Modeling the evolution of ice deuteration during the formation of low-mass protostars

Vianney Taquet[1,2], Steven Charnley[1], Martin Cordiner[1,3]

1 NASA Goddard Space Flight Center, 2 NASA Postdoctoral Program, 3 The Catholic University of America

Introduction

Extremely large deuteration of several molecules has been observed around prestellar cores and low-mass protostars for a decade. New observations performed with the Herschel Space Observatory or with ground-based interferometers have allowed astronomers to derive the D/H ratio of water, giving contrasting results (between less than 10^{-3} to a few percents; Coutens et al. 2012, Persson et al. 2013, Visser et al. 2013, Taquet et al. 2013a). In previous studies, we have successfully reproduced the high deuteration of water derived by Coutens et al. (2012) with typical molecular cloud conditions and a low value for the H_2 ortho/para ratio (opr ≤ 10^{-3}; Taquet et al. 2013b). However, this result contrasts with the long timescale needed to decrease the H_2 opr from its statistical value of 3 and, therefore, the non-detection of DCO^+ towards interstellar clouds outside dense cores (see Pagani et al. 2011).

In this poster, we study the time-dependent and spatial evolutions of the H_2 opr and the ice deuteration in the early-stages of low-mass star formation. For this purpose, we coupled our gas-grain astrochemical model GRAINOBLE (Taquet et al. 2012) with a simple dynamical model of core collapse leading to the formation of a central protostar (Whitworth & Ward-Thompson 2001).

Astrochemical model

General description

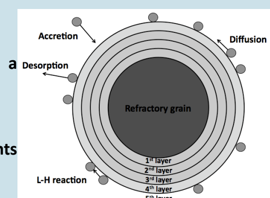
Rate equations for a time-dependent treatment of the gas-grain chemistry:

- Gas phase chemical network from KIDA (Wakelam et al. 2012) and extended to include deuterium chemistry and ortho/para spin states of H_2 and key ions
- Surface chemical network from experimental works to form main deuterated ice components
- Activation barriers of surface reactions computed from quantum calculations with the Eckart model (Taquet et al. 2013b)

Multilayer approach

Ice formation and desorption of ices with a multilayer approach:

- Processes only on the surface / bulk is inert
- Chemical differentiation within ices
- Volcano and co-desorptions as seen in experiments (Collings et al. 2004)



1D Physical model

Dynamics / Radiative transfer

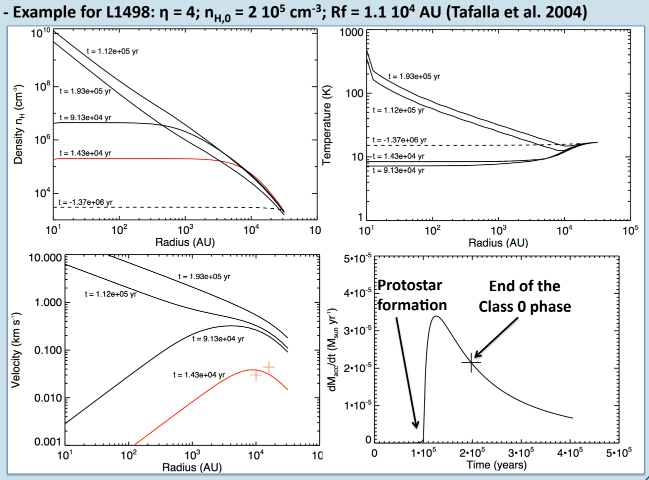
-Static formation of a dense core, in a time ≈ 3 10^6 yr with a density structure

$$n_{\rm H} = \frac{n_{\rm H,0}}{(1+(r/R_f)^2)^{\eta/2}}$$

- Free-fall collapse following Whitworth & Ward-Thompson (2001)
➔ high accretion rate at the beginning of the Class 0 phase

- Radiative transfer with DUSTY (Ivezic & Elitzur 1997) to get the T_d profile

- Example for L1498: η = 4; $n_{H,0}$ = 2 10^5 cm^{-3}; Rf = 1.1 10^4 AU (Tafalla et al. 2004)

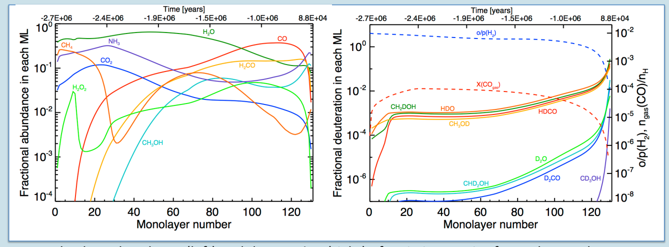


Ice deuteration and H_2 opr in dense cores

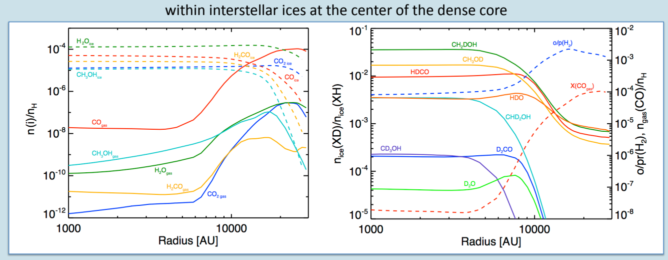
- Timescale for decreasing the H2 opr via ion-neutral reactions is similar to the timescale for ice formation (τ ≈ 10^7 yr x 10^4 cm^{-3}/n_H)

➔ most of the ice is formed when H_2 opr and X(CO) are high

➔ Since high abundances of gaseous CO and ortho-H_2 limit the formation of deuterated molecules, the deuteration is limited to the few outermost ice layers



Absolute abundance (left) and deuteration (right) of main icy species for each monolayer within interstellar ices at the center of the dense core

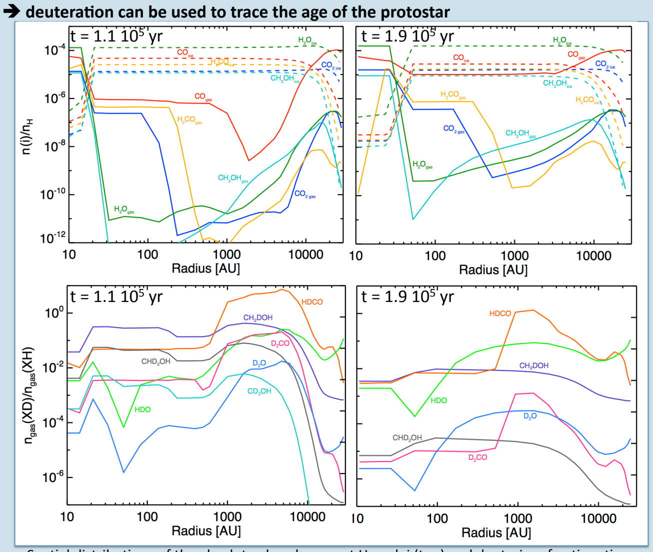


Spatial distributions of the absolute abundance wrt H nuclei (left) and deuterium fractionation (right) of main icy species at the end of the dense core phase

Ice abundances and deuterations in Class 0 protostars

- The volcano desorptions induce complex abundance profiles with double abundance jumps of icy molecules trapped in water ➔ reproduce CO and H_2CO profiles observed by Jorgensen et al. (2002) and Ceccarelli et al. (2001)
- High deuteration of formaldehyde and methanol observed by Parise et al. (2006) would mainly come from the cold external envelope
- Deuteration tends to decrease with the age of the protostar, due to the gravitational collapse of the envelope

➔ deuteration can be used to trace the age of the protostar



Spatial distributions of the absolute abundance wrt H nuclei (top) and deuterium fractionation (bottom) of main icy species at the beginning (left) and the end of the Class 0 phase

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