

Reactions of nicotine and the hydroxyl radical in the environment: Theoretical insights into the mechanism, kinetics and products

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Abstract:

Nicotine (**NCT**) is a prevalent and highly poisonous tobacco alkaloid found in wastewater discharge. Advanced oxidative processes (AOP) are radical interactions between harmful pollutants and ambient free radicals that, theoretically, result in less toxic compounds. For a better understanding of the chemical transformations and long-term environmental effects of toxic discharges, the study of these processes is crucial. Here, quantum chemical calculations are used to investigate the AOP of the **NCT** in aqueous and lipidic environments. It was found that **NCT** interacted with HO[•] in polar and nonpolar media, with an overall rate constant $k_{\text{overall}} = 10^6 - 10^{10} \text{ M}^{-1} \text{ s}^{-1}$. The computed kinetic data are reasonably accurate as seen by the comparison with the experimental rate constant in water (pH = 7.0), which results in a $k_{\text{calculated}}/k_{\text{experimental}}$ ratio of 1.4. The hydrogen transfer–single electron transfer pathways are the main mechanisms for the HO[•] + **NCT** reaction in pentyl ethanoate solvent to form the cations as the primary products of the two-step reaction. However, in aqueous environments, the degradation of **NCT** by HO[•] radicals is affected by pH variations. The results show that the breakdown of **NCT** increases with increasing pH levels, despite the fact that the AOP products of **NCT** are less harmful than **NCT** itself, especially in an aqueous environment with a pH < 7.0.

Keywords: nicotine, DFT study, advanced oxidation processes, structure-activity relationship, chemical fate

