

Neutral Na in comet tails: a chemical story

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Abstract

The origin of the neutral sodium comet tail discovered in comet Hale-Bopp in 1997 is still a matter of discussion. Here we propose a scenario which is based on chemical grounds. The starting point is the chemical trapping of the Na⁺ ion in the refractory material during the condensation phase of the protosolar nebula, followed by its incorporation in the building blocks of the comets parent bodies. In the next step, the Na⁺ ions are washed out of the refractory material by the water formed by the melting of the ice due to the heat released in the radioactive decay of short period elements. When the water freezes again, the Na⁺ ion loses its positive charge to evolve progressively toward a neutral atom when approaching the surface of the ice. As shown by high-level numerical simulations based on first principle periodic density functional theory (DFT) to describe the solid structure of the ice, it is a neutral Na that is ejected with the sublimation of the ice top layer

1. Introduction

The presence of sodium D line emission has been confirmed in a large number of comets close to perihelion over the past century. Observations of comet C/1995O1 Hale-Bopp during the spring of 1997 led to the discovery of a new tail connected with the sodium D line emission. This neutral sodium gas tail is entirely different from the previously known ion and dust tails, and its associated source is unclear. It has been proposed that this third type of tail is shaped by radiation pressure due to resonance fluorescence of Na atoms [1]. Further possibilities

were considered regarding the origin of this tail, then rejected, as photo-sputtering and/or ion sputtering of non-volatile dust grains [2]. Instead, it was proposed that the driving force would be the collisional interaction between the cometary dust coma of micron-sized particles and the very small grains [2].

Here, a completely different scenario built upon chemical grounds is proposed.

2. A three steps scenario

To obtain the solid and gaseous composition of the disk, we use the HSC chemistry package [3], based on the Gibbs energy minimization method. The equilibrium compositions of Na-bearing compounds forming over a wide range of temperatures in the protosolar nebula are represented on Figure 1. Whatever the disk's temperature, these Na-bearing compounds are all refractory materials below 900K.

It is generally admitted that comets are formed by accretion from solids consisting in a mixture of ice and rocks. At early epochs after accretion, the interior of comets has been subject to heating due to the radiogenic decay of short-lived nuclides ²⁶Al and ⁶⁰Fe. Despite the fact that specific results on the early heating of comets by radioactive isotopes alone still require detailed investigations on comet formation processes and timescales, so far all models are consistent with a potential occurrence of liquid water inside comets, for a given set of realistic initial parameters.

The evolution of the central temperature of 30km-radius bodies calculated, as a function of time after

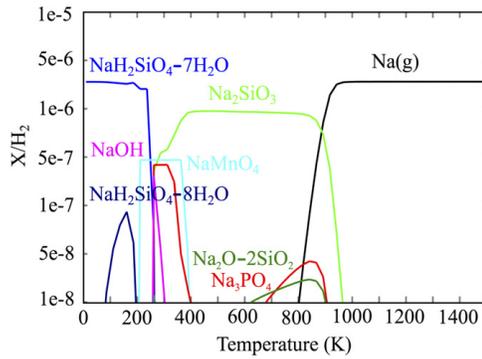


Figure 1: Equilibrium Na/H₂ abundances.

formation, is obtained by numerical simulations based on the model of Guilbert-Lepoutre [4]. It shows the melting of the ice in the nucleus, allowing the transfer of Na⁺ from refractory compounds to liquid water, with an electronic charge $q=1$.

The last step, i.e. the transformation of Na⁺ into a neutral atom when released from the sublimating cometary ice can be followed by means of high level numerical simulations based on first principle periodic density functional theory (DFT) to describe the solid structure of the ice. We used a periodic representation of solid water in the form of apolar hexagonal ice composed of bi-layers of water molecules. It is computationally justified because only apolar structures can generate slabs that are, at the same time, stable, reproduce the bulk properties, with a balanced distribution of hydrogen and oxygen sites at their surfaces. Practically, the Vienna ab initio simulation package (VASP) was used to carry out all the calculations [5]. The generalized gradient approximation (GGA) was used for geometry optimization and calculation of adsorption energies on the ice, including the Grimme correction to take care of the long-range van der Waals interactions. A plane-wave expansion of the basis set is used, coupled to projector augmented wave ultrasoft pseudo-potentials for the atomic cores.

In the ice, the periodic structure of the crystal imposes strong geometrical constraints leading to stable structures without counterpart in the liquid phase or in micro clusters. This evolution can be followed on Figure 2.

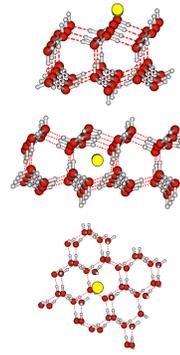


Figure 2: The path of Na, from bulk to surface.

Bottom : Substituted to H₂O molecule in the crystal, Na ($q=+0.82$) is stabilized by ~ 22 -25 kcal/mol that is stronger than the ice cohesion. *Middle* : Encapsulated in a void in the crystal, Na ($q=+0.86$) is stabilized by ~ 12 kcal/mol which is about one half of the ice cohesion. *Top* : On the surface, a quasi-neutral Na ($q=+0.20$) is attached by ~ 14 to 17 kcal/mol, i.e., by a bonding energy close to that of ~ 14 kcal/mol with which a single H₂O is attached to the ice surface.

3. Summary

Our scenario [6] is based upon chemical grounds. It is shown that the Na⁺ ions, originally trapped in the refractory materials, then washed out during the hydration phase, loose their positive charge to evolve progressively into neutral Na with their migration towards the surface of the cometary ices with which they are ejected.

References

- [1] Cremonese, G., Boehnhardt, H., Crovisier, J. et al., ApJ, Vol. 490, L199, 1997
- [2] Ip, W.H., & Jorda, L., ApJ, Vol. 496, L47, 1998.
- [3] White, W. B., Johnson, S. M., & Dantzic, G. B. J. Chem. Phys., Vol. 28, 751, 1958.
- [4] Guilbert-Lepoutre, A., Lasue, J., Federico, C., et al. A&A, Vol. 529, A71, 2011
- [5] Kresse, G., & Hafner, J., Phys. Rev. B, Vol. 49, 14251 1994.
- [6] Ellinger, Y., Pauzat, F., Mousis, O., et al. ApJ, Vol. 801, L30, 2015