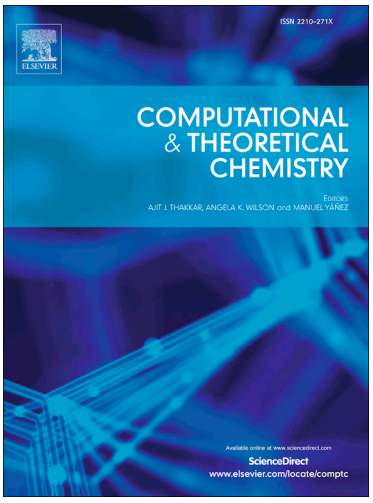

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Abdelkader M. Elhorri, Kumar D. Belaid, Mourad Zouaoui–Rabah, Redouane Chadli

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Theoretical study of the azo dyes dissociation by advanced oxidation using Fukui indices. DFT calculations.

Abdelkader M. ELHORRI[1,*], Kumar D. BELAID[2], Mourad ZOUAOUI–RABAH[1], Redouane CHADLI[3]

[1] *Laboratoire de microscopie et de spectroscopie moléculaire (L2MSM), Djillali Liabes University of Sidi–Bel–Abbes, P.O. Box 89, 22000 Sidi Bel-Abbes, Algeria*

[2] *Laboratoire de matériaux et systèmes réactifs (LMSR), Djillali Liabes University of Sidi–Bel–Abbes, P.O. Box 89, 22000 Sidi Bel-Abbes, Algeria*

[3] *Laboratoire de chimie organique, substances naturelles et analyses (COSNA), University of Tlemcen, Algeria*

Abstract:

This work focuses on the study of the degradation to four acid dyes by advanced oxidation; the dyes used are called blue acid 113, 114, 118 and 120. The goal of this study is the determination of the most reactive sites at the levels of the dyes studied, in order to understand the mechanisms of degradation of these dyes in the field of water depollution. The study was carried out theoretically by *ab initio* methods. The corresponding results were calculated by CAM–B3LYP functional combined with the 6–31++G(d, p) basis set. The calculated parameters are the local Fukui indices for radical attacks, hardnesses, dipole moments, solvation Gibbs free enthalpy ΔG_{solv}, wavelengths of the maximum absorption and oscillator Strengths. The results showed a good agreement between the mechanisms proposed experimentally and the mechanisms calculated theoretically. Hence, the confirmations of these mechanisms were obtained by local Fukui indices. The latter's revealed larger values for the nitrogen atoms constituting the four dyes, which confirm that these sites are the most reactive by radical attacks. This study is dedicated for advanced oxidation applications.

Key words: blue acid dyes, advanced oxidation, radical attacks, Fukui indices, DFT, TD–DFT.

1. Introduction

Azoic dyes have attracted the attention of researchers in recent decades because of their broad applications in the field of optics such as optical storage, holography and nonlinear optics [1]. They are also used in other fields such as the textile industry [2], fleurish cosmetics [3] and fast food [4]. Azo dyes have shown many advantages such as excellent photophysical properties [5], biological and pharmacological activities [6]. Despite the diverse applications and benefits of azo dyes, they are considered pollutants by their discharges into the waters [7]. Their effluents are harmful to human health. However, the researchers have developed several technics to eliminate these pollutants, for example: clays and activated carbon adsorption, coagulation–flocculation, advanced oxidation, electrocoagulation, flotation, ozonation and photocatalysis ... etc [8-12].