Atmospheric oxidation of 4-(2-Methoxyethyl) phenol initiated by OH radical in the presence of O2 and NOx: A mechanistic and kinetic study

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Abstract

4-(2-Methoxyethyl) phenol (MEP) is an significant methoxypheolic compound, which has been shown to play an important role in the formation of secondary organic aerosols(SOA). The present work focuses on the gas-phase oxidation mechanism and kinetics of MEP and OH radical by the density functional theory (DFT). Energetically favourable reaction channels and feasible products were identified. The initial reactions of MEP with OH radical have two different channels: OH addition and H abstraction. Subsequent reaction schemes of main intermediates in the presence of O2 and NOx are investigated using quantum chemical methods at M06-2X/6-311++G(3df,2p)//M06-2X/6-311+G(d,p) level. Ketene, Phenyldiketones and nitrophenol compounds are demonstrated to be possible oxidation products. The total rate constant(1.69×10-11 cm3 molecule-1 s-1) and individual rate constant are calculated using the traditional transition state (TST) theory at 298K and 1atm. The lifetime of MEP is estimated to be 16.4 hours, which provides a comprehensive explanation for atmospheric oxidation pathway of MEP and shows MEP would be removed by OH radical in the atmosphere.

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