**ABSTRACT**

Reaction mechanism of 2‐methoxyphenol (2MP) (guaiacol) with OH radical has been performed using density functional theory methods BH&HLYP and MPW1K method with 6‐311++G(d,p) basis set. Single‐point energy calculations were done using CCSD(T)/6‐311++G(d,p). The theoretical results reveal that the hydrogen abstraction from methoxy group is found to be the dominant reaction channel with an energy barrier of 9.31 kcal/mol. Also, time‐dependent density functional theory calculations have been performed using BH&HLYP/6‐311++G(d,p) level of theory, and the results reveal that the reactions occur in ground state than the excited state. The results of reaction force profile indicate that structural rearrangements are most influential with high percentage than the relaxation process. The calculated theoretical rate constants (12.19 × 10−11 cm3 molecule−1 s−1) are in good agreement with the experimental rate constant. The atmospheric lifetime of 2‐methoxyphenol with respect to OH radicals is 2.27 hours, which implies that OH radical plays an important role in the degradation of 2MP. The Wiberg bond index of the abstraction reaction reveals that the bond order is concerted, partially synchronic. The reactant‐like transition state satisfies Hammond postulate, which eventually results in an exothermic reaction, and the product‐like transition state reveals in endothermic nature.