SF2A 2025
A. Siebert, K. Baillié, M. Béthermin, F. Cantalloube, E. Josselin, N. Lagarde, J. Malzac, J. Richard, L. Selliez, O. Venot (eds)

CHEMICAL CONSTRAINTS ON THE DYNAMICAL EVOLUTION OF THE COLD CORE L694

A. Taillard[1], V. Wakelam[2], P. Gratier[2], E. Dartois[3], M. Chabot[4], J. A. Noble[5] and L. Chu[6]

Abstract. The trend of the chemical composition through the entire star formation process is already set at the very early phases. The cold cores, characterised by low temperatures (T<15 K), moderate densities (ranging from 10^3 to 10^6 cm^{-3}) and a high visual extinction ($A_V > 3$ mag) allow the formation of thick ices at the surface of the grains. The species in the solid-phase will enrich the gas-phase through non-thermal desorption mechanisms or remain in the mantle to form complex organic molecules. The kind of species present in the ices, and subsequently in the gas-phase, is partly set by the physical history of the grains and initial abundances. To understand how the early phases will impact the later stellar formation, it is important to trace both phases and their physical environment to add constraints on the chemistry at play in these extreme environments. In this study, we focus on the cold cores L694 and L429-C, both observed with infrared telescopes and with the IRAM 30m radiotelescope to map (300" x 300") the gas-phase abundances of a sample of molecules, focusing on CO, its isotopologues and methanol. Both cores have close physical parameters yet behave differently in their abundances, as L694 is already infalling contrary to L429-C. We present the difference in the observed abundances between the two cores, link it to the physical parameters derived in both sources and finally, focus on reproducing the observations with two types of model (static and dynamic) to understand what are the main constraints on the chemistry. We show that the static setups need far more evolutionary time to reproduce the observations within a factor of 10, whereas the dynamical setups' evolutionary time is faster but fails to reproduce the lower density. A larger sample of cores, with a systematic method to derive the abundance, is needed to fully paint the picture of the chemical trend that can be found in these early environments.

Keywords: Astrochemistry, ISM: abundances, ISM: clouds, ISM: Individual objects: LDN 694, ISM: molecules

1 Introduction

Pre-stellar cores begin to build the chemical trend that will be inherited during the proto-stellar phase, impacting the future stellar system and its composition. pre-stellar cores are defined by high densities ($n_H \sim 10^5$ cm^{-3}), a high visual extinction ($A_V > 3$ mag) and cold temperatures (T < 20 K) (Bergin & Tafalla 2007). In these particular physical conditions, the ice mantle starts to form on the dust grain as the gas starts to deplete on their surface. The depleted species will set the entire elemental budget for the next phases of the star formation since the ice mantles will grow to contain most of the initial gaseous matter. Chemical models show that the evolution of Complex Organic Molecules (COMs) is dependent on the physical parameter of the dust but also the dynamical evolution of the core (Clément et al. 2023). This evolution leads to a chemical variety of cores, despite sharing similar physical conditions (Fuente et al. 2019). To understand the different regimes that lead to these differences, we must constraint both the physical parameters and the chemical composition of pre-stellar cores. For instance, we focus on certain molecules forming only on the surface, such as CH_3OH, that is desorbed

[1] Centro de Astrobiología (CAB), CSIC-INTA, Ctra. de Ajalvir, km 4, Torrejón de Ardoz, 28850 Madrid, Spain
[2] Laboratoire d'Astrophysique de Bordeaux, Univ. Bordeaux, CNRS, B18N, allée Geoffroy Saint-Hilaire, 33615 Pessac, France
[3] Institut des sciences Moléculaires d'Orsay, CNRS, Université Paris-Saclay, Bât 520, Rue André Rivière, 91405 Orsay, France
[4] Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France
[5] Physique des Interactions Ioniques et Moléculaires, CNRS, Aix Marseille Univ., 13397 Marseille, France
[6] Institute for Astronomy, 2680 Woodlawn Drive, Honolulu, HI 96822-1897, USA

in the gas-phase through non-thermal desorption mechanisms (photo-desorption, chemical desorption, cosmic-rays (CR) induced desorption...). We study how the abundances in both phases are changing between two dense cores at different stages of development: L429-C (pre-collapse) and L694 (collapsing). These two cores have pre-JWST ice observations combining Spitzer and IRTF (Boogert et al. 2011; Chu et al. 2020) with an estimate of the methanol ice column density. We also observed them with the IRAM 30m telescope to map the gas-phase. Then, we use two different types of chemical models, static and dynamic, to constrain the chemical evolution of the two pres-tellar cores.

2 Sources description and observations

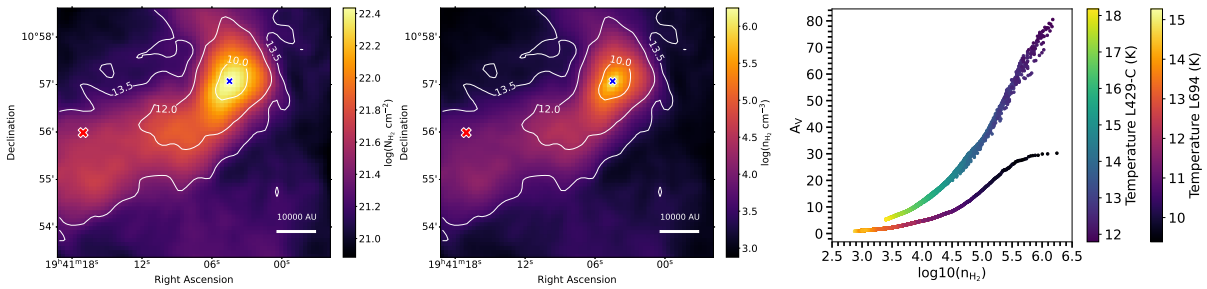

Fig. 1. Physical parameter maps of the cold core L694 derived from *Herschel* data, with temperature (K) in white contours. The blue cross indicates the dust continuum peak and the spatial scale is represented by the white bar (in AU). **Left:** H_2 column density map (N_{H_2} - cm^{-2}) **Middle:** H_2 volume density (n_{H_2} in cm^{-3}). **Right:** Visual extinction as a function of volume density, with temperature in colour-scale, for both L429-C and L694.

L429-C is a cold core located in the Aquila Rift, studied thoroughly in Taillard et al. (2023), presenting thick column densities of CH_3OH as observed with the NASA infrared telescope facility (IRTF) and *Spitzer* space telescope (Boogert et al. 2011). The core is still not infalling and rather chemically advanced considering the high ice column densities observed. L694 is also located in the Aquila Rift, labelled as infalling from molecular line profiles exhibiting redshifted self-absorption (Lee et al. 2001, 2004). L694 has been observed using the IRTF towards one background star where solid CH_3OH has been observed (Chu et al. 2020).

Both sources have been observed with the IRAM 30m radio telescope in similar setups to map the cores (300 x 300"), focusing on CH_3OH, CO and its isotopologues. We observed 11 molecules in L429-C and 10 in L694, where the full inventories are presented in Taillard et al. (2023) and Taillard et al. (2025) respectively. To compute the gas-phase abundances, we used *Herschel* dust continuum maps available for both cores, allowing us to derive the physical parameters (T_{dust}, A_V and N_{H_2}) at each pixel. The physical parameters maps of L694 are presented in Fig. 1, with on the right, the comparison with L429-C physical parameters obtained with the same method. In parallel, we extract the integrated intensity and line width of each molecular line at each pixel in our radio observations. We then use a radiative transfer inversion code to compute the theoretical intensity and compare it with the observed one. With a χ^2 minimisation, we obtain the column density of each molecule at each pixel. We then convert it to abundances w.r.t. H_2 by dividing it with H_2 column density. The full method is detailed in Taillard et al. (2023). In the end, we obtain the gas-phase abundance maps of each molecule as well as abundances as a function of physical parameters.

3 Comparison with chemical models

We run chemical models to reproduce the observations and constrain the most efficient non-thermal mechanisms. For this study, we choose to run two types of setups: a three-phase chemical model considering static physical parameters in the first case and Smooth Particle Hydrodynamics (SPH) model in the second case.

The static setup uses the gas-grain model considering constant physical parameters derived from our *Herschel* parameter maps. Nautilus (Ruaud et al. 2016; Wakelam et al. 2024) simulates the chemical evolution in the three phases (gas, ice mantle and surface). The code is based on kinetic rates and surface data from lab experiments and theoretical calculations. It takes as inputs the physical parameters (T_{gas},T_{dust}, n_H, A_V...) and it simulates the abundances of all three phases as a function of time. The input parameters are the ones derived for a few positions, covering the different densities observed (from 5×10^4 to 10^6 cm^{-3}). The dust temperature

is computed using the formalisms in Hocuk et al. (2017). We run two sets of static models, we vary the CR sputtering yield, with one set using the H_2O-rich value and the second one using CO_2-rich value (Dartois et al. 2018, 2020). We determine the "best" model using the distance of disagreement from Wakelam et al. (2006).

We then compare the resulting outputs with the observed abundances. The static model reproduces the observed gas-phase abundances within a factor of 10. It also manages to reproduce CO solid abundance almost perfectly and the model at low density using a low sputtering yield reproduces the methanol solid abundance within a factor of 3.

The second setup uses time varying physical parameters derived from a SPH model based on Bonnell et al. (2013), simulating the gas dynamic in a galactic potential in a 250 x 250 pc^2. Following the method presented in Ruaud et al. (2018), we selected a few trajectories where the final volume density is similar to the observed ones. We then selected all the particles in a radius of 0.5 pc around the peak density and derived their physical parameters evolution through time. We then ran Nautilus as post-processing, using these parameters. For both the dynamic and static models, the starting elemental abundances are the same and from Wakelam et al. (2021).

The dynamic setups exhibit a range of chemical abundances that depend on the histories of individual particles. It fails to reproduce most of the observed molecules at low density and CO abundance at high density. However, the depletion profile and abundances of CS and CH_3OH at high densities are well reproduced.

4 Discussion

4.1 Observations - Chemical comparison between the two cores

We compared the observed gas-phase abundances as a function of physical parameters of the two cores. In Fig. 2, we show the CO and CH_3OH gas-phase abundances as a function of density for L694 in red and L429-C in blue. Both cores show depletion profiles for all the observed molecules except for CH_3OH, that is rather constant through density in L429-C. This is expected as the cloud is not yet in an infalling state, where all molecules in the gas-phase are expected to drastically deplete.

4.2 Chemical modelling - Constraint on time

In the case of the static models, both L429-C and L694 chemical outputs are computed at the same "best" time no matter the density, showing that in Nautilus used as it is here, CO gas-phase abundance remains the main constraint on the chemical evolution time. Since both cold cores share similar physical parameters and CO abundances at high densities, the predictions are clearly similar, despite L429-C not infalling. This shows how strong is CO abundance on the chemical evolution time in static models.

4.3 Chemical modelling - Tracing the dynamical evolution of the cores

In the static models, we show that the time needed to reach the observed abundances in the densest part is about 10^4 yr, taking the assumption that the gas-phase elements are initially in atomic form. In the dynamical simulations, the timescale is computed depending on the physics and kinematics of the considered trajectory. Looking at the predicted CO abundances in Fig. 2, the dynamic setup strongly underestimates it at high densities. Opposite to the static simulations, the dynamic ones take much longer to form CO in the gas-phase by about an order of magnitude. Yet, CO chemistry is robust and well constrained in chemical models and is a good indicator of the depletion processes in cores (Wakelam et al. 2021). These results show that the dynamical simulations have an incompatible time-dependent density evolution compared to the CO observations at high densities. Multiple parameters impact the CO depletion: density, time and sticking coefficient. The latter could be improved with new laboratory measurements and has already shown its impact in models (Stadler et al. 2025). More recent hydrodynamic simulations with more realistic core formation timescale will need to be considered in future studies.

5 Conclusions

We studied the gas- and solid-phases of two pre-stellar cores, L429-C and L694, at different chemical stages. From the gas-phase observations, we see that all molecules show strong depletion at the dust continuum peak in both cores, except CH_3OH in L429-C where its abundance remains constant as density increases. This is expected as the core is in a less advanced dynamical state. We ran both static and dynamic models to compare

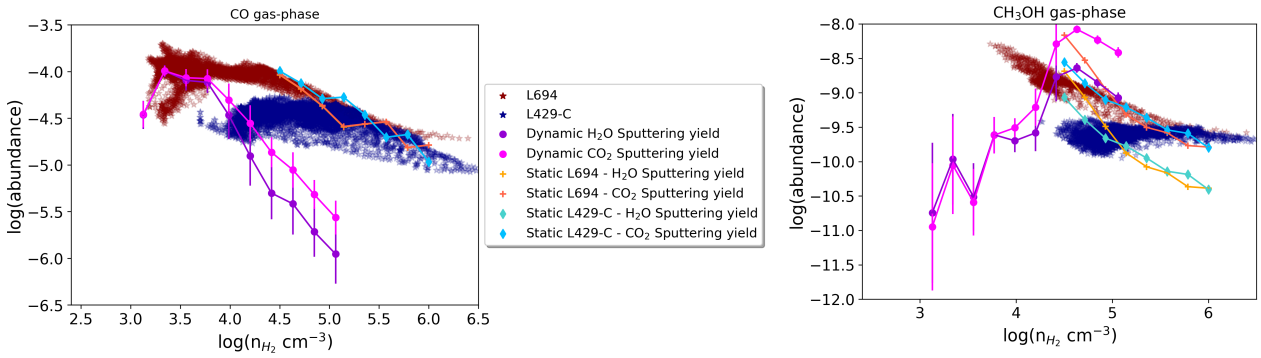

Fig. 2. Observed gas-phase abundances as a function of density of L694 (red stars) and L429-C (blue stars), with the modelled abundances of the static setups (crosses and diamonds) and the dynamic setups (points). **Left:** CO abundances. **Right:** CH_3OH abundances.

the dynamical evolution of the source. The static models reproduce the abundances within a factor of 10 and have their chemical timescale to reproduce the observations decrease with density (varying by a factor of ∼30 across the density range explored). The SPH dynamical models exhibit a range of chemical abundances that depend on the histories of individual particles. It fails to reproduce most of the observed molecules at low density and CO abundance at high density. But the depletion profiles and abundances of CS and CH_3OH at high densities are well reproduced. When tracing the dynamical evolution of the cores, we show that the dynamical setup under-predict the CO gas-phase abundance at high density, as the slow evolution of the density results in a higher depletion of CO, which is not supported by our observations. A deeper study on the parameters impacting CO depletion (sticking coefficient, density, and time) could lead to improvements.

Thank you to the organizers of the SF2A 2025! This project has received funding from the European Research Council (ERC) under the European Union's Horizon Europe research and innovation programme ERC-AdG-2022 (SUL4LIFE GA No. 101096293). AT, VW, PG, ED, MC, and JN acknowledge the thematic Action "Physique et Chimie du Milieu Interstellaire" (PCMI) of INSU Programme National "Astro", with contributions from CNRS Physique & CNRS Chimie, CEA, and CNES.

References

Bergin, E. A. & Tafalla, M. 2007, ARA&A, 45, 339
Bonnell, I. A., Dobbs, C. L., & Smith, R. J. 2013, MNRAS, 430, 1790
Boogert, A. C. A., Huard, T. L., Cook, A. M., et al. 2011, ApJ, 729, 92
Chu, L. E. U., Hodapp, K., & Boogert, A. 2020, ApJ, 904, 86
Clément, A., Taillard, A., Wakelam, V., et al. 2023, A&A, 675, A165
Dartois, E., Chabot, M., Bacmann, A., et al. 2020, A&A, 634, A103
Dartois, E., Chabot, M., Barkach, T. I., et al. 2018, A&A, 618, A173
Fuente, A., Navarro, D. G., Caselli, P., et al. 2019, A&A, 624, A105
Hocuk, S., Szűcs, L., Caselli, P., et al. 2017, A&A, 604, A58
Lee, C. W., Myers, P. C., & Plume, R. 2004, ApJS, 153, 523
Lee, C. W., Myers, P. C., & Tafalla, M. 2001, ApJS, 136, 703, arXiv: astro-ph/0105515
Ruaud, M., Wakelam, V., Gratier, P., & Bonnell, I. A. 2018, A&A, 611, A96
Ruaud, M., Wakelam, V., & Hersant, F. 2016, MNRAS, 459, 3756
Stadler, C., Laffon, C., Parent, P., Taillard, A., & Wakelam, V. 2025, A&A, 700, A83
Taillard, A., Wakelam, V., Gratier, P., et al. 2025, A&A, 698, A278
Taillard, A., Wakelam, V., Gratier, P., et al. 2023, A&A, 670, A141
Wakelam, V., Gratier, P., Loison, J. C., et al. 2024, A&A, 689, A63
Wakelam, V., Gratier, P., Ruaud, M., et al. 2021, A&A, 647, A172
Wakelam, V., Herbst, E., & Selsis, F. 2006, A&A, 451, 551