Astrochemistry: from primordial gas to present-day clouds

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Abstract. Astrochemistry plays a central role during the process of star formation, both in the primordial regime as well as in the present-day Universe. We revisit here the chemistry in both regimes, focusing first on the chemistry under close to primordial conditions, as observed in the so-called Caffau star SDSS J102915+172927, and subsequently discuss deuteration processes in present-day star-forming cores. In models of the high-redshift Universe, the chemistry is particularly relevant to determine the cooling, while it also serves as an important diagnostic in the case of present-day star formation.

Key words. Astrochemistry – Stars: formation – Primordial Universe – Molecular clouds

1. Introduction

Chemistry plays a central role in astrophysics, and particularly during star formation. In the primordial Universe consisting only of hydrogen and helium, the H_2 molecule provides the only and relatively inefficient coolant, implying relatively high temperatures of the star-forming clouds compared to Milky Way type conditions. In the absence of dust grains, H_2 abundances of order 10^{-3} start forming at gas number densities of 10^4 cm^{-3} due to gas phase reactions (Saslaw & Zipoy 1967). The gas becomes fully molecular from densities of about 10^{12} cm^{-3} due to three-body reactions (Palla et al. 1983). The resulting temperatures of 300 K or higher are commonly expected to give rise to significantly enhanced masses of the first stars.

The presence of even tiny amounts of dust grains may alter this picture, giving rise to potentially strong fragmentation at high densities (Schneider et al. 2003). The star SDSS J102915+172927 is considered as a candidate for such behavior (Klessen et al. 2012; Schneider et al. 2012), as its metal abundances are so low that only dust grains could have contributed relevantly to the cooling (Caffau et al. 2011). In the following, we will present a numerical simulation exploring how the formation of such a star may have occurred. We will subsequently turn to deuteration processes in present-day clouds, as explored by Walmsley et al. (2004). We will show that large deuteration fractions can be reached within about a free-fall time. The chemical modeling pursued in this work is based on the publicly avail-
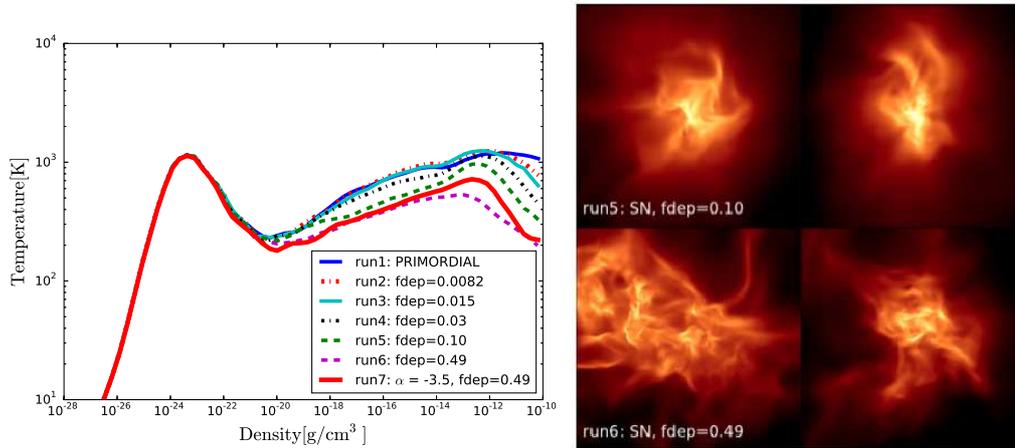
Fig. 1. Profile of the mass-weighted average temperatures for different dust depletion factors f_{dep} in the dark matter halo with 10^6 $M_\odot$ (left), as well as the density structure on a scale of 20 AU for selected runs with both halos (left: 10^6 $M_\odot$, right: 7×10^5 $M_\odot$) (Bovino et al. 2016). The calculations assume the metal abundances of the Caffau star.

able astrochemistry package KROME[1] (Grassi et al. 2014).

2. The formation of the Caffau star SDSS J102915+172927

We model the formation of the Caffau star using the cosmological hydrodynamics code Enzo (Bryan et al. 2014) combined with the astrochemistry package KROME. We explore the results for two minihalos, one with 10^6 $M_\odot$ and one with 7×10^5 $M_\odot$, forming at $z = 22$ and $z = 18$, respectively. The halos are part of a cosmological box with size of 300 kpc h^{-1}, an initial topgrid resolution of 128^3, two additional nested grids around the halo of choice and 29 levels of refinement. The Jeans length is always resolved with at least 64 cells. The details of the setup, as well as our treatment of the chemistry and the dust grains, is reported by Bovino et al. (2016). Fixing the metal abundances to the values of the Caffau star, we find that the cooling is predominantly regulated by the depletion factor $f_{dep} = D/Z$, where D denotes the dust-to-gas mass ratio and Z the metallicity.

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[1] KROME: http://www.kromepackage.org/

The resulting thermal evolution and the density structure is shown in Fig. 1, where higher depletion factors correspond to lower gas temperatures at high densities. Looking also at the density structure, we found that a strong transition from an approximately spherical collapse mode to a filamentary collapse occurs between depletion factors of 0.1 and 0.49, suggesting that the latter corresponds to the critical threshold for fragmentation induced via dust cooling for metallicities as in the Caffau star (Bovino et al. 2016).

3. Deuteration processes during present-day star formation

We further explore deuteration processes in prestellar cores, with the aim of inferring the approximate timescale to reach high deuteration fraction. For this purpose, we consider the collapse of a turbulent magnetized Bonnor-Ebert sphere (Ebert 1955; Bonnor 1956), which is modeled with the magneto-hydrodynamical code FLASH (Fryxell et al. 2000). The chemistry is modeled using the network of Walmsley et al. (2004) under the assumption of full depletion (see Körtgen et al. 2017, for a detailed description of the overall setup).
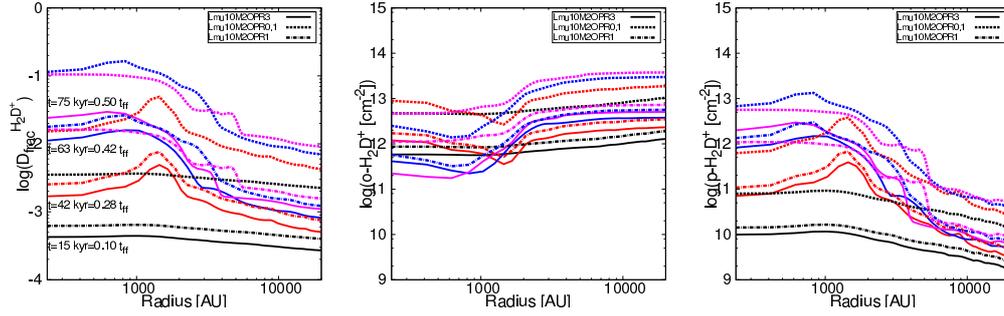
Fig. 2. Comparison of radial profiles of the deuteration fraction and the spin states of H_2D^+ for runs with initial H_2 ortho-to-para (OPR) ratio OPR=3 (solid), OPR=1 (dash–dotted) and OPR=0.1 (dashed). See Körtgen et al. (2017) for a more detailed discussion.

In Fig. 2, we show the radial profiles of the deuteration fraction and the spin states of H_2D^+ for runs with different initial H_2 ortho-to-para ratios, exploring values of 3, 1 and 0.1. Results are given at 15 kyrs, 42 kyrs, 63 kyrs and 75 kyrs, corresponding to 0.1, 0.28, 0.42 and 0.5 free-fall times. Even in the most unfavorable case with an initial H_2 ortho-to-para ratio of 3, a deuteration fraction of 0.01 is achieved within the central 1000 AU during half a free-fall time. This demonstrates the high efficiency of deuteration processes, which we will explore in more detail in future investigations including finite amounts of depletion.

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