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# A model of cometary nucleus taking into account all phase changes of water ice: amorphous, crystalline, and clathrate

**U. Marboeuf (1), B. Schmitt (1), J.-M. Petit (2), O. Mousis (2) and N. Fray (3)**
**(1) Institut de Planétologie et d'Astrophysique de Grenoble, France (marboeuf@ujf-grenoble.fr), (2) Institut UTINAM, Besançon, France, (3) Laboratoire Inter-Universitaire des Systèmes Atmosphériques, LISA/IPSL, Créteil, France**

## Abstract

We present a model of cometary nucleus which takes into account all structures of water ice (amorphous ice, crystalline ice and clathrate hydrate, or a mixture of these water ice structures) for the first time. This model describes heat transmission, latent heat exchanges, all water ices transitions (amorphous-to-pure crystalline, amorphous-to-clathrate hydrates and pure crystalline-to-clathrate hydrates and vise versa), sublimation/recondensation of volatile molecules in the nucleus, gas diffusion, gas release and trapped by crystallization and clathrate formation/dissociation processes, as well as gas and dust release and mantle formation at the surface. This model is able to predict the outgassing profile of volatile molecules that could be measured by the Rosetta mission and can be used to constrain the structural type of ice existing in the interior of the comet 67P/Churyumov Gerasimenko and, hopefully, its initial composition.

## 1. Introduction

Comets are currently supposed to be the most primitive objects in the solar system. Their chemical composition suggest that cometary material is formed at low temperature in colder regions of the protoplanetary disk or in the ISM, where most volatile molecules can condensate. The chemical composition and water ice structure included in comets are mainly affected 1) by temperature and molecular composition of the surrounding environment during both the formation of cometary materials in the protoplanetary disk or ISM and 2) by the thermodynamical evolution of comets in solar system since their formation.
Current theories [7], models of cometary nuclei [4, 6] and of ice formation in the protoplanetary disk [5, 9], and laboratory studies [1-2, 10] suggest that cometary materials could be formed of pure crystalline water ice, amorphous water ice, clathrate hydrate, or a mixture of these structures of ice, i.e. icy grains (see Figure 1), depending of the location of formation of both the cometary material (in ISM or protoplanetary disk) and the comet in the solar system [3], and the thermodynamical evolution of comets since their formation[8].
The clathrates are crystalline solids composed of water and gas (see Figure 2). The water molecule structure is organized in the form of cages which are stabilized by the inclusion of gas molecules. Each cage contains a single gas molecule trapped thanks to van der Waals interactions but the clathrate structure can trap different volatile molecules.

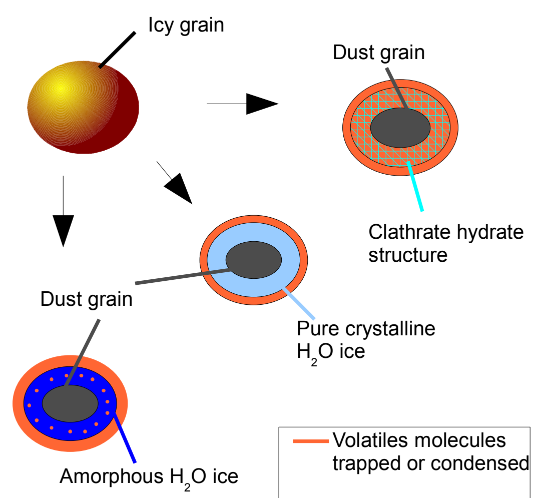


Figure 1: Schematic view of all the possible structures of water ice in icy grains of comets.

We present a 1D model of cometary nucleus, which takes into account all structures of water ices and phase changes during the thermal evolution of the comet around the sun. We pretend this model is able to interpret the outgassing observations that will be made by Rosetta mission and to constrain the chemical composition and the water ice structure in the interior of the target comet.

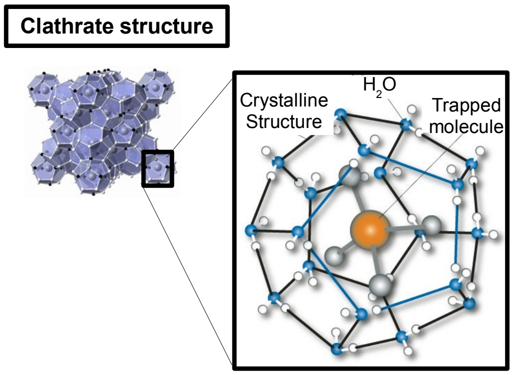


Figure 2: Schematic view of cages of clathrate hydrates structure.

## 2. The model of cometary nucleus

This model considers a sphere composed of a porous predefined mixture of water ice, volatile molecules (in gas and solid states) and dust grains in specified proportions. All initial water ice structures (amorphous, pure crystalline, clathrate hydrates or a mixture of these structure) can be taken into account in this model following assumptions considered on the formation location of the comet in the solar system and origins of formation of cometary materials. This model describes heat transmission, latent heat exchanges, sublimation/recondensation of volatile molecules in the nucleus, gas diffusion, gas release and trapped by crystallization and clathrate formation/dissociation processes, gas and dust release and mantle formation at the surface, as well as water ices transitions: all phases changes of water ice (amorphous-to-pure crystalline, amorphous-to-clathrate hydrates and pure crystalline-to-clathrate hydrates and vise versa) are taken into account in this model following the thermodynamical evolution of the comet around the sun and initial physical assumptions considered in the model.

## 3. Results

By taking into account all structures of water ice and phase changes in comets, this model allows us to predict different outgassing profiles of volatile molecules that could be measured by the Rosetta mission and used to constrain the physico-chemical processes effectively occurring as well as the structural types of ice existing in the interior of the comet 67P/Churyumov Gerasimenko. Finally, this model shows that clathrate structure can be formed in comets whatever the initial ice structure considered. The formation of clathrates induces changes in the physico-chemical behaviour and the outgassing profiles of comets compared to current models of cometary nuclei used in the literature.

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