



Gas-phase reaction of hydroxyl radicals with m-, o- and p-cresol

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The gas-phase reaction of oxygenated aromatic compounds m-cresol, o-cresol and p-cresol with hydroxyl radicals has been studied by GC-MS. Experiments have been performed in a large-volume photoreactor (8 000 Litres) at (294 ± 2) K and atmospheric pressure. The relative kinetic method was used to determine the rate constants for these reactions, with 1,3,5-trimethylbenzene as reference compound. The rate constants obtained are: $k_{OH}(\text{m-cresol}) = (5.88 \pm 0.92) \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$; $k_{OH}(\text{o-cresol}) = (4.32 \pm 0.52) \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$ and $k_{OH}(\text{p-cresol}) = (4.96 \pm 0.75) \times 10^{-11} \text{ cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$. The degradation products observed and their respective molar yields were methyl-1,4-benzoquinone (12.4 ± 1.2 %), 5-methyl-2-nitrophenol (1.5 ± 0.3 %) and 3-methyl-2-nitrophenol (1.4 ± 0.3 %) from m-cresol, methyl-1,4-benzoquinone (5.6 ± 0.9 %) and 6-methyl-2-nitrophenol (4.7 ± 0.8 %) from o-cresol, and 4-methyl-2-nitrophenol (17.2 ± 2.5 %) from p-cresol.

This kinetic and product data are compared with the literature and the reaction mechanisms are discussed.