**ABSTRACT**

A detailed density functional theory investigation has been performed on the gas phase reaction mechanism of 2,4,5-TMP with OH radical by considering both abstraction and addition channels at three different functionals with 6-311++G(d,p) basis sets. Among the H-abstraction channel, phenol group reaction is favorable with barrier height of 5.27 kcal/mol whereas the addition channel results show that the OH-addition to C6 (ortho position) is more energetically favorable with small barrier height of 1.39 kcal/mol. The reaction force analysis also indicates that both H-atom abstraction and OH addition pathways are dominated by structural rearrangement than the electronic reordering. The rate constants are calculated over the temperature range of 278–350 K. The Arrhenius plot shows positive temperature dependence of both abstraction and addition reactions in the whole temperature range indicating its occurrence in the upper troposphere. However, the addition reaction rate constant is found to be favourable than abstraction reaction, and agrees reasonably well with the experimental study. The calculated atmospheric lifetime of 2,4,5-TMP and OH radical with respect to addition reaction is 14.69 h and seems competitive to photolysis process of methoxyphenols