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Modelling the trapping of noble gases in comets ices

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Abstract

Among the information impatiently awaited from the observation of comet 67P/Churyumov-Gerasimenko were those concerning noble gases. From these observations, it is surmised that there is a relation between abundances in the nucleus and volatiles in the coma. However, their origin is still under debate. We consider a scenario according which the noble gases have been integrated in an early time to the icy grains precursors of comets in the interstellar medium, and this strongly enough to persist till now through the comet formation and aging. In this contribution we report theoretical investigations focusing on two key parameters of this scenario, i.e. the ability of noble gases to adsorb onto ices surfaces (first step of the process in the ISM) and their stability within cavities of the icy bulk.

1. Observational background

The recent observations of comet 67P/Churyumov-Gerasimenko brought valuable information concerning noble gases; as a matter of fact, the nature of their source in different space bodies was still unknown and their relative abundances subject to debate. Analysis of the data delivered by the ROSINA instrument showed depletion of Xe with respect to Kr, and of Kr itself with respect to Ar. These relative abundances were found consistent, within observational errors, with solar relative abundances [1, 2, 3].

2. A primordial scenario

We might assume that the noble gases have been integrated to the icy grains precursors of comets in the interstellar medium, first stuck on the surfaces by adsorption, then covered by the successive layers of ices. Thus, they could have been kept embedded in the voids of the compact ices till they desorbed with ices and other volatiles by sputtering or sublimation of the surface ice layers. Such a scenario implies that Ar, Kr and Xe were trapped as a function of their solar abundances and strongly enough into ices holes not to migrate efficiently to the surface. It is most probably the reason why we are still able to observe them to day.

3. Two key points checked

In this contribution we report theoretical investigations of two key parameters of this scenario, i.e. the ability of noble gases to adsorb onto ices surfaces (first step of the process in the ISM) and their stability in cavities. In all situations we assume that the surrounding ice is made of H_2O (testing different shapes and sizes of cavities). For this purpose, we have used quantum numerical simulations based on first principle periodic density functional theory (DFT) [4, 5, 6]. These methods have shown to be well adapted to the description of compact and porous ices and are capable to describe the trapping of volatiles in the ice matrix [7, 8]. Our theoretical results were checked against the adsorption and inclusion energies obtained by the Bertin team using technics of Temperature Programmed Desorption (TPD) [9, 10].

3.1 Adsorption step

The three noble gases are found able to adsorb on icy surfaces in different locations with averaged energies going from 0.10 eV for Ar to 0.13 eV for Kr and 0.16 eV for Xe (Table 1).

Table 1: Adsorption energies of NG on water ices (eV)

NG	max	min	aver.	exp.[11]
Ar	0.12	0.07	0.10	0.08
Kr	0.15	0.10	0.13	0.13
Xe	0.19	0.10	0.16	0.17

Concerning the adsorption process, the specificity of crystalline versus amorphous ices is found irrelevant, giving no energetic differences [11].

3.2 Inclusion step

Voids of different shapes and sizes have been created within the crystalline structure in order to simulate irregular compact water ices. We found that Ar, Kr and Xe could stabilize in such voids (Table 2) with energies close enough to H_2O ice binding energy, implying that they can be trapped without disturbing the ice matrix.

Table 2: Stabilization energies of NG in holes (size of 2/4 water molecules) within the bulk of water ices (eV)

NG	hole 2	hole 4
Ar	0.2	0.22
Kr	0.2	0.27
Xe	0.2	0.34

In fine, these noble gases should leave the icy matrix only when this latter sublimates.

4. Summary and Conclusions

Noble gases detected in the coma of 67P/C-G might issue from the icy bulk where they might have been trapped in the constitutive planetesimals at the time of their formation in the interstellar medium. Using computational chemistry models based on first principle periodic density functional theory (DFT), we have evaluated their adsorption energies on top of ices, checking the possibility of their trapping, and then, the stability of these species in the irregular cavities of the compact ices, revealing a stabilisation efficient enough to keep them trapped until the ices sublimate.

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