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Evaluation of the chemical composition of gas and particle phase products of aromatic oxidation – implications for ambient measurements and modelling studies

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Volatile organic compounds are released into the atmosphere from both natural sources such as vegetation, and from anthropogenic sources such as fuel combustion and industry. In developing megacities, emissions can be dominated by the anthropogenic activity. The range of VOCs emitted varies from city to city and it has been seen in recent work that substituted aromatics are some of the key species for anthropogenic SOA formation as they are highly reactive and produce high SOA yields. In megacities such as Beijing, regulation of these aromatics could be important for managing ozone levels as overall PM levels continue to decrease.

Here we present a comprehensive study of the chemical composition of gas and particle phase products from the oxidation of 1,3,5-trimethyl benzene, 1,2,4-trimethyl benzene, 1-methyl naphthalene, propyl benzene and isopropyl benzene using an Aerodyne Potential Aerosol Mass Oxidation Flow Reactor (PAM-OFR). Composition was evaluated using a VOCUS-PTR and a FIGAERO-I-CIMS and the volatility of SOA was probed using the FIGAERO inlet.

Mass spectral peak identification has been carried out for > 70 % of product signal and a smaller subset of around 30 ions account for over half of the ion signal from the different precursors. Comparison of results with the range of species which could be observed from the Master Chemical Mechanism (MCM) shows that the yield of oxidised products is consistently underestimated across the precursors. The actual product distribution observed is much more oxidised than the MCM predicts and there are a range of products missing from the MCM which contribute significantly to observed signal from both I-CIMS and VOCUS-PTR measurements. Many of the product ions observed are common between some or all of the precursors, and some are common with biogenic marker species. This will have implications in the interpretation of ambient measurements and for modelling studies.