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What is the link of the abundances of volatile species in the coma with the ones in the nucleus ?

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Abstract

The chemical composition of comets is frequently assumed to be directly provided by the observations of the abundances of volatile molecules in the coma. The present work aims to determine the relationship between the chemical composition of the coma, the outgassing profile of volatile molecules and the physico-chemical composition of the nucleus. To do this, we have developed a quasi 3D model of a cometary nucleus which takes into account all phase changes and water ice structures and applied this model to the comet 67P/Churyumov-Gerasimenko, the target of the Rosetta mission. We find that the outgassing profile of volatile molecules is a strong indicator of the physical and thermal properties of the solid nucleus. The relative abundance (to H_2O) of volatile molecules released from the nucleus interior varies by some orders of magnitude as a function of the distance to the sun, the volatility of species, their abundance and distribution between the 'trapped' and 'condensed' states, the structure of water ice, and the thermal inertia and other physical assumptions (dust mantle, ...) on the nucleus.

1. Introduction

Comets are expected to be the most primitive objects in the solar system. The study of these objects is crucial to determine the chemical composition and the thermodynamic conditions of ice formation in the protoplanetary disc and the early (primitive) solar system. Observations of these bodies [2,3] show variations of abundances of all the species (relative to H_2O) up to 2 orders of magnitude [1] whatever the position of comets around the sun. The present work aims to determine the relationship between the abundance of gas species in the coma of comets and the primitive internal abundance of ice species within the nucleus. In particular, we study the effects of the physical and thermodynamical properties such as the water ice structure, the thermal inertia, the abundance and distribution of species between the 'trapped' and 'condensed' states, and the presence of a dust mantle on the surface of nuclei on the relative abundances and the outgassing profiles of volatile molecules at the surface of comets. The main objective of this study is to constrain some general observational keys for the interpretation of outgassing observations of comets, in particular the future one of the comet 67P/Churyumov-Gerasimenko, the target comet of the Rosetta mission.

2. Quasi 3D model of cometary nucleus

The model simulates the cometary material as an icy porous matrix composed of dust grains with an icy mantle formed of water and some other volatile species in solid states. The numerical model uses the quasi 3D approach which allows us to take into account spatial (latitudinal and longitudinal) variations of the temperature on the surface of nuclei. This model represents a spherical nucleus whose surface is divided numerically in several sections as illustrated in Fig.1, and below which the interior of the nucleus is divided in several radial layers (i index) whose thickness follows initially a power law.

The model takes into account several volatile species together (H_2O, CO, CO_2 , CH_4, and H_2S) and several types of water ice structures: amorphous with trapped gases, pure crystalline, clathrate with trapped gases or a mixture of these structures [4]. Within the cometary nucleus, the model describes radial heat transfers, latent heat exchanges, H_2O ice phase transitions (amorphous → crystalline, crystalline ↔ clathrate, and amorphous → clathrate), sublimation/condensation of volatile molecules in the porous network of the nucleus, radial gas diffusion, as well as the allowed gas releases/trapping by/in the water ice structures.

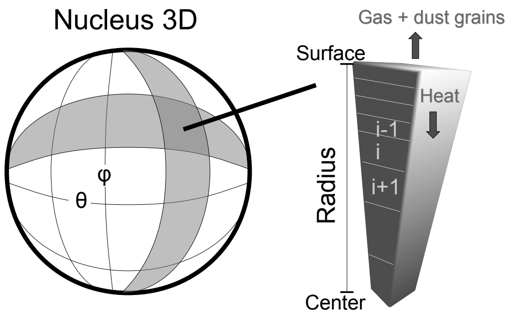

Figure 1: Schematic view of the quasi 3D nucleus model of comet. Heat conduction and gas diffusion occur only radially throughout the nucleus.

3. Results

The relative (to H_2O) abundance in coma of the less volatile molecules CO_2 and H_2S remain similar to the primitive composition of the nucleus (relative deviation less than 25%) only around the perihelion passage (in the range -3-2 to + 2-3 AU), whatever is the water ice structure and chemical composition, and under the conditions that the nucleus is not fully covered by a dust mantle (see Fig.2). The relative (to H_2O) abundance of highly volatile molecules CO and CH_4 in the coma remain approximately equal to the primitive nucleus composition only for nuclei made of clathrates. The nucleus releases systematically lower relative abundances of highly volatile species (up to one order of magnitude) around perihelion (in the range -3-2 to + 2-3 AU) in the cases of the crystalline and amorphous water ice structures in the nuclei. The rate of production, the outgassing profile and the relative abundances (to H_2O) of volatile molecules are the key parameters allowing one to retrieve the chemical composition and thermodynamic conditions of cometary ice formation in the early solar system. The coming observations of the coma and nucleus by the Rosetta mission instruments (VIRTIS, MIRO, ...) should provide the necessary constraints to the model to allow it to infer the primordial ice structure and composition of the comet.

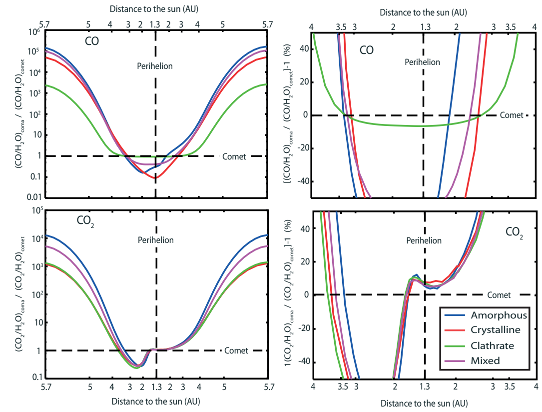

Figure 2: Ratio X/H_2O of the gas productions in the coma relative to this ratio in the primitive nucleus (left column) and the deviation from the primitive composition of the nucleus (right column) for volatile species CO and CO_2 as a function of the distance to the sun, for 4 initial structures of water ice: amorphous, crystalline, clathrate and mixed. The values 1 and 0 (horizontal dashed lines) correspond respectively to the primitive abundance (left column) and to the case where no deviation is observed between the coma and the nucleus (right column).

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