

Insights into the Alkene Triol Conundrum: Characterization and Quantitation of Isoprene-Derived C₅H₁₀O₃ Reactive Uptake Products

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Abstract

2-Methyltetrols and a group of C₅H₁₀O₃ isomers referred to as “alkene triols,” are chemical tracers used to estimate the contribution of isoprene oxidation to atmospheric PM_{2.5}. The molecular structures and the mass contribution of alkene triols are uncertain, and their origin as analytical artifacts is contentious. Here, we report that the alkene triols are uptake products and present evidence of partitioning into the gas phase. Based on the hypothesis that rearrangement of IEPOX yields C₅H₁₀O₃ isomers on reactive uptake, we synthesized “alkene triol” candidates and investigated their behavior under conventional derivatization gas chromatography/electron impact mass spectrometry (GC/EI-MS) and, in parallel, by non-destructive hydrophilic interaction liquid chromatography coupled with high-resolution quadrupole time-of-flight electrospray mass spectrometry (HILIC/ESI-HR-QTOFMS). Synthetic targets were 3-methyltetrahydrofuran-2,4-diol (**1**) and 3-methylene-1,2,4-trihydroxybutane (**2**).

Using the standards, we confirmed **1** and **2** in chamber-generated cis- and trans-β-IEPOX SOA both by HILIC/ESI-HR-QTOFMS and derivatization GC/EI-MS. In ambient SOA collected in Research Triangle Park, NC, **1** and **2** were confirmed and quantitatively estimated by GC-EI/MS. Trimethylsilyl derivatization of **1** is problematic, yielding predominantly bis- but also a small amount (<10%) of tris-trimethylsilyl forms. Our findings are consistent with reports that the tris-trimethylsilyl derivatives **1** and **2** represent largely thermal decomposition of 2-methyltetrol sulfate esters; however, based on HILIC/ESI-HR-QTOFMS analysis of chamber-generated SOA, we estimate up to 10% and 50% of **1** and **2**, respectively are not artifact-derived, and may arise from isomerization of IEPOX upon reactive uptake. Significant quantities of **1** and **2** were detected in impinger samples downstream from a denuder in series with a filter indicating partitioning into the gas phase. Results suggest that isoprene-derived “alkene triols” do form and are preferentially in the gas phase rather than particle phase, warranting studies on partitioning and gas-phase oxidation pathways.