

ABSTRACT

The intensive emission of halogen compounds into the Earth's atmosphere is one of the main reasons for the progressive degradation of the environment. Among these compounds, halogenated *n*-alkanes play a particularly infamous role. It is caused by the large-scale production of these substances in industrial processes and their high chemical reactivity.

The deactivation of chloroalkanes in the Earth's atmosphere is the subject of intensifying research in various branches of environmental chemistry. Currently, the most promising method of neutralising these compounds is their oxidation by radical reactions using chlorine atoms. In their most essential part, these processes boil down to the abstraction of a hydrogen atom from the chloroalkane molecules. Reactions of this type are characterised by much higher rates than those using, for example, a hydroxyl radical as an oxidant.

The first part of this dissertation presents the results of theoretical studies on the mechanism, thermodynamics, and kinetics of radical reactions of a hydrogen and deuterium atom abstraction from four selected chloroalkanes, i.e. chloroethane, 1,2-dichloroethane, 2-chloropropane and 1-chloropropane. The model processes were carried out in a simulated vacuum using advanced quantum chemistry methods.

The halogen bond (XB) is one of the three main specific non-bonding interactions. However, despite its undeniably great importance in nature, especially in the proper functioning of biological systems, it is the least studied interaction of this type.

The second part of the dissertation concerned theoretical investigations of the nature of the interaction through the halogen bond, mainly from the perspective of its energy. The results obtained are described in the fourth publication appended to this guide. The subjects of the studies were six model complexes with linear structure and formula $\text{O}\equiv\text{C}\cdots\text{X}-\text{Y}$, where $\text{X}-\text{Y}$ denotes $\text{Br}-\text{Br}$, $\text{Cl}-\text{Cl}$, $\text{F}-\text{F}$, $\text{Br}-\text{Cl}$, $\text{Br}-\text{F}$ and $\text{Cl}-\text{F}$, respectively. In addition, a distinct XB characterises them. The systems obtained by optimising the geometrical structure were subjected to the procedure of interaction energy decomposition using the LMOEDA (localised molecular orbital energy decomposition) method. It allows for the separation and complete analysis of all components of the total interaction energy.