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A DFT study of disperse yellow 119 degradation mechanism by hydroxyl radical attack

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Abstract:
Previous experimental studies had proposed two possible mechanisms, that is, N-N or C-N bond cleavage, for azo dye degradation. However, the relative feasibility of these mechanisms based on their energetics has not been properly explored. In this work, the mechanisms of azo dye degradation by hydroxyl (OH) radical were investigated theoretically for disperse yellow 119 (DY119) dye using density functional theory (DFT) method. This was done with the view to provide useful theoretical insights on photodegradation mechanism of azopyridone dyes. The role of hydrogen bonding on the mechanism was investigated, and the possibility of nitrogen evolution during the process was also examined. Potential energy profiles (PEPs) for the two possible mechanisms were predicted at VWN-BP/DNP level of theory. Local reactivity indices and energy parameters revealed that the C–N bond cleavage mechanism is preferred to the N-N cleavage for the photodegradation of DY119. Removal of one intramolecular hydrogen bond from DY119 structure enhanced both the C–N and N–N bond cleavages, but with greater effect on C–N. Loss of nitrogen molecule via the C–N bond cleavage was predicted to be highly spontaneous.