Ozonation of Phosmet Insecticide in the Gas Phase: Mechanistic and Kinetics Studies

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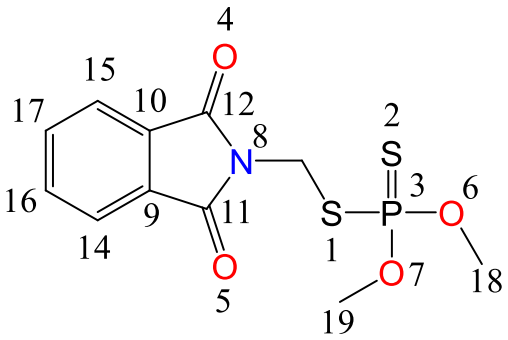
Abstract

Phosmet (Phos) (*O*,*O*-Dimethyl S-phthalimidomethyl phosphorodithioate) ($C_{11}H_{12}NO_4PS_2$) is a phthalimide-derived, non-systemic, organophosphate insecticide that has widely been used to control insects and mites in fruit, potatoes, sweet potatoes, vines, cotton, and other crops. Phos is a dangerous compound as it inhibits the acetylcholinesterase enzyme available in the central nervous system. [1] Other adverse effects of phosmet include dizziness, slowed heartbeat, convulsions, severe respiratory irritation, and even fatality. [2] Understanding decomposition in environmental conditions is crucial for better controlling the water treatment processes, and further predicting its ecotoxicity and human health effects.

Thus, thermodynamics and kinetics for phosmet insecticide decomposition by ozone (O_3) in the gas phase were investigated using the DFT/M06-2X/6-311++G(3df,3pd)//M06-2X/6-31+G(d,p) level of theory at a temperature from 283 to 333 K. The results show that the O_3 addition to the C16=C17 double bond of the benzyl ring is recognized as the dominant reaction with Gibbs free energies of reaction ($\Delta_r G^0$) and free energy barrier ($\Delta G^{\#}$) being -89.2 and 95.3 kJ mol^{-1}, respectively, and the rate constant being 3.78×10^{-3} M^{-1} s^{-1}. The total rate constant of the reaction is equal to 6.64×10^{-3} M^{-1} s^{-1} at 298 K. The total rate constants as function of the studied temperature range is also presented. Subsequent reactions of the major addition-intermediates with O_3 and lifetimes of phosmet as function of the O_3 concentration are computed to further assess the atmospheric effect of phosmet.



References:

[1] H. Bagheri, Z. Ayazi, E. Babanezhad, *Microchem. J.* 2010, 94, 1–6.

[2] Y. Fan, K. Lai, B. A. Rasco, Y. Huang, *Food Control* 2014, 3,153–157.