International Master 2 Atmospheric Sciences: Research Training 2020-2021

Laboratory: PC2A

Supervisor: LOUIS Florent

Tél : 03.20.33.63.32, E-mail : florent.louis@univ-lille.fr

CaPPA Work Package: WP-6 Radionuclides – their fate

Unraveling the atmospheric degradation of iodinated organic compounds

Abstract

The goal of this internship is to improve the understanding of the gas-phase reactivity of iodine-containing species with major photo-oxidants, to better address the lack of data in the field of atmospheric chemistry and nuclear safety, and to provide a set of reliable kinetic and mechanistic data on gas-phase iodine reactivity.

Quantum chemistry is more and more used to determine rate constants for gas-phase elementary reactions because the power of the current generation of computers allows obtaining reliable kinetic parameters. It permits to understand the mechanism of global and elementary reactions. It allows calculating the molecular properties (geometrical data, molecular mass, vibrational frequencies, inertia moments) of reactants, products, transition states, and molecular complexes for an elementary reaction. Then, the macroscopic quantities such as the thermodynamical functions (internal energy, enthalpy, and Gibbs free energy) are calculated from molecular properties using statistical thermodynamics. Finally, temperature and pressure dependencies of rate constants will be determined using kinetic theories from thermodynamical functions.

Key words: iodine, atmospheric chemistry, reactivity, molecular simulations