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# Partially oxidised organic components in urban aerosol using GCXGC-TOF/MS

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Abstract. Partially oxidised organic compounds associated with PM2.5 aerosol collected in London, England, have been analysed using direct thermal desorption coupled to comprehensive gas chromatography-time of flight mass spectrometry (GCXGC-TOF/MS). Over 10000 individual organic components were isolated from around 10µg of aerosol material in a single procedure and with no sample pre-treatment. Chemical functionalities observed using this analytical technique ranged from alkanes to polyoxygenated species. The chemical band structures commonly used in GCXGC for group type identifications overlap for this sample type, and have required mass spectrometry as an additional level of instrument dimensionality. An investigation of oxygenated volatile organic compounds (o-VOC) contained within urban aerosol has been performed and in a typical sample around 130 o-VOCs were identified based on retention behaviour and spectral match. In excess of 100 other oxygenated species were also observed but lack of mass spectral library or pure components prevents positive identification. Many of the carbonyl species observed could be mechanistically linked to gas phase aromatic hydrocarbon oxidation and there is good agreement in terms of speciation between the urban samples analysed here and those degradation products observed in smog chamber experiments of aromatic oxidation. The presence of partially oxidised species such as linear chain aldehydes and ketones and cyclic products such as furanones suggests that species generated early in the oxidative process may undergo gas to particle partitioning despite their relatively high volatility.

■ Final Revised Paper (PDF, 1106 KB) ■ Discussion Paper (ACPD)

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