DEVELOPMENT OF CHEMICAL MODELS BASED ON LABORATORY DATA

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INTRODUCTION

Several complex organic molecules are routinely detected, in high abundaces, toward hot cores and hot corinos (Herbst & van Dischoek 2009). Yet, for many of them, their paths of formation in space is unknown as gas phase reactions alone seem to be insufficient.
It is believed that grain surface reactions could play a pivotal role in reproducing the abundances of molecules in the interstellar medium (ISM) and in understanding their formation.

Unlike for gas-phase chemical models (for which we have a fairly complete network of the reaction rates and the column densities), there are not observational clues on how molecules may form on grains.

Experiments in solid state under astrophysical conditions are the key to investiagate the production of new species in astrochemical environments (Burke & Brown 2010).

The aim of my project is to couple UCL_CHEM chemical model with the new experimental results on grain surfaces in order to reproduce the observed abundances of molecules into the ISM.

The work presented here is part of the LASSIE European Network.

Background

Complex organic molecules are detected in high abundances in some interstellar environments such as:

•Hot cores, compact objects found in the vicinity of massive protostars, characterized by high densities (10^7 cm^{-3}) and high temperature (300-500K);

•Hot corinos, very compact objects (10^8 cm^{-3}) surrounding low-mass stars, where the temperature is about 100K;

•Dark cores, colder regions (~ 10K) with density in the 10^2-10^4 cm^{-3} range.

UCL_CHEM

UCL_CHEM is a time-depth dependent gas-grain chemical model, first developed in the 1999 by Viti & Williams.

It simulates the formation of stars in two steps:

•Phase I starts with a free-fall collapse during wich molecules freeze onto grain surfaces and new species can form.

•Phase II reproduce the desorption of molecules from the grain surfaces as investigated by Viti et al. (2004).

Reactions are separated in two different networks as reported in the scheme below.

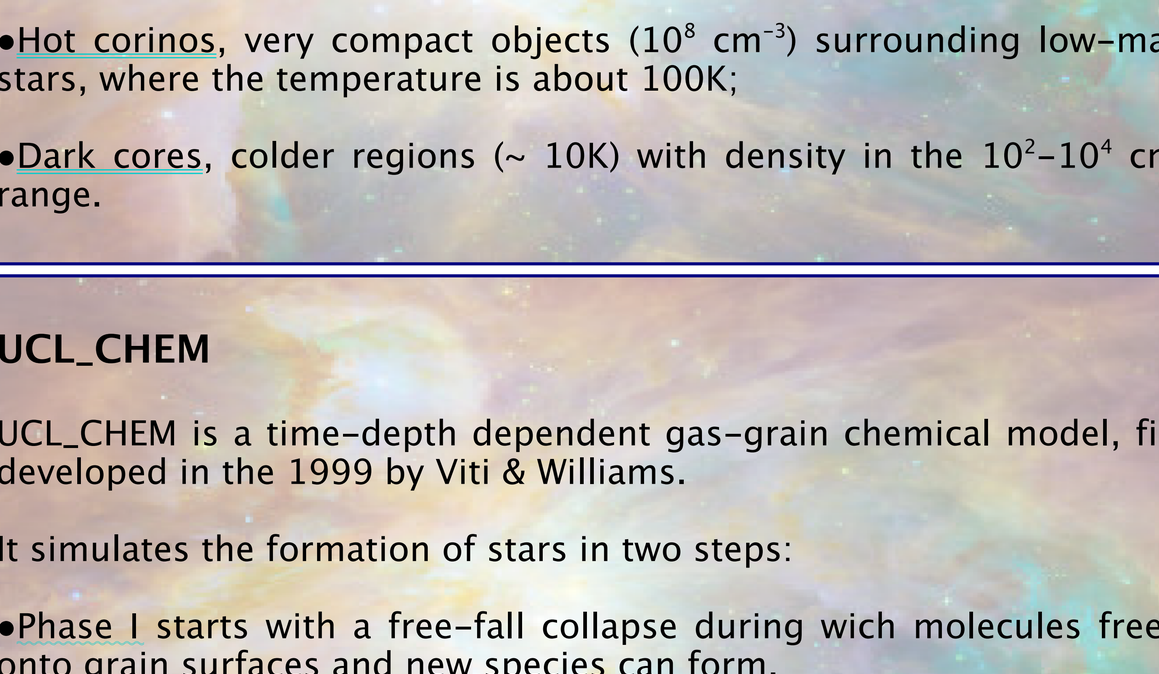

Illustration 1: Type of gas-phase and grain-surface reactions included in UCL_CHEM model.

Acknowledgments

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First Results

A study of methyl formate in astrochemical environments
Occhiogrosso A., Viti S., Modica P. & Palumbo M. E.,
2011, MNRAS

We investigated the viability of a new path of formation of methyl formate on grain surfaces in hot and cold regions:

$$mCO + mCH_3OH \rightarrow mHCOOCH_3$$

The reaction is summarised in the picture below. The *m* before the molecular formulæ stands for *mantle*.

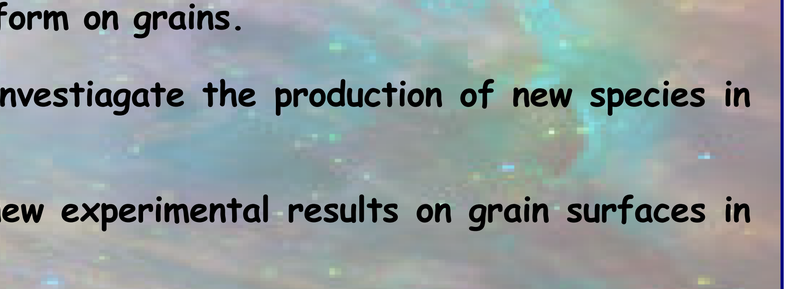

Illustration 2: Solid state path of formation of methyl formate induced by coscmic rays. Starting from the left panel, CO undergoes subsequent hydrogenation to form methanol. Once produced, methanol originates methyl formate by interaction with cosmic rays. The picture is taken from Modica & Palumbo (2010).

By comparing our theoretical results with the observations (Obërg et al. 2010), we found a good agreement in reproducing the methyl formate column density in the case of cold regions such as the dark core B1-b (see Table 1 below).

Source	Distance (pc)	Temperature (K)	Observed column density (cm^{-2})	Theoretical column density (cm^{-2})
B1-b dark core	350	<30	8.3×10^{12}	1.2×10^{12}

Table 1: Comparison between the observational and theoretical methyl formate column densities.

Work in progress

♦ Electron stimulated desorption of species from H_2O ices in order to study the role of H bonds in the excitation of molecules. (Secondment's project in collaboration with prof. McCoustra at the Heriot-Watt University)

♦ The chemistry of sulfur-bearing species in the ISM:
- Cosmic ray interactions (Collaboration with dr. M. E. Palumbo, INAF, Catania, Italy);
- Temperature programmed Desorption (TPD)(Collaboration with dr. W. A. Brown, UCL, London, UK);
- Formation, proprierties and reactivity of products (Collaboration with prof. S. D. Price, UCL, London, UK).

References

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