Isoprene nitrates: preparation, separation, identification, yields, and atmospheric chemistry

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Isoprene is an important atmospheric volatile organic compound involved in ozone production and NOx (NO+NO2) sequestration and transport. Isoprene reaction with OH in the presence of NO can form either isoprene hydroxy nitrates ("isoprene nitrates") or convert NO to NO2 which can photolyze to form ozone. While it has been shown that isoprene nitrate production can represent an important sink for NOx in forest impacted environments, there is little experimental knowledge of the relative importance of the individual isoprene nitrate isomers, each of which has a different fate and reactivity. In this work, we have identified the 8 individual isomers and determined their total and individual production yields. The overall yield of isoprene nitrates at atmospheric pressure and 295 K was found to be 0.070(+0.025/−0.015). Three isomers, representing nitrates resulting from OH addition to a terminal carbon, represent 90% of the total IN yield. We also determined the ozone rate constants for three of the isomers, and have calculated their atmospheric lifetimes, which range from ~1–2 h, making their oxidation products likely more important as atmospheric organic nitrates and sinks for nitrogen.

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