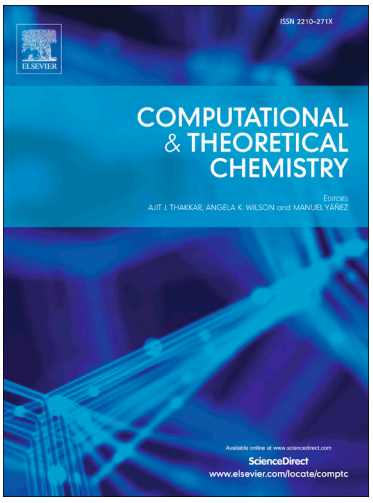

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ABSTRACT

Density Functional Theory was used to explore the protonation of the amine/imine byproducts of the alloxydim herbicide. An extensive exploration of the possible protonation sites of anionic and neutral fragments was performed. Doubly charged species were also considered. The structure and relative stabilities of different tautomers were determined. The results were analyzed by