Elucidation of the dechlorination pathway of 1,2,3,4-TCDD through atomic charge calculation

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\begin{abstract}
The atomic charge of 1,2,3,4-TCDD as a model compound of dioxin using the Gaussian 03 program was compared with the radical dechlorination decomposition pathway reported in the literature. In the case of the atomic charge, the chlorine combined at the position of the carbon with a large negative charge value was found to have been dissociated first. Among the atomic charges, the CHelpG charge had the best agreement with the dechlorination degradation results in the literature. Based on the results, it is suggested that the radical dechlorination decomposition pathway of organic chlorinated compounds, including dioxins, can be predicted through atomic charge calculation.

Keywords: Dioxins; Atomic charge; Radical; Dechlorination pathway
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