



Investigations on the atmospheric chemistry of nitrophenolic-type compounds

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Aromatics are an important class of VOCs present in the urban atmosphere. They are mainly emitted by anthropogenic activities and make a sizable contribution to SOA formation; it has been estimated that their oxidation may be responsible for up to 40% of photochemically produced ozone in troposphere. Nitroaromatics are compounds with carcinogenic and phytotoxic properties. Nitrophenols have been identified to play a role in forest decline and a recent study in our laboratories has shown that their photolysis produces nitrous acid (HONO). HONO plays an important role in tropospheric chemistry since its photolysis leads to the formation of OH radicals.

In this study we present preliminary investigations on the gas-phase reaction of nitrophenols with chlorine atoms. Experiments were performed in two cylindrical smog chambers, a 480 l Duran glass and a 1080 l quartz glass photoreactor, at 298 K and 1 atm of air. FT-IR spectroscopy was used to monitor both reactants and products.

A relative kinetic technique was used to determine the rate coefficients for the reactions of chlorine atoms with methyl-o-nitrophenol isomers. In product studies of Cl with o-nitrophenols, IR features attributable to formation of 2-chlorophenol, HCl, CO, NO₂ and ClNO₂ were observed. Formation yields for 2-chlorophenol, HCl, CO and the total N-balance (ClNO₂+ NO₂) have been derived from a preliminary linear least squares analysis of the concentration-time data. The results are supportive of a mechanism involving both displacement of NO₂ in 2-nitrophenol by Cl and H-atom

abstraction from the OH group.