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Stable Carbon Isotope Ratios of Specific Products in Secondary Particulate Organic Matter Formed by Photo-Oxidation of Toluene

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Laboratory experiments for stable carbon isotope studies of secondary particulate organic matter (POM) in the gas-phase were conducted. Secondary POM was generated using a 2.5 L flow reactor or an 8 $m\hat{3}$ smog chamber. The initial mixing ratio of toluene and the initial toluene/NO ratio were 20 ppmV - 40 ppmV and 4 - 8 for the flow reactor experiments and ∼0.5 ppmV and 0.3 - 2 for the smog chamber experiments, respectively. The flow reactor experiments were made without seed particles, while the smog chamber experiments were done with ammonium sulfate seed particles. Using these different experimental set-ups/conditions, POM generated under different extent of toluene consumption was collected on filters for compound-specific stable carbon isotope analysis as well as for the stable carbon isotope analysis of total POM carbon. For the compound specific analysis, the collected filter samples were extracted with acetonitrile, and the extracts were then concentrated under a gentle flow of pure nitrogen gas. The concentrated extracts were derivatized using N, O-bis(trimethylsilyl)trifluoroacetoamide (BSTFA). The derivatives were qualitatively and quantitatively/isotopically analyzed by GC-MS and GC-C-IRMS, respectively.

The qualitative analysis by the GC-MS identified 7 nitromonohydroxy/nitrodihydroxy aromatic compounds in the POM extracts. The results from the compound-specific stable carbon analysis show that, for 6 out of the 7 identified products, the isotope ratios were the similar to that of the total POM carbon, which is predictable using the kinetic isotope effect of the initial toluene+OH reaction, the initial isotope ratio of toluene, and fraction of toluene consumed (Irei et al., 2006). In this presentation, comparison of these observations with the reaction mechanisms postulated by others will be discussed.

Reference

Flow reactor studies for stable carbon isotopic composition of secondary particulate organic matter generated by toluene/OH radical-induced reactions, S. Irei, L. Huang, F. Collin, W. Zhang, D. Hastie and J. Rudolph, Atmospheric Environment, 2006, vol. 40, p 5858