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New trace of secondary organic aerosol from oxidation of acetonitrile with radical hydroxyl

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Abstract

Gas phase oxidation reaction of acetonitrile as a volatile organic compound and hydroxyl radical are investigated in this work. The studied chemical reaction can have important role in the formation of secondary organic aerosol based on acetonitrile. The B3LYP in connection with 6-311++G(3df,3pd) basis set and G3B3 levels of computation were used to optimize geometries of reactants, products, intermediates, and transition states. Then, CCSD(T)/ 6-311++G(3df,3pd) level was used to obtain accurate energies. Eleven kinds of products were obtained. Three of them have enough thermodynamic stability and one of them is kinetically favorable. The reaction pathways corresponding to each product is discussed and the potential energy surface was drawn. The rate constant for P2 as kinetic adduct was calculated at atmospheric pressure over the temperature range 200-2500 K. Finally, the formation of secondary organic aerosol has been discussed.

Key words VOC, SOA, acetonitrile, radical hydroxyl, reaction pathway, potential energy surface

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