

Methanol formation: A Monte Carlo study

Ankan Das¹, Kinsuk Acharyya², Sonali Chakrabarti^{3,1}, and
Sandip K. Chakrabarti^{2,1}

¹Indian Centre for Space Physics,
Chalantika 43, Garia Station Road, Kolkata 700084, India
email: ankan@csp.res.in

²S. N. Bose National Centre for Basic Sciences
Salt Lake, Kolkata 700098, India
email: acharyya@bose.res.in, chakraba@bose.res.in

³Maharaja Manindra Chandra College
20 Ramakanta Bose Lane, Kolkata 700003, India
email: sonali@csp.res.in

Abstract. We carry out a Monte-Carlo simulation to study the formation of methanol on the grain surfaces. We found that the recombination efficiencies are strongly dependent on the extrinsic properties of the grain, such as the number of sites on the grain surface and the flux of the accreting matter. This uses the concept of effective grain surface (denoted through a factor α) area which changes as the grain is populated.

Keywords. ISM: abundances, ISM: molecules, methods: numerical, molecular processes

1. Introduction

It is now well known that the grain chemistry plays a vital role in the chemical evolutions of the molecular cloud. The rate equation method is very extensively used by several authors to study the grain surface chemistry (Hasegawa *et al.* 1992, Roberts & Herbst 2002, Acharyya *et al.* 2005). However, this method is only applicable when there are large number of reactants on the grain surface. Given the fact that the interstellar medium is very dilute, very often the criteria for using the rate equation are not fulfilled. Furthermore, it is assumed that the recombination efficiency is independent of the surface area of the grain. The only advantage of this method is that computationally it is faster and it can very easily be coupled with the gas phase reactions. More realistic method to handle the grain chemistry is the Monte-Carlo approach. This is very accurate method because here we can trace each and every species over the entire period of time. The major disadvantage of this is that it is computationally time consuming. Using Monte-Carlo approach Chakrabarti *et al.* (2006a, b) introduced a new concept of the effective grain surface area and showed that it is this effective area which must be used for the grain chemistry. It was argued that the surface area S in the usual rate equation is to be replaced by S^α where α is to be determined from Monte-Carlo method for a few cases and extrapolated value is to be used in the equation. Its usefulness was demonstrated while computing the formation of H_2 molecules on the grains. In the present work, we carry out a similar analysis to study the formation of water and methanol on the grains.

2. Procedure

We study the chemical evolution on grains assuming H, O and CO as the sole accreting species. For the sake of simplicity, we assume that a grain surface is a square lattice S number of sites. We assume further that each site has four nearest neighbours, as in an fcc[100] lattice. In order to mimic the spherical grain structure, we assume a periodic

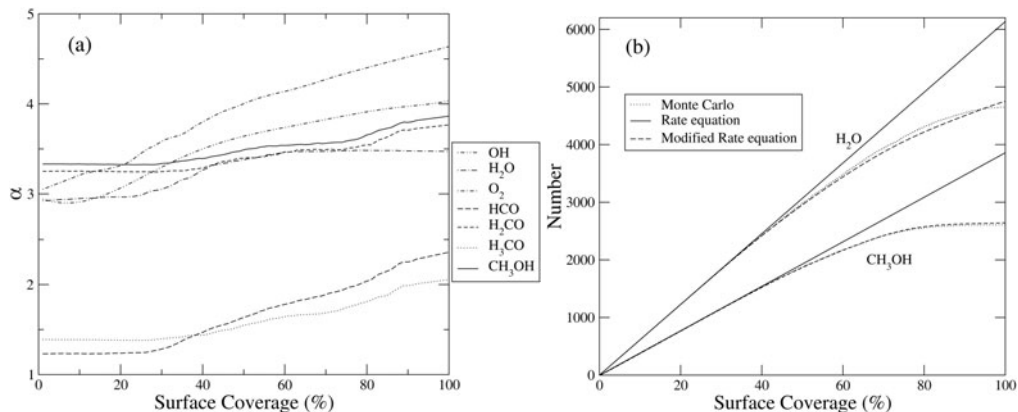


Figure 1. In (a) we plot α for various species. In (b) we compare our results with the modified rate equation method, where we replaced S by S^α and with the original rate equation method.

boundary condition. The four major steps to handle the grain chemistry are the accretion, diffusion, reaction and evaporation. We execute every step by the appropriate use of the random number generator. Keeping in mind that there are two types of reaction schemes (Eley-Rideal and Langmuir-Hinselwood), we continue our simulations for different models assuming different procedure for the accretion of the gas phase species.

3. Results

In Figure 1a, we plot α for various species as a function of the surface coverage for an Olivine grain at 10K having 10^4 sites. We note that α is not unity for any of these species. Up to about 30% of the surface coverage α remains roughly constant, but after that they rise as the surface gets filled up. In Figure 1b, we made a comparison of the abundances of two of the most important species, namely, H₂O and CH₃OH in different methods. The results of our simulation clearly agree with those from the modified rate equation, but not with those from the original rate equation. This indicates that the α s we introduced are very important and their effects are to be taken into account for an accurate estimation of the species from the grain chemistry.

4. Concluding Remarks

According to the observations, the solid state methanol abundance should be 5% to 30% (Gibb *et al.* 2000) with respect to H₂O. We carried out our simulation for the low gas phase abundance (Case I: density of H₂ 10^3 cm⁻³) and for the high gas phase abundance (Case II: density of H₂ 10^5 cm⁻³). We found that for different models this number varies from ($\sim 43\%$ – $\sim 57\%$) for Case I and from (4% – 6%) for Case II. Thus the observed abundance must be from some intermediate region of the cloud. One of our important findings is that the parameter α strongly depends on the surface population of the grain surface. This deviates significantly from unity, the usual value in existing rate equation.

References

- Acharyya, K., Chakrabarti, S. K., & Chakrabarti, S. 2005, *MNRAS*, 361, 550
 Chakrabarti, S. K., Das, A., Acharyya, K., & Chakrabarti, S. 2006a, *A&A*, 457, 167
 Chakrabarti, S. K., Das, A., Acharyya, K., & Chakrabarti, S. 2006b, *BASI*, 34, 299
 Gibb, E. L., *et al.* 2000, *ApJ*, 536, 347
 Hasegawa, T., Herbst, E., & Leung, C. M. 1992, *ApJS*, 82, 167
 Roberts, H. & Herbst, E. 2002, *A&A*, 395, 233