Gas-Phase Reaction of OH Radicals with Benzene: Temperature-Dependence of the Product Yields

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Benzene and a series of alkylated derivatives (toluene, xylenes, etc.) are predominantly emitted into the atmosphere by human activities (road travel, solvent use). In urban areas, atmospheric mixing ratios up to 30 ppb have been measured (Finlayson-Pitts and Pitts, 2000). The degradation process of benzene is exclusively initiated by the attack of OH radicals forming an OH/adduct radical. The atmospheric fate of the resonance stabilized OH/adduct radical is governed by the reaction with O_2 (Knispel et al., 1990). The first stable products of this process are still subject of intense research.

In the present work the gas-phase reaction of OH radicals with benzene was studied in O_2/He mixtures under flow conditions in the temperature range of 276 - 353 K at a total pressures of 500 mbar using on-line FT-IR spectroscopy and GC-MS measurements. OH radicals were produced via the reaction sequence:

$$H + O_2 \rightarrow HO_2 \quad (1)$$

$$HO_2 + NO \rightarrow OH + NO_2 \quad (2)$$

The initial ratio [NO] / [O_2] ranged from 1 x 10^{-6} to 2 x 10^{-5}. In order to prevent reactions of products with OH radicals benzene was used in a large excess and the amount of consumed benzene was in the order of 0.1 %.

Detected main products were phenol and up to now unidentified carbonylic substances as well as in low amounts *p*-benzoquinone, nitrobenzene, glyoxal and furan. For the highest NO concentrations in the gas mixture, the formation of 2,4-hexadienedials was observed. In the whole temperature range, with increasing NO concentrations the formation yield of phenol decreased. On the other hand, for a constant [NO] / [O_2] ratio, the phenol yield increased with increasing temperature; [NO] / [O_2] = 1 x 10^{-6}, phenol yield: 0.18 (276 K) and 0.68 (353 K). Generally, the total yield of carbonylic substances was found to be anticorrelated with the phenol yield.

A simple model describing the temperature- and NO-dependence of the phenol yield is presented. The application of these results for the real atmosphere is discussed.

References

Finlayson-Pitts B.J. and J.N. Pitts, Jr. in *Chemistry of the Upper and Lower Atmosphere*, Academic Press, 2000.

Knispel R., R. Koch, M. Siese and C. Zetzsch, *Ber. Bunsenges. Phys. Chem.* 94 (1990) 1375.