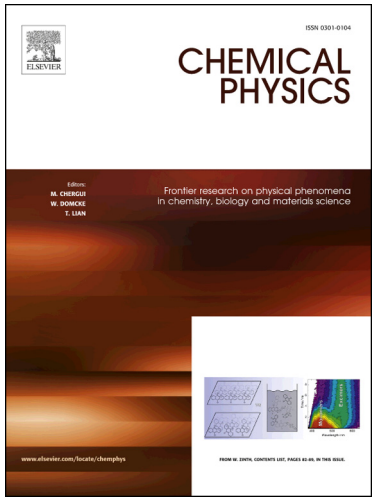
Accepted Manuscript



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PII: S0301-0104(17)30795-4
DOI: https://doi.org/10.1016/j.chemphys.2017.12.013
Reference: CHEMPH 9894

To appear in: *Chemical Physics*

Received Date: 23 September 2017
Accepted Date: 21 December 2017

Please cite this article as: S. Ponnusamy, L. Sandhiya, K. Senthilkumar, Reaction Mechanism and Kinetics of the Degradation of Terbacil initiated by OH radical - A Theoretical Study, *Chemical Physics* (2017), doi: https://doi.org/10.1016/j.chemphys.2017.12.013

Reaction Mechanism and Kinetics of the Degradation of Terbacil initiated by OH radical - A Theoretical Study

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Abstract:

The reaction of terbacil with OH radical is studied by using electronic structure calculations. The reaction of terbacil with OH radical is found to proceed by H-atom abstraction, Cl-atom abstraction and OH addition reactions.The initially formed alkyl radical will undergo atmospheric transformation in the presence of molecular oxygen leading to the formation of peroxy radical. The reaction of peroxy radical with other atmospheric oxidants, such as HO_2 and NO radicals is studied. The rate constant is calculated for the H-atom abstraction reactions over the temperature range of 200 to 1000 K. The results obtained from electronic structure calculations and kinetic study show that the H-atom abstraction reaction is more favorable. The calculated lifetime of terbacil is 24 hours in normal atmospheric OH concentration. The rate constant calculated for H-atom abstraction reactions is $6x10^{-12}$, $4.4x10^{-12}$ and $3.2x10^{-12}$ $cm^3molecule^{-1}s^{-1}$, respectively which is in agreement with the previous literature value of $1.9x10^{-12}$ $cm^3molecule^{-1}s^{-1}$.

Keywords: Terbacil, atmospheric reactions, OH radical, kinetics, secondary organic aerosol.