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New results on the atmospheric chemistry of oxygenated aromatic compounds

I. Bejan (1,2), **I. Barnes (1),** R. Olariu (2), K. H. Becker (1), R. Mocanu (2)

(1) Bergische Universität Wuppertal, FB C - Physikalische Chemie, Gaußstraße 20, D-42097 Wuppertal, Germany, (2) "Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry, Department of Analytical Chemistry, Carol I Boulevard 11, 700506 Iasi, Romania (barnes@uni-wuppertal.de)

Large quantities of harmful VOCs are emitted into the troposphere from anthropogenic sources. Aromatic hydrocarbons are an important class of VOCs present in the atmosphere and contribute significantly to the chemistry of urban air. Due to the atmospheric reactivity of aromatic hydrocarbons and the strength of their emission sources, it has been estimated that their oxidation may be responsible for up to 40% of photochemically produced tropospheric ozone in troposphere. In the atmosphere, phenols are produced in substantial yields by the reactions of OH with BTX (benzene, toluene, xylene isomers), benzene producing phenol, toluene a mixture of $o-$, $m-$ and $p-$cresols and the xylene isomers a series of hydroxydimethylbenzenes. Studies in Wuppertal, have shown that the major products in the OH-radical initiated oxidation of phenols are 1,2-benzenediols (1,2-dihydroxybenzenes). Apart from rate constants for the reaction of OH radicals, NO_3 radicals and O_3 with these compounds, nothing is presently known about the atmospheric chemistry of 1,2-benzenediols.

As part of a systematic study of the gas-phase atmospheric chemistry of dihydroxybenzenes we present here preliminary results from investigations on the products formed from their reaction with OH radicals. Using FTIR several different types of products have been observed in a 1080 L reactor in Wuppertal. The products formation from the reactions of OH with 1,2-dihydroxybenzene, 3-methyl-1,2-dihydroxybenzene and 4-methyl-1,2-dihydroxybenzene have been studied. For 1,2-dihydroxybenzene and 4-methyl-1,2-dihydroxybenzene formation of (as yet unidentified) ketene-type compounds has been observed. For the reaction of OH radicals with 4-methyl-1,2-dihydroxybenzene, formation of methylated orthobenzoquinone

has been observed. In the reaction of OH radicals with 1,2-dihydroxybenzene formation of maleic anhydride (2,4-furandione) has been observed with a yield of between 5 and 10 %. Possible mechanistic pathways leading to the products will be presented and possible implications of the results for SOA formation from the photooxidation of the 1,2-benzenediols will be considered.