DFT study on hydrolysis pathway of herbicide naphtalam

Wichien Sang-aroon1*, Vithaya Ruangpornvisuti2

1Department of Chemistry, Faculty of Engineering, Rajamangala University of Technology Isan, KhonKaen campus, KhonKaen 40000, Thailand
2Molecular Modeling and Computational Chemistry Research Group, Supramolecular Chemistry research unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10320, Thailand
*E-mail: wichien.sa@rmuti.ac.th

Abstract: Naphtalam is phthalic acid herbicide-family which is selectively active to suppress the growth of herbicide seed. The herbicide contaminated in environment will be directly toxic to farmers or resided in animals and also human life cycle. In this work, degradation of naphtalam via direct (concerted and step-wise) and cyclic intermediate hydrolysis reaction pathways were explored computationally. The energetics, thermodynamic properties, rate constants, and equilibrium constants of all hydrolysis reactions, as well as their energy profiles were computed at the B3LYP/6-311++G(d,p) level of theory. The concerted and the step-wise hydrolysis resulted in naphthylamine and phthalic acid as products. 1-naphthol and isoindoline-1,3-dione are degradation products of cyclic intermediate hydrolysis pathway. The result indicated that hydrolysis of naphtalam occurred most preferentially via the cyclic intermediate hydrolysis pathway. The overall reaction rate constants of cleavage pathways assisted by a water molecule were, in increasing order: concerted < step-wise < cyclic intermediate.

Keywords: Naphthalam; Direct hydrolysis; Cyclisation hydrolysis; DFT; Rate constant