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Theoretical investigation on iodine oxides formation and their role in the production of atmospheric aerosols

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Atmospheric iodine has received considerable attention in the past two decades due to both its potential role in the catalytic destruction of ozone (1) and its contribution to the formation of ultrafine particles (2). Seaweeds, marine phytoplankton, and abiotic processes release iodocarbons and I_2 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 carried out to investigate this process (see e.g. (3)), however the complete mechanism of formation of such particles and the role of water, and other condensable vapors, in this process have not yet been elucidated. In this context, quantum calculations could help to unravel essential steps of these processes and to evaluate relevant physicochemical properties that can be incorporated into atmospheric models.

In this contribution, we show results of a theoretical study on different reactions that iodine oxides, in the presence of water, can undergo to form IOPs. Thermodynamic and kinetic properties of these reactions have been obtained at high level *ab initio* correlated calculations that included relativistic corrections. In these calculations, we have used a relativistic effective potential (REP) and REP-optimized basis sets for iodine atom developed in our group, which have previously been employed in a theoretical study about several iodinated species (4).

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