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Oxidative Activation and Degradation of Organophosphorus Pesticides Mediated by Iron Porphyrins

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Abstract:

Biomimetic oxidation mediated by three types of iron porphyrins was examined for five organophosphorus pesticides, fenitrothion (**I**), cyanophos (**II**), tolclofos-methyl (**III**), butamifos (**IV**) and fenthion (**V**). The major products from **I–IV** were the corresponding phenols and each oxon formed *via* a phosphoxathiirane intermediate by oxidation at the P=S moiety similarly as reported for their mammalian metabolism by cytochrome P450 enzymes. Stepwise oxidation of the methylthio sulfur *via* sulfoxide to sulfone, and ester cleavage and oxidative desulfuration primarily proceeded for **V**. Both the electron distribution of the highest occupied molecular orbital and its energy level of the pesticides calculated by MNDO-PM3 were shown to control the reaction site and rate of oxidation at sulfur atoms. © Pesticide Science Society of Japan

Keywords:

oxidation mediated by iron porphyrin, organophosphorus pesticides, MNDO-PM3 calculations

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