**ABSTRACT**

 In the present study, a possible reaction mechanism for the degradation through Cl initiated atmospheric oxidation of methyl salicylate (MeSA) was studied using density functional theory at B3LYP and M06-2X levels of theory with 6-311++G(d,p) basis set. The degradation occurred through an abstraction process at the meta position of MeSA along the entire reaction path. The barrier height values indicated that the reaction of the benzoate radical of MeSA and NO was a favourable route for degradation, which was thermodynamically exothermic and exergonic in nature. The lifetime calculations indicated a short life span for MeSA at 1.14 days. The rate constant values displayed good Arrhenius character with respect to temperature. The activation hardness predicted a rapid reaction between MeSA and NO. The HOMO and LUMO values along with their plot indicated that the NO radical and benzene ring in the MeSA were highly reactive. Topological analysis revealed that during the reaction the interaction between reactants was covalent in nature.