

# AstroChemical Newsletter #98

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## Abstracts

### The GUAPOS project: G31.41+0.31 Unbiased ALMA sPectral Observational Survey. IV. Phosphorus-bearing molecules and their relation with shock tracers

Fontani, F., Mininni, C., Beltran, M.T., Rivilla, V.M., Colzi, L., et al.

The astrochemistry of the important biogenic element phosphorus (P) is still poorly understood, but observational evidence indicates that P-bearing molecules are likely associated with shocks. We study P-bearing molecules, as well as some shock tracers, towards one of the chemically richest hot molecular core, G31.41+0.31, in the framework of the project "G31.41+0.31 Unbiased ALMA sPectral Observational Survey" (GUAPOS), observed with the Atacama Large Millimeter Array (ALMA). We have observed the molecules PN, PO, SO, SO<sub>2</sub>, SiO, and SiS, through their rotational lines in the spectral range 84.05-115.91 GHz, covered by the GUAPOS project. PN is clearly detected while PO is tentatively detected. The PN emission arises from two regions southwest of the hot core peak, "1" and "2", and is undetected or tentatively detected towards the hot core peak. The PN and SiO lines are very similar both in spatial emission morphology and spectral shape. Region "1" is in part overlapping with the hot core and it is warmer than region "2", which is well separated from the hot core and located along the outflows identified in previous studies. The column density ratio SiO/PN remains constant in regions "1" and "2", while SO/PN, SiS/PN, and SO<sub>2</sub>/PN decrease by about an order of magnitude from region "1" to region "2", indicating that SiO and PN have a common origin even in regions with different physical conditions. Our study firmly confirms previous observational evidence that PN emission is tightly associated with SiO and it is likely a product of shock-chemistry. We propose the PN emitting region "2" as a new astrophysical laboratory for shock-chemistry studies

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### Observational Chemical Signatures of the Past FU Ori Outbursts

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FU Ori-type stars are young stellar objects (YSOs) experiencing luminosity outbursts by a few orders of magnitude, which last for  $\sim 10^2$  years. A dozen of FUors are known up to date, but many more currently quiescent YSOs could have experienced such outbursts in the last  $\sim 10^3$  years. To find observational signatures of possible past outbursts, we utilise ANDES, RADMC-3D code as well as CASA ALMA simulator to model the impact of the outburst on the physical and chemical structure of typical FU Ori systems and how it translates to the molecular lines' fluxes. We identify several combinations of molecular lines that may trace past FU Ori objects both with and without envelopes. The most promising outburst tracers from an observational perspective are the molecular flux combinations of the N<sub>2</sub>H<sup>+</sup> J = 3 - 2, C<sub>18</sub>O J = 2 - 1, H<sub>2</sub>CO (J<sub>K<sub>a</sub></sub>-J<sub>K<sub>c</sub></sub>) = 4<sub>04</sub>-3<sub>03</sub>, and HCN J = 3 - 2 lines. We analyse the processes leading to molecular flux changes and show that they are linked with either thermal desorption or enhanced chemical reactions in the molecular layer. Using observed CO, HCN, N<sub>2</sub>H<sup>+</sup> and H<sub>2</sub>CO line fluxes from the literature, we identify ten nearby disc systems that might have undergone FU Ori outbursts in the past  $\sim 10^3$  years: [MGM2012] 556, [MGM2012] 371 and [MGM2012] 907 YSOs in L1641, Class II protoplanetary discs around CI Tau, AS 209 and IM Lup and transitional discs DM Tau, GM Aur, LkCa 15 and J1640-2130.

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### JWST: Deuterated PAHs, PAH-nitriles, and PAH Overtone and Combination Bands I: Program Description and First Look

Boersma, C., Allamandola, L.J., Esposito, V.J., Maragkoudakis, A., Bregman, J.D., Temi, P., Lee, T.J., Fortenberry, R.C., Peeters, E.

A first look is taken at the NIRSpec 1–5  $\mu$ m observations from James Webb Space Telescope program 1591 that targets seven objects along the low-mass stellar life cycle with polycyclic aromatic hydrocarbon (PAH) emission. Spectra extracted from a 1".5 radius circular aperture are explored, showing a wealth of features, including the 3  $\mu$ m PAH complex, the PAH continuum, and atomic and molecular emission lines from H I, He, H<sub>2</sub>, and other species. CO<sub>2</sub>- and H<sub>2</sub>O-ice absorption and CO emission is also seen. Focusing on the bright-PDR position in M17, the PAH CH stretch falls at 3.29  $\mu$ m (FWHM = 0.04  $\mu$ m). Signs of its 1.68  $\mu$ m overtone are confused by line emission in all targets. Multicomponent decomposition reveals a possible aliphatic deuterated PAH feature centered at 4.65  $\mu$ m (FWHM = 0.02  $\mu$ m), giving [D/H]<sub>alip</sub> = 31%  $\pm$  12.7%.

However, there is little sign of its aromatic counterpart between 4.36 and 4.43  $\mu\text{m}$ . There is also little sign of PAH nitrile emission between 4.34 and 4.39  $\mu\text{m}$ . A PAH continuum rises from  $\sim 1$  to 3.2  $\mu\text{m}$ , after which it jumps by about a factor of 2.5 at 3.6  $\mu\text{m}$ , with bumps at 3.8, 4.04, and 4.34  $\mu\text{m}$  adding structure. The CO<sub>2</sub> absorption band in M17 is matched with 10:1 H<sub>2</sub>O:CO<sub>2</sub> ice at 10 K. The  $v = 0$  pure rotational molecular hydrogen population diagram reveals  $>2200$  K UV-pumped gas. The hydrogen Pfund series runs from levels 10 to  $>30$ . Considering  $\text{Br}\alpha/\text{Br}\beta = 0.381 \pm 0.01966$  and Case B recombination results in  $AV \approx 8$ . CO emission in IRAS 21282+5050 originates from 258 K gas. In-depth spectral–spatial analysis of all features and targets is planned for a series of forthcoming papers.

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## JOYS+: mid-infrared detection of gas-phase SO<sub>2</sub> emission in a low-mass protostar. The case of NGC 1333 IRAS2A: hot core or accretion shock?

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JWST/MIRI has sharpened our infrared eyes toward the star formation process. This paper presents the first mid-infrared detection of gaseous SO<sub>2</sub> emission in an embedded low-mass protostellar system. MIRI-MRS observations of the low-mass protostellar binary NGC 1333 IRAS2A are presented from the JWST Observations of Young protoStars (JOYS+) program, revealing emission from the SO<sub>2</sub>  $v_3$  asymmetric stretching mode at 7.35 micron. The results are compared to those derived from high-angular resolution SO<sub>2</sub> data obtained with ALMA. The SO<sub>2</sub> emission from the  $v_3$  band is predominantly located on  $\sim 50$ – $100$  au scales around the main component of the binary, IRAS2A1. A rotational temperature of  $92 \pm 8$  K is derived from the  $v_3$  lines. This is in good agreement with the rotational temperature derived from pure rotational lines in the vibrational ground state (i.e.,  $v=0$ ) with ALMA ( $104 \pm 5$  K). However, the emission of the  $v_3$  lines is not in LTE given that the total number of molecules predicted by a LTE model is found to be a factor  $2 \times 10^4$  higher than what is derived for the  $v=0$  state. This difference can be explained by a vibrational temperature that is  $\sim 100$  K higher than the derived rotational temperature of the  $v=0$  state. The brightness temperature derived from the continuum around the  $v_3$  band of SO<sub>2</sub> is  $\sim 180$  K, which confirms that the  $v_3=1$  level is not collisionally populated but rather infrared pumped by scattered radiation. This is also consistent with the non-detection of the  $v_2$  bending mode at 18–20 micron. Given the rotational temperature, the extent of the emission ( $\sim 100$  au in radius), and the narrow line widths in the ALMA data (3.5 km/s), the SO<sub>2</sub> in IRAS2A likely originates from ice sublimation in the central hot core around the protostar rather than from an accretion shock at the disk-envelope boundary.

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## Single-atom catalysis in space: Computational exploration of Fischer–Tropsch reactions in astrophysical environments

Pareras, Cabedo, McCoustra & Rimola

Gas-phase chemistry at extreme conditions (low densities and temperatures) is difficult, so the presence of interstellar grains is especially important for the synthesis of molecules that cannot form in the gas phase. Interstellar grains are advocated to enhance the encounter rate of the reactive species on their surfaces and to dissipate the energy excess of largely exothermic reactions, but less is known of their role as chemical catalysts that provide low activation energy pathways with enhanced reaction rates. Different materials with catalytic properties are present in interstellar environments, like refractory grains containing space-abundant d-block transition metals. In this work we report for first time mechanistic insights on the Fischer–Tropsch methanol (CH<sub>3</sub>OH) synthesis under astrophysical conditions using single-atom Fe-containing silica surfaces as interstellar heterogeneous catalysts. Quantum chemical calculations considering extended periodic surfaces were carried out in order to search for the stationary points and transitions states to finally construct the reaction potential energy surfaces. Binding energy and kinetic calculations based on the Rice–Ramsperger–Kassel–Marcus (RRKM) scheme were also performed to evaluate the catalytical capacity of the grain and to allocate those reaction processes within the astrochemical framework. Our mechanistic studies demonstrate that astrocatalysis is feasible in astrophysical environments. Thermodynamically the proposed process is largely exergonic, but kinetically it shows energy barriers that would need from an energy input in order to go through. Kinetic calculations also demonstrate the strong temperature dependency of the reaction process as tunnelling is not relevant in the involved energetic barriers. The present results can explain the presence of CH<sub>3</sub>OH in diverse regions where current models fail to reproduce its observational quantity. The evidence of astrocatalysis opens a completely new spectrum of synthetic routes triggering chemical evolution in space. From the mechanistic point of view the formation of methanol catalysed by a single atom of Fe<sup>0</sup> is feasible; however, its dependency on the temperature makes the energetics a key issue in this scenario.

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## $\alpha$ -enhanced astrochemistry: the carbon cycle in extreme galactic conditions

Bisbas, T.G., Zhang, Z-Y., Gjergo, E., Zhao, Y-H., Luo, G., Quan, D., Jiang X-J., Sun, Y., Topkaras, T., Li, D., and Guo, Z.

Astrochemistry has been widely developed as a power tool to probe physical properties of the interstellar medium (ISM) in various conditions of the Milky Way (MW) Galaxy, and in near and distant galaxies. Most current studies conventionally apply linear scaling to all elemental abundances based on the gas-phase metallicity. However, these elements, including carbon and oxygen, are enriched differentially by stellar nucleosynthesis and the overall galactic chemical evolution, evident from  $\alpha$ -enhancement in multiple galactic observations such as starbursts, high-redshift star-forming galaxies, and low-metallicity dwarfs. We perform astrochemical modeling to simulate the impact of an  $\alpha$ -enhanced ISM gas cloud on the abundances of the three phases of carbon (C<sup>+</sup>, C, CO) dubbed as 'the carbon cycle'. The ISM environmental parameters considered include two cosmic-ray ionization rates ( $\zeta_{\text{cr}}=1\text{e-}17$  and  $1\text{e-}15$  s<sup>-1</sup>), two isotropic FUV radiation field strengths ( $\chi/\chi_0=1$  and  $1\text{e}2$ ), and (sub-)linear dust-to-gas relations against metallicity, mimicking the ISM conditions of different galaxy types. In galaxies with  $[\text{C}/\text{O}]<0$ , CO, C and C<sup>+</sup> all decrease in both abundances and emission, though with differential biases. The low-J CO emission is found to be the most stable tracer for the molecular gas, while C and C<sup>+</sup> trace H<sub>2</sub> gas only under limited conditions, in line with recent discoveries of [C I]-dark galaxies. We call for caution when using [C II] $\sim$ 158 $\mu\text{m}$  and [C I](1-0) as alternative H<sub>2</sub>-gas tracers for both diffuse and dense gas with non-zero [C/O] ratios.

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### JWST Observations of Young protoStars (JOYS+): Detection of icy complex organic molecules and ions. I. CH<sub>4</sub>, SO<sub>2</sub>, HCOO<sup>-</sup>, OCN<sup>-</sup>, H<sub>2</sub>CO, HCOOH, CH<sub>3</sub>CH<sub>2</sub>OH, CH<sub>3</sub>CHO, CH<sub>3</sub>OCHO, CH<sub>3</sub>COOH

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Complex organic molecules (COMs) detected in the gas phase are thought to be mostly formed on icy grains, but no unambiguous detection of icy COMs larger than CH<sub>3</sub>OH has been reported so far. Exploring this matter in more detail has become possible with the JWST the critical 5-10  $\mu\text{m}$  range. In the JOYS+ program, more than 30 protostars are being observed with the MIRI/MRS. This study explores the COMs ice signatures in the low and high-mass protostar, IRAS 2A and IRAS 23385, respectively. We fit continuum and silicate subtracted observational data with IR laboratory ice spectra. We use the ENIIGMA fitting tool to find the best fit between the lab data and the observations and to performs statistical analysis of the solutions. We report the best fits for the spectral ranges between 6.8 and 8.6  $\mu\text{m}$  in IRAS 2A and IRAS 23385, originating from simple molecules, COMs, and negative ions. The strongest feature in this range (7.7  $\mu\text{m}$ ) is dominated by CH<sub>4</sub> and has contributions of SO<sub>2</sub> and OCN<sup>-</sup>. Our results indicate that the 7.2 and 7.4  $\mu\text{m}$  bands are mostly dominated by HCOO<sup>-</sup>. We find statistically robust detections of COMs based on multiple bands, most notably CH<sub>3</sub>CHO, CH<sub>3</sub>CH<sub>2</sub>OH, and CH<sub>3</sub>OCHO. The likely detection of CH<sub>3</sub>COOH is also reported. The ice column density ratios between CH<sub>3</sub>CH<sub>2</sub>OH and CH<sub>3</sub>CHO of IRAS 2A and IRAS 23385, suggests that these COMs are formed on icy grains. Finally, the derived ice abundances for IRAS 2A correlate well with those in comet 67P/GC within a factor of 5. Based on the MIRI/MRS data, we conclude that COMs are present in interstellar ices, thus providing additional proof for a solid-state origin of these species in star-forming regions. The good correlation between the ice abundances in comet 67P and IRAS 2A is in line with the idea that cometary COMs can be inherited from the early protostellar phases.

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### Sulphur ion implantation into O<sub>2</sub>, CO, and CO<sub>2</sub> ices: Implications for the formation of sulphur-bearing molecules in the Kuiper Belt

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Previous experimental work has systematically investigated the radiolytic sulphur chemistry arising as a result of the implantation of reactive sulphur ions into various oxygen-bearing molecular ices (e.g., H<sub>2</sub>O, CO<sub>2</sub>) so as to better understand the surface chemistry of the Galilean moons of Jupiter, where sulphur ions are sourced from the giant Jovian magnetosphere. However, significantly less attention has been paid to analogous sulphur chemistry occurring under conditions relevant to the Kuiper Belt, where sulphur ions supplied by the solar wind may implant into the surfaces of icy bodies that are rich in volatile oxygen-bearing molecular ices such as O<sub>2</sub>, CO, or CO<sub>2</sub>. This paper presents the results of a study on the implantation of 290–400 keV S<sup>+</sup> ions into pure O<sub>2</sub>, CO, and CO<sub>2</sub> ices under temperature, pressure, radiation dose, and ice deposition conditions relevant to the Kuiper Belt, with a particular focus on the potential synthesis of simple inorganic sulphur-bearing molecules (e.g., SO<sub>2</sub>, OCS, CS<sub>2</sub>). Experiments involving CO<sub>2</sub> ices were also performed at higher temperatures more typically associated with the Galilean moon system so as to determine whether there exist any differences in the chemistry resulting from the implantation of reactive sulphur ions in these two regions of the Solar System. Our results constitute the first systematic investigation of solid-phase sulphur chemistry in the Kuiper Belt mediated by the

sulphur ion component of the solar wind, and thus represent an important step forward in our understanding of the astrochemical processes occurring in the outermost depths of the Solar System.

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