Theoretical Studies of the Hydrodehalogenation Reactions of $CBrX_3$ (X= H, F, Cl)

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INTRODUCTION

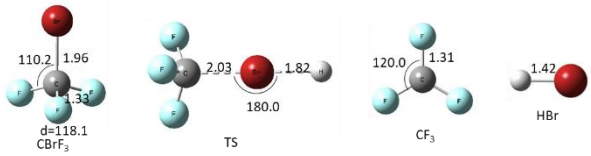
Halons, a group of chemicals with diverse industrial and consumer applications such as refrigeration, fire suppression, and foam manufacturing, possess desirable properties. Unfortunately, they are also potent ozone-depleting substances (ODSs) and greenhouse gases (GHGs), contributing to environmental harm. Their widespread use has led to significant ozone layer depletion and exacerbated global warming. To address this, the Montreal Protocol mandated the gradual phase-out of ODS production globally, sparking research into ODS treatment[1]. Developing models for the thermal degradation of halogenated compounds in flames requires a deep understanding of reaction mechanisms, kinetic data, and thermodynamics. This knowledge is crucial for comprehending the incineration of hazardous industrial waste and developing more environmentally friendly incineration methods. It's particularly relevant when studying halogen abstraction from $CBrF_3$ (halon-1301) by hydrogen atoms during combustion, a process central to incineration but capable of producing toxic by products. Their potency to destroy ozone is measured by their Ozone Depleting Potential (ODP). Ozone depleting substances controlled by Montreal Protocol include:

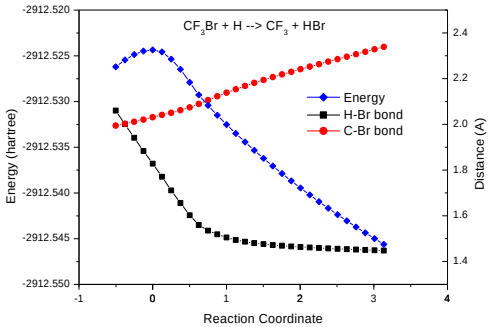
- CFCs
- Halon (CFxClyBrz)
- Chlorocarbons
- Hydrochlorofluorocarbons (HCFCs)
- Hydrobromofluorocarbons (HBFCs)
- Bromocarbons
- Bromochloromethane

METHODS

The several Method was employed in our work to determine the potential energy surface (PES), geometries, vibrational frequencies and energies of the reactants, transition states and products of the $CBrX_3 + H_2$ (X = H, F, Cl) reactive process. Vibrational frequencies were used to characterize the stationary points as minimum or transition states; the number of imaginary frequencies (0 or 1) indicates whether a minimum or a transition state has been located. To confrm that the transition state really connects reactants and products, the intrinsic reaction coordinate (IRC) calculations were determined. All calculations were performed with Gaussian16 program. Researchers employ advanced tools like RRKM/Master Equation, Transition State Theory (TST), and programs like MESMER[2] and Apuama[3] to investigate the kinetics of hydrodehalogenation reactions of $CBrX_3$ (where X = H, F, Cl) across a wide temperature range (298-1500 K). These studies involve detailed potential energy surface mapping and utilize density functional theory (DFT) with various basis sets for all reaction species.

RESULTS





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