institute is home to the Cryogenic Storage Ring (CSR), exploring reactions at interstellar medium conditions. The meeting is co-organized by the Max Planck Institute for Astronomy (MPIA), which is operating a laboratory astrophysics facility - the "Origins of Life Lab". We will open the website for pre-registration in fall. The City of Heidelberg is easy to reach by train and plane (Frankfurt International Airport). We hope to see as many of you as possible next year in Heidelberg.
Holger Kreckel, Thomas Henning (for the SOC) and C. Joblin (for the ECLA standing SOC)