Effects of initial condition and cloud density on the composition of the grain mantle

Ankan Das,[1,2]★ Kinsuk Acharyya[2] and Sandip K. Chakrabarti[1,2]

[1]Indian Centre for Space Physics, Chalantika 43, Garia Station Rd, Kolkata, 700084, India
[2]S. N. Bose National Centre for Basic Sciences, Salt Lake, Kolkata 700098, India

ABSTRACT

The evolution of grain mantles in various interstellar environments is studied. We concentrate mainly on water, methanol and carbon dioxide, which constitute nearly 90 per cent of the grain mantle. We investigate how the production rates of these molecules depend on the relative gas-phase abundances of oxygen and carbon monoxide and constrain the relevant parameter space that reproduces these molecules close to the observed abundances. Allowing the accretion of only H, O and CO on the grains and using the Monte Carlo method, we follow the chemical processes for a few million years. We allow the formation of multilayers on the grains and incorporate the freeze-out effects of accreting O and CO. We find that the formation of these molecules depends on the initial conditions as well as on the average cloud density. Specifically, when the number density of accreting O is less than three times that of CO, methanol is always overproduced. Using the available reaction pathways it appears to be difficult to match the exact observed abundances of all three molecules simultaneously. Only in a narrow region of parameter space are all three molecules produced within the observed limits. Furthermore, we found that the incorporation of the freeze-outs of O and CO leads to an almost steady state on the grain surface. The mantle thickness grows anywhere between 60 and 500 layers in a period of two million years. In addition, we consider a case in which the gas number density changes with time owing to the gradual collapse of the molecular cloud and present the evolution of the composition of different species as a function of the radius of the collapsing cloud.

Key words: hydrodynamics – molecular processes – stars: protostars – ISM: abundances – ISM: molecules.

1 INTRODUCTION

The study of the chemical evolution of the interstellar medium (ISM) is recognized to be a challenging task. The ISM is a rich reservoir of complex molecules. So far, around 150 gas-phase molecules and around 20 molecular species on the grain surface have been detected in various regions of the ISM, especially in regions of star formation. In the last decade it has become well established that the gas-phase reactions alone cannot explain the molecular abundances in the ISM. The chemical reactions that occur on the interstellar dust grains are essential for explaining the formation of several molecules, especially hydrogenated species, including the simplest and most abundant molecule, H_2. Interstellar grains provide a surface on which the accreted species can meet and react. Therefore, an understanding of the formation of molecules on grain surfaces is of prime importance. In this paper, we follow the evolution of the grain mantle mainly as a function of the initial conditions. We concentrate only on water, methanol and carbon dioxide, as these molecules constitute nearly 90 per cent of the grain material in dense regions of the ISM. These molecules are detected on the grain surface as a result of their strong absorption bands arising out of multiple vibrational modes. Water is the most abundant species on grains in the dense ISM. It has an abundance of 10^{-4} with respect to the total hydrogen column density (Tielens et al. 1991). The ice band, at 3.07 μm (3280 cm^{-1}), is attributable to the O-H stretch mode of H_2O ice and was first discovered by Gillett & Forrest (1973) in Becklin & Neugebour (1967, hereafter BN) objects. CO_2 is the second most abundant molecule in the ISM, with an abundance of around 20 per cent with respect to H_2O. However, this abundance can vary from cloud to cloud, and in clouds such as W 33A it could be even less than 5 per cent of the water abundance (Keane et al. 2001). Several strong CO_2 features are observed (de Graauw et al. 1996; Keane et al. 2001). Generally, it is found that the CO_2 correlates best with H_2O ice, suggesting that these molecules may have similar chemical histories. The next most abundant molecule is CO, which is a well-studied ice, with an abundance varying between 2 and 15 per cent of that of water and with a characteristic absorption

★E-mail: ankan@csp.res.in