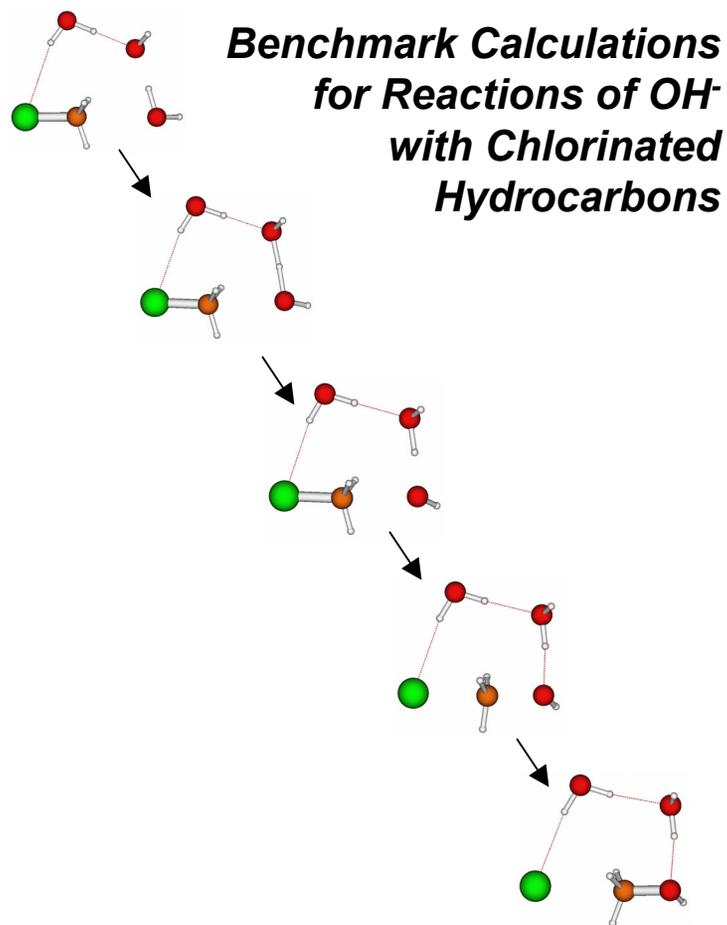


## Chemical Fate of Contaminants in the Environment



A major challenge for computational chemistry is the accurate calculation of rate constants for reactions in aqueous solution, such as those involving environmental contaminants such as chlorinated hydrocarbons. We have developed a systematic approach to study the effects of molecular environments on the energetics and dynamics of chemical reaction in liquids. This approach uses a hierarchy of computational tools from highly accurate ab initio calculations on cluster models to approximate treatments of bulk solvation. We have recently reported benchmark calculations on the energetics for reactions of OH<sup>-</sup> with methyl chloride, dichloromethane, chloroform, and carbon tetrachloride. These studies have been extended to include the effects of small numbers of water molecules (microsolvation) and to approximate bulk solvation effects using hybrid quantum mechanical/molecular mechanics techniques.

EE Arcia, YA Borisov, BC Garrett, TH Dunning, Jr.,  
SL Mielke *J. Phys. Chem. A* **105**, 7724 (2001)