Modeling reactivity and trapping of O2 in the bulk of cometary ices

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The search for (di-oxygen) O_2 in space has been carried out for years to no avail. It suddenly arose a new interest following its observation in comet 67P/Churyumov-Gerasimenko (Bieler et al 2015; Le Roy et al 2015). As a matter of fact, three years later, the nature of its source is still in debate.

We propose that di-oxygen was formed inside the icy grains precursors of comets by irradiation (photolysis and/or radiolysis) of the H_2O molecules of the ice itself. In this scenario, the irradiation is assumed to be responsible of two simultaneous events: i) to create hyper-reactive fragments (H, O, OH), from the broken water molecules, ii) voids in the compact ices, in which these fragments recombine into molecules including HO_2, H_2O_2 and ultimately O_2.

We have investigated the stability of O_2 molecules in such cavities, testing different shapes and volumes. For this purpose, we have used theoretical chemistry numerical models based on "first principle" periodic density functional theory (DFT). These models have shown to be well adapted to the description of compact ice and are capable to describe the trapping of volatiles in the ice matrix (Ellinger et al 2015).

We found that the stabilization energy of O_2 in such voids is slightly less than that of the H_2O ice binding energy, implying that these di-oxygen molecules are well trapped in the ices without disturbing the icy matrix. Dimers of O_2 are also stabilized in the same way. The net consequence is that these molecules can accumulate in the voids and then survive to the formation of pebbles and ultimately comets. They can leave the icy matrix only when this latter sublimates.

More important is the fact that the cavities encapsulating O_2 are formed with ~ 20-30 surrounding H_2O molecules, i.e. a ratio O_2/H_2O of 5% to 3%, well in line with the data collected between May 2015 (equinox) and August 2015 (perihelion) by the ROSINA mass spectrometer, showing a clear correlation of O_2 with H_2O with a ratio O_2/H_2O of 3.8%.