AstroChemical Newsletter #86

January 2023

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Abstracts

A large (~1 pc) contracting envelope around the prestellar core L1544

E. Redaelli, A. Chacón-Tanarro, P. Caselli, M. Tafalla, J. E. Pineda, S. Spezzano, O. Sipilä

Prestellar cores, the birthplace of Sun-like stars, form from the fragmentation of the filamentary structure that composes molecular clouds, from which they must inherit at least partially the kinematics. Furthermore, when they are on the verge of gravitational collapse, they show signs of subsonic infall motions. How extended these motions are, which depends on how the collapse occurs, remains largely unknown. We want to investigate the kinematics of the envelope that surrounds the prototypical prestellar core L1544, studying the cloud-core connection. To our aims, we observed the HCO+ (1-0) transition in a large map. HCO+ is expected to be abundant in the envelope, making it an ideal probe of the large-scale kinematics in the source. We modelled the spectrum at the dust peak by means of a non local-thermodynamical-equilibrium radiative transfer. In order to reproduce the spectrum at the dust peak, a large (~1pc) envelope is needed, with low density (tens of cm^{-3} at most) and contraction motions, with an inward velocity of ~0.05km/s . We fitted the data cube using the Hill5 model, which implements a simple model for the optical depth and excitation temperature profiles along the line-of-sight, in order to obtain a map of the infall velocity. This shows that the infall motions are extended, with typical values in the range 0.1−0.2km/s . Our results suggest that the contraction motions extend in the diffuse envelope surrounding the core, which is consistent with recent magnetic field measurements in the source, which showed that the envelope is magnetically supercritical.

Accepted for publication in ApJ (Oct 22)
DOI: [10.3847/1538-4357/ac9d8b](10.3847/1538-4357/ac9d8b)
Full-text URL: https://arxiv.org/abs/2210.13571

The Core Population and Kinematics of a Massive Clump at Early Stages: An Atacama Large Millimeter/submillimeter Array View

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High-mass star formation theories make distinct predictions on the properties of the prestellar seeds of high-mass stars. Observations of the early stages of high-mass star formation can provide crucial constraints, but they are challenging and scarce. We investigate the properties of the prestellar core population embedded in the high-mass clump AGAL014.492-00.139, and we study the kinematics at the clump and clump-to-core scales. We have analyzed an extensive data set acquired with the Atacama Large Millimeter/submillimeter Array interferometer. Applying a dendrogram analysis to the Band 7 o-H2D+ data, we identified 22 cores. We fitted their average spectra in local thermodynamic equilibrium conditions, and we analyzed their continuum emission at 0.8 mm. The cores have transonic to mildly supersonic turbulence levels and appear to be mostly low-mass, with Mcore<30Msun . Furthermore, we have analyzed Band 3 observations of the N2H+ (1-0) transition, which traces the large-scale gas kinematics. Using a friend-of-friend algorithm, we identify four main velocity coherent structures, all of which are associated with prestellar and protostellar cores. One of them presents a filament-like structure, and our observations could be consistent with mass accretion toward one of the protostars. In this case, we estimate a mass accretion rate of Macc≈2×10−4 Msun/yr. Our results support a clump-fed accretion scenario in the target source. The cores in the prestellar stage are essentially low-mass, and they appear to be subvirial and gravitationally bound, unless further support is available, for instance, due to magnetic fields.

The Astrophysical Journal, Volume 936, Issue 2, id.169, 26 pp.
DOI: [10.3847/1538-4357/ac85b4](https://doi.org/10.3847/1538-4357/ac85b4)
Full-text URL: https://arxiv.org/abs/2208.01675

Gas kinematics around filamentary structures in the Orion B cloud

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Understanding the initial properties of star-forming material and how they affect the star formation process is key. From an observational point of view, the feedback from young high-mass stars on future star formation properties is still poorly constrained. In the framework of the IRAM 30m ORION-B large program, we obtained observations of the translucent and moderately dense gas, which we used to analyze the kinematics over a field of 5 deg2 around the filamentary structures. We used the ROHSA algorithm to decompose and de-noise the C18O(1-0) and 13CO(1-0) signals by taking the spatial coherence of the emission into account. We produced gas column density and mean velocity maps to estimate the relative orientation of their spatial gradients. We identified three cloud velocity layers at different systemic velocities and extracted the filaments in each velocity layer. The filaments are preferentially located in regions of low centroid velocity gradients. By comparing the relative orientation between the column density and velocity gradients of each layer from the ORION-B observations and synthetic observations from 3D kinematic toy models, we distinguish two types of behavior in the dynamics around filaments: (i) radial flows perpendicular to the filament axis that can be either inflows (increasing the filament mass) or outflows and (ii) longitudinal flows along the filament axis. The former case is seen in the Orion B data, while the latter is not identified. We have also identified asymmetrical flow patterns, usually associated with filaments located at the edge of an HII region. This is the first observational study to highlight feedback from HII regions on filament formation and, thus, on star formation in the Orion B cloud. This simple statistical method can be used for any molecular cloud to obtain coherent information on the kinematics.

Accepted to A&A
Full-text URL: https://arxiv.org/abs/2211.14350

The complex organic molecular content in the L1517B starless core

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Recent observations of the pre-stellar core L1544 and the younger starless core L1498 have revealed that complex organic molecules (COMs) are enhanced in the gas phase toward their outer and intermediate-density shells. Our goal is to determine the level of chemical complexity toward the starless core L1517B, which seems younger than L1498, and compare it with the other two previously studied cores to see if there is a chemical evolution within the cores. We have carried out 3 mm high-sensitivity observations toward two positions in the L1517B starless core: the core's centre and the position where the methanol emission peaks (at a distance of ~5000 au from the core's centre). Our observations reveal that a lower number of COMs and COM precursors are detected in L1517B with respect to L1498 and L1544, and also show lower abundances. Besides methanol, we only detected H2CCO, CH3CHO, CH3CN, CH3NC, HCCCN, and HCCNC. Their measured abundances are ~3 times larger toward the methanol peak than toward the core's centre, mimicking the behaviour found toward the more evolved cores L1544 and L1498. We propose that the differences in the chemical complexity observed between the three studied starless cores are a consequence of their evolution, with L1517B being the less evolved one, followed by L1498 and L1544. Chemical complexity in these cores seems to increase over time, with N-bearing molecules forming first and O-bearing COMs forming at a later stage as a result of the catastrophic depletion of CO.

Monthly Notices of the Royal Astronomical Society, 2022, accepted
DOI: 10.1093/mnras/stac3449
Full-text URL: https://arxiv.org/abs/2211.16119

The spectral features and detectability of small, cyclic silicon carbide clusters

Christopher M. Sehring, C. Zachary Palmer, Brent R. Westbrook, and Ryan C. Fortenberry

Rovibrational spectral data for several tetra-atomic silicon carbide clusters (TASCCs) are computed in this work using a CCSD(T)-F12b/cc-pCVTZ-F12 quartic force field. Accurate theoretical spectroscopic data may facilitate the observation of TASCCs in the interstellar medium which may lead to a more complete understanding of how the smallest silicon carbide (SiC) solids are formed. Such processes are essential for understanding SiC dust grain formation. Due to SiC dust prevalence in the interstellar medium, this may also shed light on subsequent planetary formation. Rhomboidal Si2C2 is shown here to have a notably intense (247 km mol-1) anharmonic vibrational frequency at 988.1 cm-1 (10.1 um) for v2, falling into one of the spectral emission features typically associated with unknown infrared bands of various astronomical regions. Notable intensities are also present for several of the computed anharmonic vibrational frequencies including the cyclic forms of C4, SiC3, Si3C, and Si4. These features in the 6-10 µm range are natural targets for infrared observation with the James Webb Space Telescope (JWST)'s MIRI instrument. Additionally, t-Si2C2, d-Si3C, and r-SiC3 each possess dipole moments of greater than 2.0 D making them

interesting targets for radioastronomical searches especially since d-SiC3 is already known in astrophysical media.

Front. Astron. Space Sci., 9, 1074879, 2022.
DOI: [10.3389/fspas.2022.1074879](https://doi.org/10.3389/fspas.2022.1074879)
Full-text URL: https://www.frontiersin.org/articles/10.3389/fspas.2022.1074879/full

Reparameterized Semi-Empirical Methods for Computing Anharmonic Vibrational Frequencies of Multiply-Bonded Hydrocarbons

B. R. Westbrook, J. P. Layfield, T. J. Lee, and R. C. Fortenberry

Reparameterized semi-empirical methods can reproduce gas-phase experimental vibrational frequencies to within 24 cm^{-1} or better for a 100-fold decrease in computational cost in the anharmonic fundamental vibrational frequencies. To achieve such accuracy and efficiency, the default parameters in the PM6 semi-empirical model are herein optimized to reproduce the experimental and high-level theoretical vibrational spectra of three small hydrocarbon molecules, C_2H_2, c-C_3H_2, and C_2H_4, with the hope that these same parameters will be applicable to large polycyclic aromatic hydrocarbons (PAHs). This massive cost reduction allows for the computation of explicit anharmonic frequencies and the inclusion of resonance corrections that have been shown to be essential for accurate predictions of anharmonic frequencies. Such accurate predictions are necessary to help to disentangle the heretofore unidentified infrared spectral features observed around diverse astronomical bodies and hypothesized to be caused by PAHs, especially with the upcoming influx of observational data from the James Webb Space Telescope. The optimized PM6 parameters presented herein represent a substantial step in this direction with those obtained for ethylene (C_2H_4) yielding a 37% reduction in the mean absolute error of the fundamental frequencies compared to the default PM6 parameters.

2022, Electronic Structure, 4, 045003.
DOI: [10.1088/2516-1075/aca458](https://doi.org/10.1088/2516-1075/aca458)
Full-text URL: https://iopscience.iop.org/article/10.1088/2516-1075/aca458

Direct measurements of carbon and sulfur isotope ratios in the Milky Way

Yan Y. T., Henkel C., Kobayashi C., Menten K. M., Gong Y., Zhang J. S., Yu H. Z., Yang K., Xie J. J., Wang Y. X.

With the IRAM 30-m telescope, we performed observations of the J = 2-1 transitions of CS, C33S, C34S, C36S, 13CS, 13C33S, and 13C34 S as well as the J = 3-2 transitions of C33S, C34S, C36S, and 13CS toward a large sample of 110 HMSFRs. We measured the 12C/13C, 32S/34S, 32S/33S, 32S/36S, 34S/33S, 34S/36S, and 33S/36S abundance ratios with rare isotopologues of CS, thus avoiding significant saturation effects. With accurate distances obtained from parallax data, we confirm previously identified 12C/13C and 32S/34S gradients as a function of galactocentric distance (RGC). In the CMZ 12C/13C ratios are higher than suggested by a linear fit to the disk values as a function of RGC. While 32S/34S ratios near the Galactic center and in the inner disk are similar, this is not the case for 12C/13C, when comparing central values with those near RGC of 5 kpc. As was already known, there is no 34S/33S gradient but the average ratio of 4.35~ ± ~0.44, derived from the J = 2-1 transition lines of C34S and C33S, is well below previously reported values. A comparison between solar and local interstellar 32S/34S and 34S/33S ratios suggests that the solar system may have been formed

from gas with a particularly high 34S abundance. For the first time, we report positive gradients of 32S/33S, 34S/36S, 33S/36S and 32S/36S in our Galaxy. The predicted 12C/13C ratios from the latest GCE models are in good agreement with our results, while 32S/34S and 32S/36S ratios show larger differences at larger RGC, 32S/33S ratios show an offset across the entire inner 12 kpc of the Milky Way.

71 pages, 12 tables, 18 figures. Accepted for publication in A&A
Full-text URL: https://arxiv.org/abs/2212.03252

Direct Determination of the Activation Energy for Diffusion of OH Radicals on Water Ice

A. Miyazaki, M. Tsuge, H. Hidaka, Y. Nakai, and N. Watanabe

Using a combination of photostimulated desorption and resonance-enhanced multiphoton ionization methods, the behaviors of OH radicals on the surface of an interstellar ice analog were monitored at temperatures between 54 and 80 K. The OH number density on the surface of ultraviolet-irradiated compact amorphous solid water gradually decreased at temperatures above 60 K. Analyzing the temperature dependence of OH intensities with the Arrhenius equation, the decrease can be explained by the recombination of two OH radicals, which is rate-limited by thermal diffusion of OH. The activation energy for surface diffusion was experimentally determined for the first time to be 0.14 +/- 0.01 eV, which is larger than or equivalent to those assumed in theoretical models. This value implies that the diffusive reaction of OH radicals starts to be activated at approximately 36 K on interstellar ice.

2022 ApJL 940 L2
DOI: [10.3847/2041-8213/ac9d30](https://doi.org/10.3847/2041-8213/ac9d30)
Full-text URL: https://arxiv.org/abs/2210.13753

Star formation time-scale in the molecular filament WB 673

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We present the observations of ammonia emission lines toward the interstellar filament WB 673 hosting the dense clumps WB 673, WB 668, S233-IR, and G173.57+2.43. LTE analysis of the lines allows us to estimate gas kinetic temperature (<=30K in all the clumps), number density (7-17*1e3 cm-3), and ammonia column density (approx. 1-1.5*1e15 cm-2) in the dense clumps. We find signatures of collapse in WB 673 and presence of compact spatially unresolved dense clumps in S233-IR. We reconstruct 1D density and temperature distributions in the clumps and estimate their ages using astrochemical modelling. Considering CO, CS, NH3, and N2H+ molecules (plus HCN and HNC for WB 673), we find a chemical age of tchem = 1-3*1e5 yrs, providing the best agreement between the simulated and observed column densities in all the clumps. Therefore, we consider tchem as the chemical age of the entire filament. A long preceding low-density stage of gas accumulation in the astrochemical model would break the agreement between the simulated and observed column densities. We suggest that rapid star formation over a 10(5) yrs time-scale take place in the filament.

MNRAS, 2022, 517, 4669
DOI: [10.1093/mnras/stac2877](https://doi.org/10.1093/mnras/stac2877)
Full-text URL: https://arxiv.org/abs/2210.01576

Sulfur Ion Implantations Into Condensed CO2: Implications for Europa

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The ubiquity of sulfur ions within the Jovian magnetosphere has led to suggestions that the implantation of these ions into the surface of Europa may lead to the formation of SO2. However, previous studies on the implantation of sulfur ions into H2O ice (the dominant species on the Europan surface) have failed to detect SO2 formation. Other studies concerned with similar implantations into CO2 ice, which is also known to exist on Europa, have offered seemingly conflicting results. In this letter, we describe the results of a study on the implantation of 290 keV S+ ions into condensed CO2 at 20 and 70 K. Our results demonstrate that SO2 is observed after implantation at 20 K, but not at the Europa-relevant temperature of 70 K. We conclude that this process is likely not a reasonable mechanism for SO2 formation on Europa, and that other mechanisms should be explored instead.

Geophysical Research Letters, 2022, 49(24), e2022GL100698
DOI: 10.1029/2022GL100698
Full-text URL: https://arxiv.org/abs/2212.08947

The opaque heart of the galaxy IC 860: Analogous protostellar, kinematics, morphology, and chemistry

M. D. Gorski, S. Aalto, S. König, C. Wethers, C. Yang, S. Muller, S. Viti , J. H. Black, K. Onishi, and M. Sato

Compact Obscured Nuclei (CONs) account for a significant fraction of the population of luminous and ultraluminous infrared galaxies (LIRGs and ULIRGs). These galaxy nuclei are compact, with radii of 10-100 pc, with large optical depths at submm and far-infrared wavelengths, and characterized by vibrationally excited HCN emission. It is not known what powers the large luminosities of the CON host galaxies because of the extreme optical depths towards their nuclei. CONs represent an extreme phase of nuclear growth, hiding either a rapidly accreting supermassive black hole or an abnormal mode of star formation. Regardless of their power source, the CONs allow us to investigate the processes of nuclear growth in galaxies. Here we apply principal component analysis (PCA) tomography to high-resolution (0.06”) ALMA observations at frequencies 245 to 265 GHz of the nearby CON (59 Mpc) IC 860. PCA is a technique to unveil correlation in the data parameter space, and we apply it to explore the morphological and chemical properties of species in our dataset. The leading principal components reveal morphological features in molecular emission that suggest a rotating, infalling disk or envelope, and an outflow analogous to those seen in Galactic protostars. One particular molecule of astrochemical interest is methanimine (CH2NH), a precursor to glycine, three transitions of which have been detected towards IC 860. We estimate the average CH2NH column density towards the nucleus of IC 860 to be ~1e17 cm−2, with an abundance exceeding 1e−8 relative to molecular hydrogen, using the rotation diagram method and non-LTE radiative transfer models. This CH2NH abundance is consistent with those found in hot cores of molecular clouds in the Milky Way. Our analysis suggests that CONs are an important stage of chemical evolution in galaxies, that are chemically and morphologically similar to Milky Way hot cores.

A&A accepted
DOI: 10.1051/0004-6361/202245166
Full-text URL: https://arxiv.org/abs/2210.04499

Announcements

Post-doc position at IPAG, Grenoble, France

University of Grenoble, France
Post-doctoral position in molecular astrophysics

Applications are invited for a postdoctoral research associate at the Institute of Planetology and Astrophysics of Grenoble (IPAG) to conduct research in molecular excitation and radiative transfer for astrochemistry applications. The project, supported by a grant from the ERC project COLLEXISM (PI François Lique), involves the investigation of collisional, radiative and chemical pumping effects in the excitation of reactive hydride ions (H3+, HeH+, CH+, etc.) in harsh environments of the interstellar medium (e.g. photo-dissociation regions, planetary nebulae). Suprathermal processes, in particular, will be explored. A custom version of public radiative transfer codes will be combined with accurate collisional and reactive state-to-state data computed within the COLLEXISM project. The results will be compared to submillimeter and infrared rotational and ro-vibrational spectra of hydride ions observed, in particular, with the space/airborne observatories Herschel, SOFIA and JWST. The goal is to provide the best possible ion column densities and physical conditions (kinetic temperature and hydrogen density) and to make comparisons with available chemical models in order to determine relevant physical parameters such as the cosmic-ray ionization rate.

The successful candidate will work closely with Alexandre Faure and Pierre Hily-Blant at IPAG on the radiative transfer calculations and will tightly collaborate with the COLLEXISM group led by François Lique in Rennes.

The position is expected to be available starting March-June 2023 for an initial contract of 18 months. Candidates should have a PhD in astrophysics, with a good background in molecular excitation processes. Solid experience in radiative transfer and strong interest in numerical modeling including code development are highly desirable.

Inquires and applications, including a CV, statement of research interests, and the names and addresses of three references, should be addressed before January 13, 2023 to Alexandre Faure (alexandre.faure@obs.ujf-grenoble.fr), Pierre Hily-Blant (pierre.hily-blant@obs.ujf-grenoble.fr) and François Lique (francois.lique@univ-rennes1.fr).

2023 Kavli-IAU Astrochemistry Symposium. Astrochemistry VIII - From the First Galaxies to the Formation of Habitable Worlds. (REGISTRATION OPEN!)

2023 Kavli-IAU Astrochemistry Symposium.
Astrochemistry VIII - From the First Galaxies to the Formation of Habitable Worlds.
https://events.mpe.mpg.de/event/14/
Traverse City, MI, USA
10 – 14 Jul 2023

Astrochemistry is at the heart of many astrophysical fields, from the early Universe to local galaxies, to star- and planet-formation and evolution in our Milky Way, to exoplanet atmospheres, and to our Solar System. Decades-long concerted efforts of astronomers and theoretical/experimental chemists have provided a solid base for using molecules as powerful diagnostic tools of the physical and chemical structure, dynamics, and history of a multitude of astrophysical objects, allowing connections and glimpses into the life cycle of the interstellar medium, as well as into the growth of chemical complexity in space. The great sensitivity, high angular resolution and frequency coverage of telescopes such as ALMA have allowed unprecedented views of stellar and planet nurseries. JWST with its sensitive near- to mid-infrared spectrometers will soon open a new sensitive and sharp observing window into major molecular ingredients such as water, carbon dioxide as well as other key organic species. JWST will allow us to probe the composition of ices on interstellar and planet-forming scales, enabling studies of the linked-chemistry of exoplanetary atmospheres and protoplanetary disks. It is therefore timely for the eighth IAU Symposium on Astrochemistry that will allow the ever-growing astrochemical community to meet and discuss recent achievements and future progress including the possibilities of new connections to other fields.