

# Atmospheric reactivity of iodoalkanes towards OH radicals

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The importance of iodine in the atmosphere is known for more than two decades. Among the frequently discussed effects of atmospheric iodine are: *i*) the ozone depletion in the lower stratosphere due to the presence of IO and OIO species, *ii*) the role of iodine compounds in new particle formation in marine environments, *iii*) chemistry of halogens in troposphere through the interaction of iodine compounds with bromides and chlorides. Besides iodomethane (CH<sub>3</sub>I), several other organic iodine-containing compounds have been detected in marine boundary layer in the coastal water or in open ocean. Iodomethane and diiodomethane are produced by microalgae and phytoplankton in marine boundary layer and belong to the most abundant and reactive alkyl iodides in the troposphere. They participate in the generation of aerosols in coastal zones. While the former can persist from several hours to several days, the latter has shorter lifetime – from minutes to hours. In both cases, these time windows represent a potential for long distance atmospheric transport of iodine and the potential for chemical reactivity that can affect various atmospheric cycles, including ozone cycle.

Iodoalkanes can undergo several decomposition pathways. For instance, CH<sub>3</sub>I is easily photolyzed producing iodine atoms that enter ozone cycle or can react with NO, HO<sub>2</sub>, ClO, BrO, or IO. CH<sub>3</sub>I can abstract either H or I under attack of OH radicals, or Cl atoms, provided the concentration of the reactant radicals is high enough to compete with the photolysis.

High-level *ab initio* molecular orbital studies offer a viable alternative to provide reliable thermodynamic and kinetic data for the gas-phase chemical reactions. Modelling H- or I-abstraction from alkyl iodides is rather demanding task because for predicting the kinetic parameters one has to reach at least the chemical accuracy of the underlying thermodynamic data (better than  $\pm 4$  kJ mol<sup>-1</sup>). This implies to choose the computational chemistry tools that include all necessary and accurate corrections to molecular energies (basis set saturation, valence and core-valence electron correlation, relativistic effects, spin-adaptation, vibration contributions, and tunnelling corrections).

In this talk, we will report the results of *ab initio* calculations obtained for the reactivity of a series of iodoalkanes towards OH radicals.