Chemical Composition of Secondary Organic Aerosol Formed from the Oxidation of Isoprene-Derived C5H10O3 Reactive Uptake Products

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Abstract

Isoprene, the largest non-methane volatile organic species emitted into Earth's atmosphere, reacts with hydroxyl radicals to initiate formation of secondary organic aerosol (SOA). Under low nitric oxide conditions, the major oxidative pathway proceeds through acid catalyzed reactive uptake of isoprene-epoxydiol isomers (IEPOX). We have recently established the structures of the semivolatile C5H10O3 uptake products (formerly designated "C5-alkene triols) of cis- and trans-β-IEPOX as 3-methylenebutane-1,2,4-triol and isomeric 3-methyltetrahydrofuran-2,4-diols. Importantly, both uptake products showed significant partitioning into the gas phase. Here, we report evidence that the uptake products along with their gas phase oxidation products constitute a hitherto unrecognized source of SOA. We show that partitioning into the gas phase results in further oxidation into low volatility products, including highly oxygenated C5-polyols, organosulfates, and dimers. In the chamber studies, gas phase products were characterized by online by iodide-Chemical Ionization Mass Spectrometry (I-CIMS) and particle phase products by offline analysis of filter extracts by HILIC/(-)ESI-HR-QTOFMS using authentic standards. The chamber studies show the potential for a substantial contribution to SOA from reactive uptake of the second generation gas phase oxidation products onto both acidified and non-acidified ammonium bisulfate seed aerosols. Identification of these previously unrecognized early-generation oxidation products will improve estimates of atmospheric carbon distribution and advance our understanding of the fate of isoprene oxidation products in the atmosphere.