Complex molecule formation in TMC-1: A new approach using the physicochemical ProDiMo code

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ABSTRACT

The Taurus Molecular Cloud (TMC) has been used as astrochemical laboratory to test new approach in computational methods to solve the chemical abundances in ISM. In particular, this cloud presents a rich inventory of complex molecular species such as Acids, Alcohols and hydrocarbons that can be synthetized by ionizing radiation to produce astrobiological molecules. However, it is understood in astrochemistry that complex molecules are formed on the dust grains surface in dense and cold region of the Interstellar Medium. In this context, we use the physico-chemical ProDiMo code with newest improvements in surface chemistry to address the molecular abundances in TMC-1. Such method regards to H_2 and HD formation on cold and warm grain surfaces, as well as via hydrogenated PAHs considering a time-dependent chemistry. This subject worth because the chemical evolution is treated as function of the hydrogen abundance available to join reactions. The results will be compared with other approximations available in literature about this cloud.

1. INTRODUCTION AND MOTIVATION

Since 1960s-70s with the development of radioastronomy, several complex molecules have been detected in Molecular Clouds such as TMC-1 (see Review by Agúndez & Wakelam 2013). In order to understand how molecular species survive in space, new computational approaches were created since then, focused in dense (10^4 cm^{-3}) and cold (T ~ 10K) regions of Interstellar Medium. However, how complex molecules are formed in warm regions, with temperature around 100K? To answer this question, the ProDiMo code with warm surface chemistry (Woitke et al. 2009, 2016; Kamp et al. 2010,2017; Thi et al. 2011, 2018 - *submitted*) is employed, addressing the gas and solid-phase abundance of CH_3OH in TMC-1. Methanol is a precursor of several prebiotic molecules such as $C_2H_4O_2$ isomers (de Barros et al. 2011), as well as amino acids (methylamine - Aponte et al. 2017) and sugars (ribose - Meinert et al. 2016).

2. ASTROPHYSICAL SCENARIO

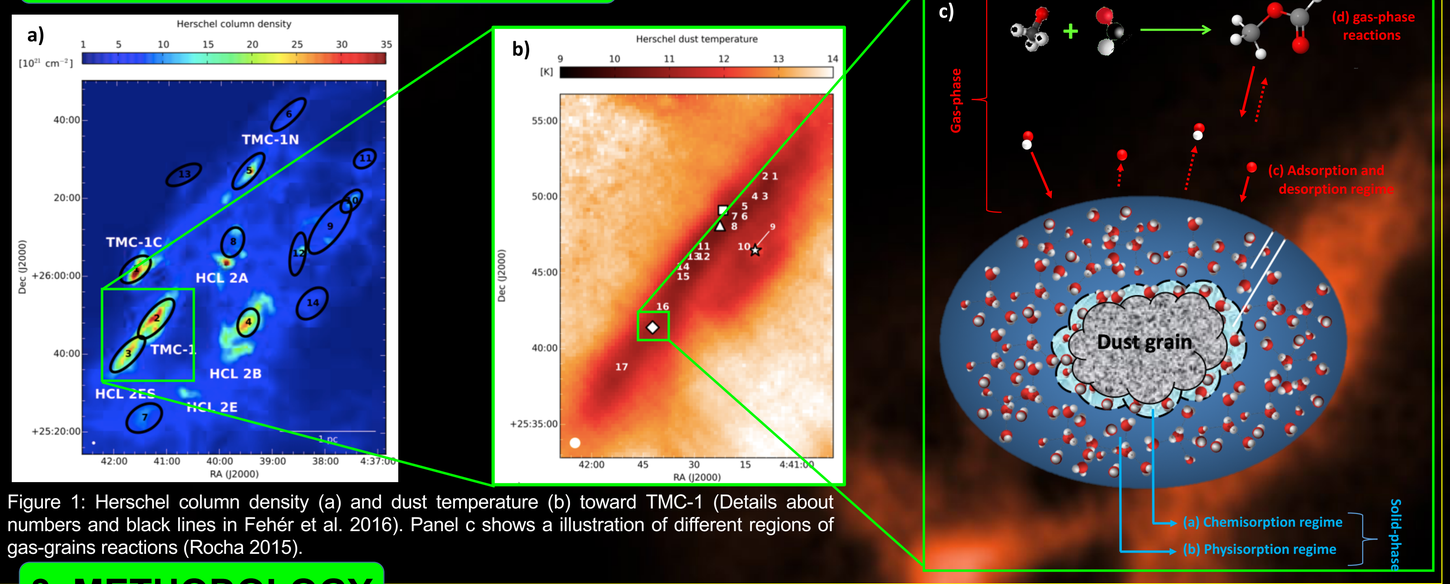


Figure 1: Herschel column density (a) and dust temperature (b) toward TMC-1 (Details about numbers and black lines in Fehér et al. 2016). Panel c shows a illustration of different regions of gas-grains reactions (Rocha 2015).

3. METHODOLOGY

3.1 Model Description

The model used here describes the chemical evolution of a Molecular Cloud simulated in 1D with the ProDiMo code using the Large DIANA network (Kamp et al. 2017). The general parameters are: ρ=2x10^{4}cm^{-3}, A_V=30 mag and ζ =1.3x10^{-17}s^{-1}. The initial elemental abundances were taken from Agúndez and Wakelam (2013).

3.2 Chemical processes (gas-gas and gas-grain)

The models include reactions in the gas-phase, as well as the interation gas-grain by adsorption and desoprtion mechanism as described in Woitke et al. (2009). The surface chemistry is a new approach in the code described in the next section.

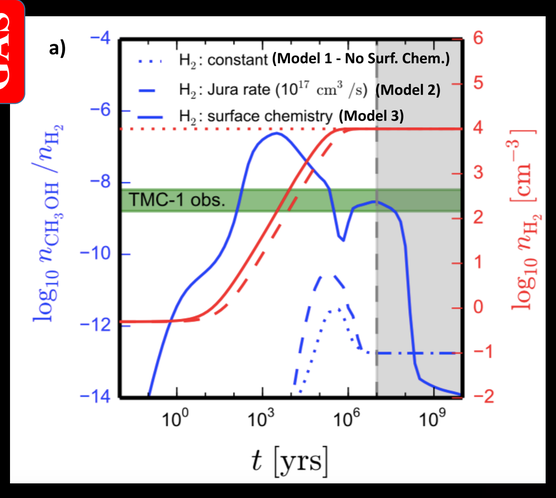
3.3 Surface Chemistry

The major difference between the surface chemistry of ProDiMo with other codes is the treatment of the Eley-Rideal and Langmuir-Hishelwood mechanims both at the physisorption and chemisorption sites (Thi et al. submitted). In this sense, the general rates are rewrite in function of the tunneling-corrected Arrhenius equation, called Bell's formula (Bell 1980), given by:

$$Q_{Bell} = Q_{Bell}\left[a_i^{gc}, E_i^{gc}, T_g\right],$$

where a_i^{gc} is the width of the rectangular activation barrier of height E_i^{gc} in a chemisorption site of temperature T_g.

4. RESULTS AND DISCUSSION



(Model 3: different temperatures)

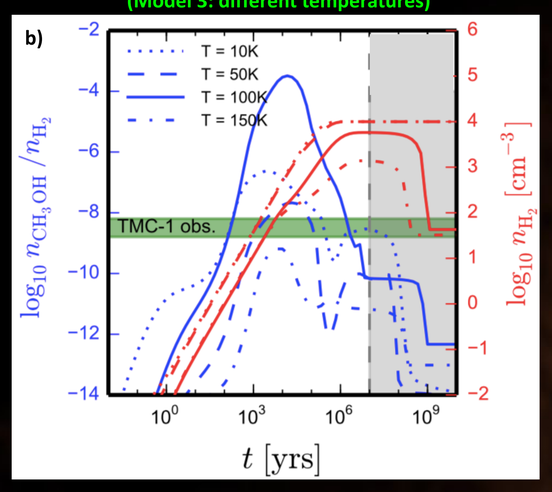
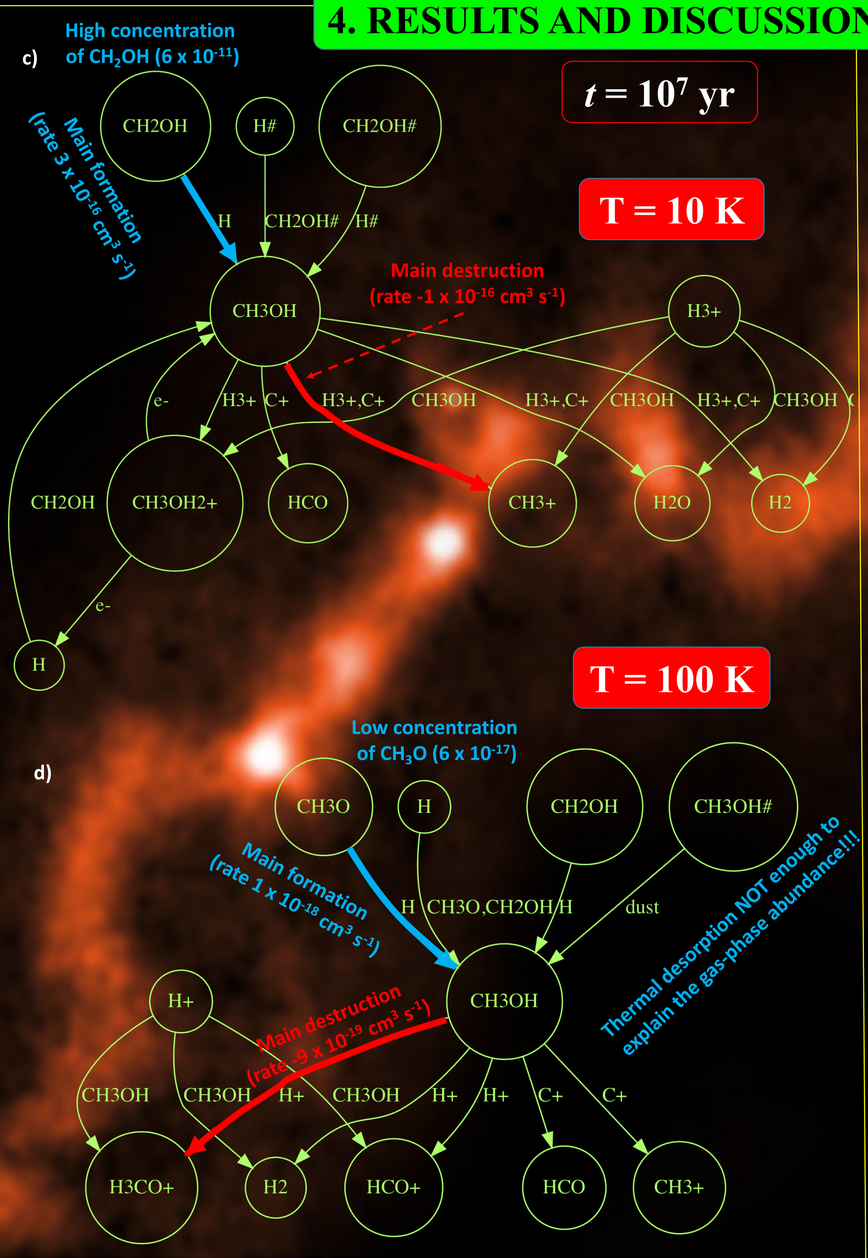


Figure 2: Relative abundances in different scenarios (Panels a nd b) of CH_3OH and H_2 calculated with ProDiMo and compared with the observed abundance in TMC-1. Panels c and d show the networks for the Model 3 at 10K and 100K.



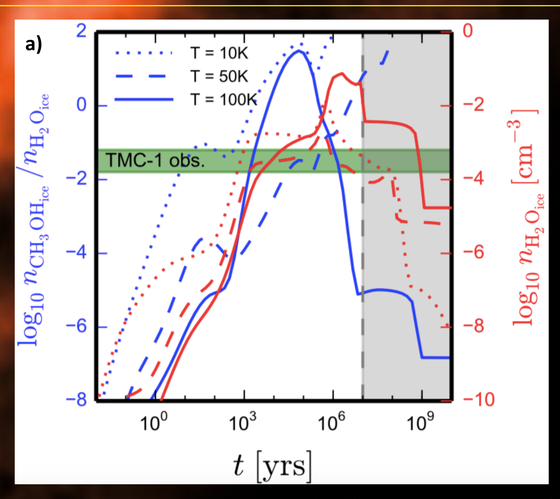
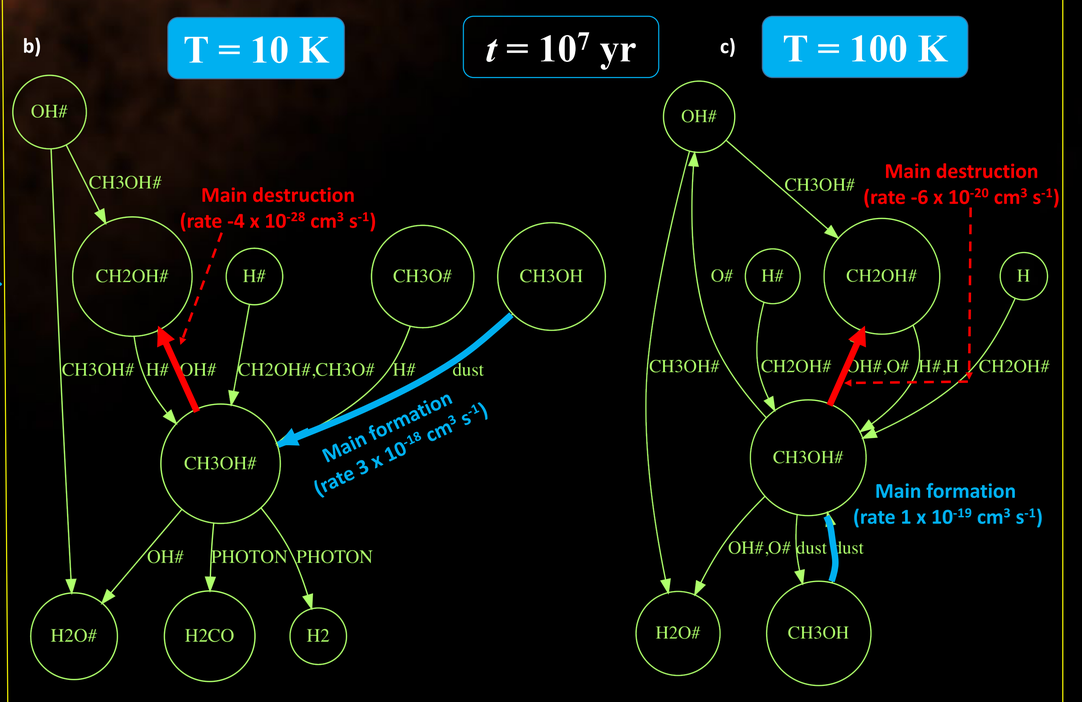


Figure 3: Relative abundances of methanol ice and water ice in different temperatures (Panels a) calculated with ProDiMo and compared with the observed abundance in TMC-1. Panels c and d show the networks at 10K and 100K.



5. CONCLUSIONS

This work was focused in showing the new approach in surface chemistry of the ProDiMo code and its impact on the formation of complex molecules as CH_3OH. The results are summarized bellow:

- Methanol is efficiently formed in a model with surface chemistry at low temperature (10K);
- Although H_2 is efficiently formed at high T, the abundance of methanol is affected by the low concentration of CH_3O;
- The ice abundance of methanol is also affected by the temperature, and decreases several magnitude orders from 10K and 100K by increasing the main destruction rate.
- Once a low concentration of methanol is available at high T, the thermal desorption remains not enough to explain the gas-phase abundance.

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