

Which origin for molecular oxygen and sulfur in Comet 67P/Churyumov-Gerasimenko?

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The observation of O₂ and S₂ in comet 67P/Churyumov-Gerasimenko^{1,2} has led to a new interest regarding the origin of volatiles detected in comets. A priori, the situation seems different for those two volatiles. The former had not been detected in space for years, whereas the latter has been observed for decades in comets.

However, basing on observations, we assume that O₂ and S₂ have a similar primordial origin and we propose that they formed in the ISM, by irradiation (photolysis and/or radiolysis) of the H₂O molecules of the icy grains precursors of comets, and of the S-bearing molecules embedded in, creating voids in ices simultaneously, within which the produced volatiles can accumulate.

We have investigated the stability of O₂ and S₂ molecules in cavities formed by the irradiation, assuming that the surrounding material is made of pure H₂O ice in the case of O₂ and a mixed H₂O/H₂S ice in the case of S₂. To support this scenario, we used chemistry numerical models based on first principle periodic density functional theory (DFT). These models are shown to be well adapted to the description of compact ice and are capable to describe the trapping of the volatiles in the ice matrix. We showed that the stabilization energies of both O₂ and S₂ molecules in such voids are close to that of the H₂O ice binding energy, implying that they can only leave when the icy matrix sublimates. This is consistent with the observations and also supports our scenario of a common origin for both volatiles O₂ and S₂.

Differences can also be explained within this scenario. Unlike O₂ whose abundance correlates to H₂O, no global trend should be drawn between the variation of S₂ and H₂O abundances if S₂ can accumulate in both S₂-bearing and H₂O ices. Such results are supported by the ROSINA data collected between May 2015 (equinox) and August 2015 (perihelion), showing that, contrary to O₂, there is no correlation observed for S₂ with H₂O or H₂S in 67P/C-G.³

Références

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