



Quantum chemical investigation on iodine oxides and their role in the formation of atmospheric aerosols

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Atmospheric iodine has received considerable attention in the two past decades due to both its potential role in the catalytic destruction of ozone (1) and its contribution to the formation of aerosol particles (2). Seaweeds and marine phytoplankton release iodocarbons and I₂ to the atmosphere, which are photo-oxidized giving iodine oxides that polymerize to finally form iodine oxide particles (IOPs). In the last years, some laboratory studies have been done to investigate this process (see e.g. (3)), however the complete mechanism of formation of such particles and the role of water in this process have not yet been elucidated. In this context, quantum calculations could help to unravel essential steps of these processes.

In this contribution, we will show preliminary results of a theoretical study on different reactions that iodine oxides and water can undergo to form IOPs. Thermodynamic properties of these reactions have been obtained at high level ab initio correlated calculations that included relativistic correction. In these calculations, we have used optimized basis sets and relativistic effective potentials for iodine atom developed in our group, which have been recently employed in a theoretical study on several iodinated species (4).

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