The rate constants calculations and the potential energy surface for indenyl C_9H_7 +O_2 reaction by ab initio methods

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Polycyclic aromatic hydrocarbons, which are considered among the most abundant pollutants and as soot precursors, exert a great impact on environment and health. The C_9H_7 + O_2 reaction may play a significant role in combustion processes. Ab initio calculations were employed to calculate the energies of various reaction pathways and final products; geometries of the reactants, various intermediates, transition states, and products on the C_9H_7 + O_2 PESs were optimized at the density functional B3LYP/6-311G(d,p) level of theory and single-point energies were refined at the G3(MP2,CC) level (Figure 1).

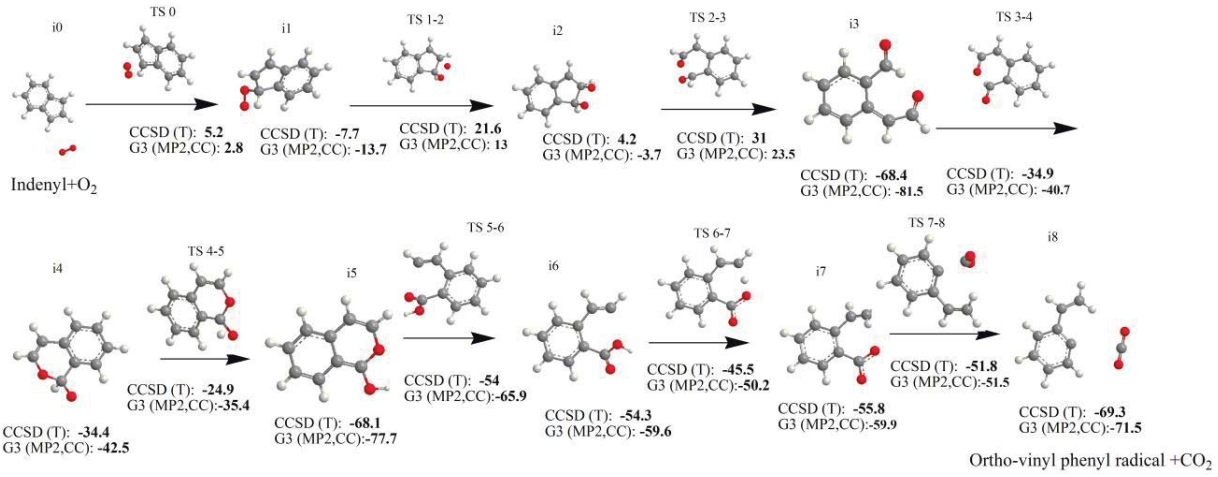
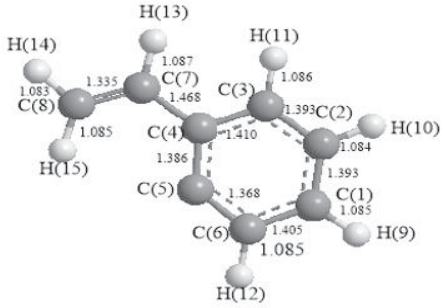


Fig. 1 The C_9H_7 + O_2 reaction pathway leading to the ortho-vinylphenyl radical C_8H_7 formation: the energies are indicated for both CCSD(T) and G3(MP2,CC) levels of theory.



The reaction can proceed by two possible pathways; both of them involve O_2 insertion into the 5-membered ring eventually leading to CO_2 elimination with formation of ortho-vinylphenyl radical (Fig. 2) and styrenyl as main reaction products. Rate constants and product branching ratio calculations have been performed for all reaction pathways.

Fig. 2 Optimized geometry of the ortho-vinyl phenyl radical; the numbers show bond lengths in Å.