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Insights in the reactivity of CH_2ICH_2OH with OH radicals: implications for atmospheric iodine chemistry

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In the case of a nuclear power plant accident, fission products may be released into the atmosphere like during the Fukushima Daichi accident. To better understand the radiological consequences of such releases, especially for iodine 131, different theoretical simulation tools were developed and used to predict its chemical atmospheric evolution. Nevertheless, significant differences have been observed between the measured and modeled atmospheric Japan concentrations of iodine 131. This can be attributed to the high reactivity of atmospheric iodine that is not fully considered in the current atmospheric dispersion codes. The main objective of this work is to provide reliable kinetic and thermodynamic data for the gas phase reaction of CH2ICH2OH with the hydroxyl radical (OH) using high-level ab initio calculations. The potential energies have been calculated at the DK-CCSD(T)/ANO-RCC-VQZP(or -VTZP)//MP2/cc-pVTZ level of theory.

