Hydrolysis reaction of 2,4-dichlorophenoxyacetic acid. A kinetic and computational study

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The degradation of the 2,4-dichlorophenoxyacetic acid in aqueous solution is an hydrolysis reaction. Two products are identified: 2,4-dichlorophenol and glycolic acid. Reaction is investigated as a function of pH and temperature, and it is first-order kinetics and pH-dependent. Reaction is modeled in gas phase, where a proton catalyses the reaction. Critical points of PES are calculated at B3LYP/6-311++G(3df,2p), and aug-cc-pvqz//6-311++G(3df,2p) levels plus ZPE at 6-311++G(3df,2p) level. The activation barrier is 21.2 kcal/mol. Theoretical results agree with the experimental results. A second mechanism related with a Cl<inf>2</inf>Ph-O-CH<inf>2</inf>-COOH...H<inf>2</inf>O complex is found, but with a rate limiting step of 38.4 kcal/mol.