Birth and life of sulphur dimers (*S2*) in cometary ices

F. Pauzat, O. Ozgurel, Y. Ellinger,

Sorbonne Université, UMR 7616-CNRS, Laboratoire de Chimie Théorique, 75005 Paris, France

O. Mousis

Aix Marseille Université, UMR 7326-CNRS, Laboratoire d'Astrophysique de Marseille 13388, Marseille, France

S_2 has been observed for decades in comets, but its recent observation in comet 67P/Churyumov-Gerasimenko (le Roy et al 2015) has reactivated new interest. As a matter of fact, the nature of its source is still in debate. Relying upon our scenario for O_2, we propose that S_2 is formed according an analogous process, i.e. by irradiation (photolysis and/or radiolysis) of S-bearing molecules embedded in the icy grains precursors of comets. As O_2 could be issued from the fragments of H_2O produced by irradiation, S_2 could come from the fragmentation of H_2S. This precursor is known as the most abundant sulfur-containing molecule present in comets ices, and could exist scattered or as clumps in the bulk of H_2O ices. The irradiation is assumed to create simultaneously voids in ices within which the produced molecules can accumulate. We investigate the stability of S_2 molecules in such cavities, considering that the surrounding ice is made whether of H_2S or of H_2O. We have studied this scenario by using quantum chemistry numerical models based on first principle periodic density functional theory (DFT). Such models have proved to be well adapted to the description of compact ice and are capable at the same time to describe the trapping of volatiles in cavities inside the ice matrix (Ellinger et al 2015, Mousis et al 2016). We show that the stabilization energy of S_2 molecules in such voids is close to that of the H_2O ice binding energy, which implies that they can only leave the icy matrix when this latter sublimates. Unlike O_2 whose abundance correlated to H_2O, no global trend should be drawn between the variation of S_2 and H_2O abundances, which can be explained by the fact that S_2 can accumulate in both S-bearing and H_2O ices. This interpretation is supported by the ROSINA data collected between May 2015 (equinox) and August 2015 (perihelion), showing that there is no clear correlation of S_2 with H_2O or H_2S in 67P/C-G (Calmonte et al. 2016).