

Hydration and reactivity of iodic acid of atmospheric and nuclear issues

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Behaviour of iodine in the reactor coolant system (RCS) as well as in the nuclear containment building of a pressurized water reactor during a severe accident has been a subject of several experimental programs and modelling studies. Indeed ¹³¹I is one of the most important radiotoxic fission products that may be released through the RCS and next in the containment and further possibly into the environment by the direct leakages or the venting procedures. A detailed understanding of the evolution of the chemical speciation of all iodine compounds formed is necessary to assess the radiological consequences during the accident progress for a wide range of accidental scenarios.

This work focused on the reactivity of iodic acid (HIO₃) that can be formed by radiolytic oxidation of volatile iodine (I₂ and CH₃I) inside the containment or by UV radiation in the atmosphere. Their microhydration processes have first been studied to elucidate the role of hydrating water molecule(s) (Figure 1). The reactivity of iodic acid towards OH radicals, O, and H atoms are then presented. Reaction rate constants were further calculated by transition state theory and implications for both atmospheric chemistry and nuclear safety will be discussed.

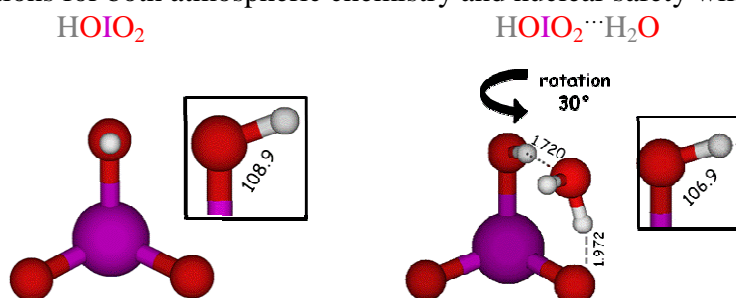


Figure 1: Optimized structures for HOIO₂ and HOIO₂ with one water molecule. Bond lengths are in angstroms and bond angles in degrees.

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