

Thermochemistry and Kinetic Modeling for OH Addition to Trifluoroethene

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Fluorinated halocarbons (CFCs and HCFCs) are widely used as refrigerants and heat transfer fluids. Partially oxidized CFCs are routinely found in environmental waters and in the atmosphere, and concerns exist for their influence on global warming and health. The study is focused on the initial OH radical reactions with $\text{CF}_2=\text{CHF}$ (Trifluoroethylene) which being considered as a refrigerant heat transfer fluid and is also an important monomer in fluoro-polymer synthesis. The reaction of OH with $\text{CF}_2=\text{CHF}$ and the subsequent reactions of the energized complex (adduct) are studied using density functional theory and CBS-QB3 ab initio theoretical methods. Enthalpies of formation, entropies and heat capacities (T) are determined. Detailed potential energy surfaces and kinetic parameters for the reactions of the two hydroxyl adducts, subsequent intra-molecular H atom and F atom transfer, HF and atom eliminations and beta scission reaction paths are calculated. Kinetics are calculated using quantum Rice-Ramsperger-Kassel (QRRK) theory for $k(E)$, and master equation analysis for falloff. The reaction system is modeled versus time and temperature with CHEMKIN under conditions for atmospheric and combustion. HF molecular elimination from the initially formed, chemically activated, HOCHF-CF_2^* and $\text{HO-CF}_2\text{-CHF}^*$ adducts is endothermic relative to the energy of the reactants, and an observed channel under atmospheric conditions.