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Oxidation of 4-methylphenol (p-cresol) by atmospheric radicals in aqueous solution - A product study

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Atmospheric oxidation processes are not only a sink for organic compounds, but also a source for new species. These compounds may have different toxic as well as phytotoxic properties than the precursor compounds or they are affecting other important atmospheric processes (e.g. particle mass production). Therefore, detailed product studies are very interesting for the further development of oxidation mechanisms in atmospheric models.

Nitro substituted phenols could be identified as the main reaction products by the oxidation of cresol with NO₃/NO₂/OH radicals. Since the phytotoxic properties of these nitro substituted compounds are well known, the characterization and quantification of possible secondary atmospheric formation processes is of importance. Product distribution of the cresol oxidation was studied applying an offline coupling of laser photolysis experiments and liquid chromatography/mass spectrometry (LP-LC/MS). This analytical technique provides on the one hand a sensitive detection system and on the other hand more structural information on not yet identified products. Additionally, a solid phase extraction (SPE) step was done, directly after the laser photolysis experiments, in order to purify and enrich the aqueous samples. The obtained results from the reaction between p-cresol and NO₃/NO₂/OH in aqueous solution will be presented and compared with the product distribution from the phenol oxidation as well as available literature data.