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DISPOSAL OF POISONOUS ORGANIC HALIDES BY USING THE ELECTROCHEMICAL METHOD: DFT SIMULATION

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Abstract. Geometry optimizations at the UBP86/6-311++G** level of electronic structure theory have been performed for DDT, *β*-hexachlorocyclohexane, and heptachlor organic polychlorides as well for their positive and negative ions. The HOMO composition of these neutral molecules show no participation of the carbon-chlorine atomic orbitals, while LUMO of the calculated molecules include a major contribution of the anti-bonding character atomic orbitals from the two or three carbon-chloride bonds of each calculated molecule. Consequently, the negative ions were the most sensitive structure during the geometry optimization, showing the carbon-chloride bonds cleaving during the electronic structure calculations. Further geometry optimization of the obtained neutral intermediate molecules after the first and second reducing by two electrons show that the electrochemical dehalogenation of the organic poychlorides is sequential.

Keywords: poisonous pesticides, organic chlorides, electrochemistry, DFT, carbon-chloride bonds.

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