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Alkyl halides at the liquid water–vapor and ice–vapor interfaces

Martina Roeselova (1), Alena Habartova (1), Babak Minofar (2), Hasan Pašalić (3), and Hans Lischka (3)

(1) Institute of Organic Chemistry and Biochemistry Academy of Sciences of the Czech Republic, Prague, Czech Republic (roesel@uochb.cas.cz), (2) Institute of Physical Biology, University of South Bohemia, Nove Hrady, Czech Republic, (3) Institute for Theoretical Chemistry, University of Vienna, Vienna, Austria

Alkyl halides of both biogenic and anthropogenic origin play an important role in atmospheric chemistry as a source of organic halogens in the atmosphere. They are known to participate in heterogeneous atmospheric chemistry, however, information about the exact reaction mechanisms is often missing. We investigate the interaction of alkyl halide molecules with the surface of liquid water and ice using both classical and ab initio molecular dynamics simulations as well as quantum chemistry calculations. A systematic study included alkyl chlorides, bromides and iodides, from methyl halides (CH3X) up to pentyl halides (C5H11X), where X = Cl, Br, or I. The results provide a molecular level insight into the surface orientation and hydration shell structure of alkyl halides on water and ice. While for most of the alkyl halide species a parallel alignment of the molecule at the surface is found with the hydrocarbon chain pointing slightly to the gas phase, methyl halide molecules are located at the surface preferentially with the methyl group oriented more toward the aqueous interface and the halide atom exposed to the gas phase. The observed difference in preferred surface orientation between the methyl halides and the longer chain alkyl halides is likely to have consequences for the chemistry of alkyl halides adsorbed on the surface of aqueous and ice particles in the atmosphere.