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Secondary organic aerosol (trans)formation through aqueous phase guaiacol photonitration: chemical characterization of the products

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One of the largest primary sources of organic aerosol in the atmosphere is biomass burning (BB) (Laskin et al. 2009); in Europe its contribution to annual mean of PM10 is between 3 and 14 % (Maenhaut et al. 2012). During the process of wood burning many different products are formed via thermal degradation of wood lignin. Hardwood burning produces mainly syringol (2,6-dimetoxyphenol) derivatives, while softwood burning exclusively guaiacol (2-methoxyphenol) and its derivatives. Taking into account physical properties of methoxyphenols only, their concentrations in atmospheric waters might be underestimated. So, their aqueous phase reactions can be an additional source of SOA, especially in regions under significant influence of wood combustion. An important class of compounds formed during physical and chemical aging of the primary BBA in the atmosphere is nitrocatechols, known as strong absorbers of UV and Vis light (Claeys et al. 2012). Very recently, methyl-nitrocatechols were proposed as suitable markers for highly oxidized secondary BBA (Iinuma et al. 2010, Kitanovski et al. 2012).
In the present work, the formation of SOA through aqueous phase photooxidation and nitration of guaiacol was examined. The key objective was to chemically characterize the main low-volatility products and further to check their possible presence in the urban atmospheric aerosols. The aqueous phase reactions were performed in a thermostated reactor under simulated sunlight in the presence of H_2O_2 and nitrite. Guaiacol reaction products were first concentrated by solid-phase extraction (SPE) and then subjected to semi-preparative liquid chromatography.The main product compounds were fractionated and isolated as pure solids and their structure was further elucidated by using nuclear magnetic resonance spectroscopy (1H, 13C and 2D NMR) and direct infusion negative ion electro-spray ionization tandem mass spectrometry (( )ESI-MS/MS). The main photonitration products of guaiacol (4-nitroguaiacol, 6-nitroguaiacol and 4,6-dinitroguaiacol) were examined for their presence in winter aerosol samples by using an optimized HPLC-(−)ESI-MS/MS. 4-nitroguaiacol and 4,6-dinitroguaiacol were unambiguously identified in winter PM10 from Ljubljana, Slovenia, whereas the absence of 6-nitroguaiacol was further explained with the help of long-term reaction monitoring. To our knowledge, our study represents the first report on the identification of 4,6-dinitroguaiacol in ambient aerosols.

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