Supplement of

Determination of the Photochemical Age of Nitrophenols in Secondary Organic Aerosols from Stable Carbon Isotope Ratios

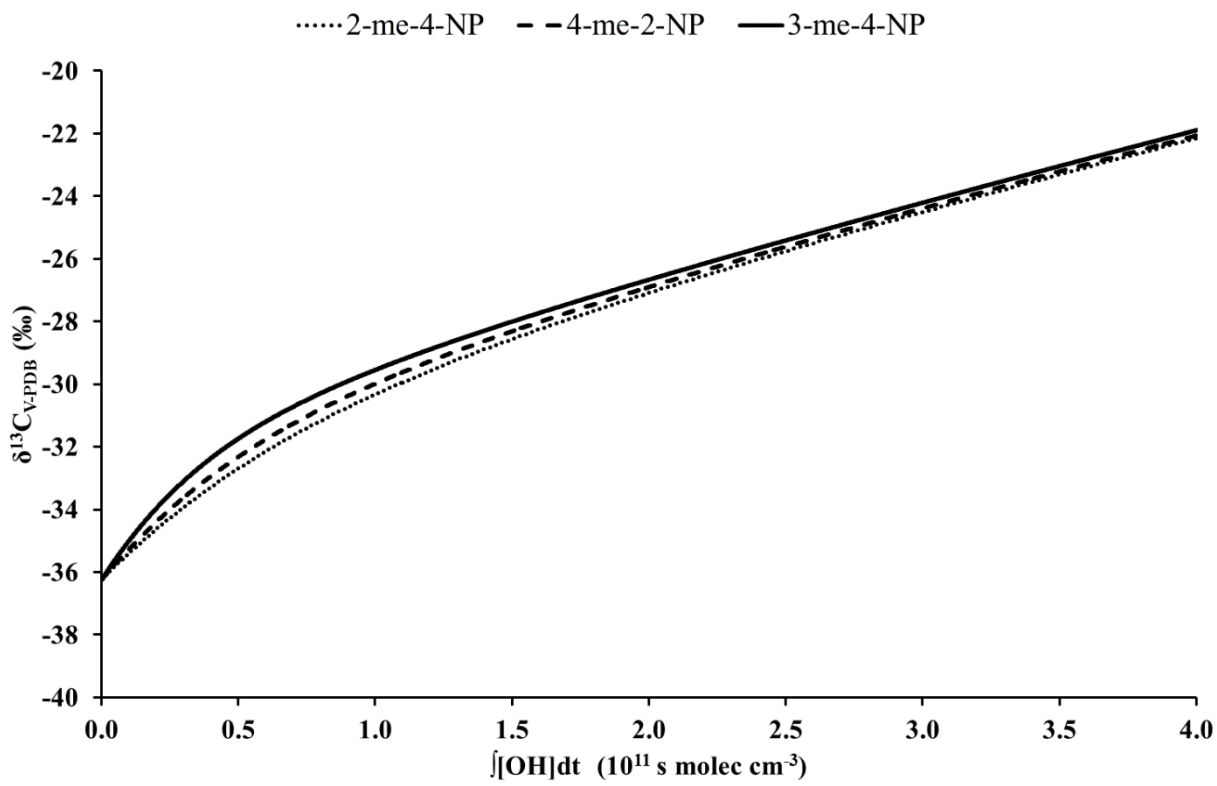
M. Saccon et al.

Figure S1. Comparison of the dependence between carbon isotope ratio and PCA (∫[OH]dt) predicted by the mechanistic model (Scenario 3) for different methylnitrophenol isomers.

Figure S2. Influence of changes in rate constant and kinetic isotope effect for the reaction of 2-methyl-4-nitrophenol with the OH-radical on the dependence between carbon isotope ratio and PCA (∫[OH]dt). The calculations are based on Scenario 3 for the base case. The other curves show the results of calculations for kinetic isotope effects changed by approximately ± 1 ‰ (ε=5 ‰ and ε=7 ‰) and the reaction rate constant changed by ± 30 % (slow loss and fast loss). Also shown are the median, 10 and 90 percentiles as well as the lowest and highest carbon isotope ratios measured by Saccon at al. (2015) in an urban area.

Figure S3. Influence of uncertainty in rate constant and kinetic isotope effect for predictions of the carbon isotope ratio of 2-methyl-4-nitrophenol as function of PCA (∫[OH]dt). The calculations are based on Scenario 3 and changes in reaction rate constants for the precursor are ± 10 % (k pre +10% and k pre -10%), for the reaction rate constant of the intermediate ± 20 % (k int +20 % and k int -20 %), and for the kinetic isotope effect of precursor reactions ± 0.5 ‰ (ε pre +0.5 ‰ and ε pre -0.5 ‰).

Figure S4. Impact of mixing two air masses with different PCAs on PCA derived from carbon isotope ratios of benzene and 4-nitrophenol. Fig.a shows the PCA derived from the precursor (benzene, thin line) and the reaction product (4-nitrophenol, thick lines) for mixing air masses with ∫[OH]dt of 5×10^{11} s molecules cm^{-3} (dashed line)**,** 10^{12} s molecules cm^{-3} (solid line)**,** and 3×10^{12} s molecules cm^{-3} (dotted line)**,** with air masses of lower values for ∫[OH]dt (x-axis). The relative weight of the aged air mass is 10% and the calculation does not consider loss of 4-nitrophenol by deposition. Fig. b shows the impact of loss by deposition on the observed PCA for mixing of air masses with ∫[OH]dt = 10^{12} s molecules cm^{-3} with an air mass of lower PCA (x-axis). The depositional loss rates are given as multiples of the chemical loss rate of 4-nitrophenol due to reaction with OH-radicals. For comparison, the PCA calculated from the precursor carbon isotope ratio is also shown (solid line).



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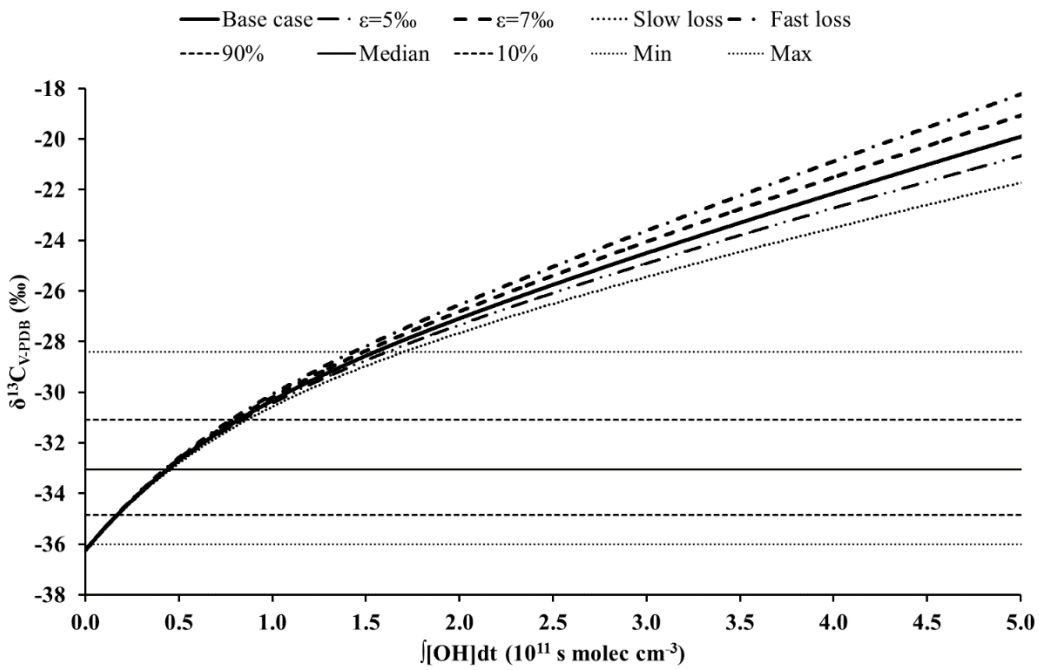

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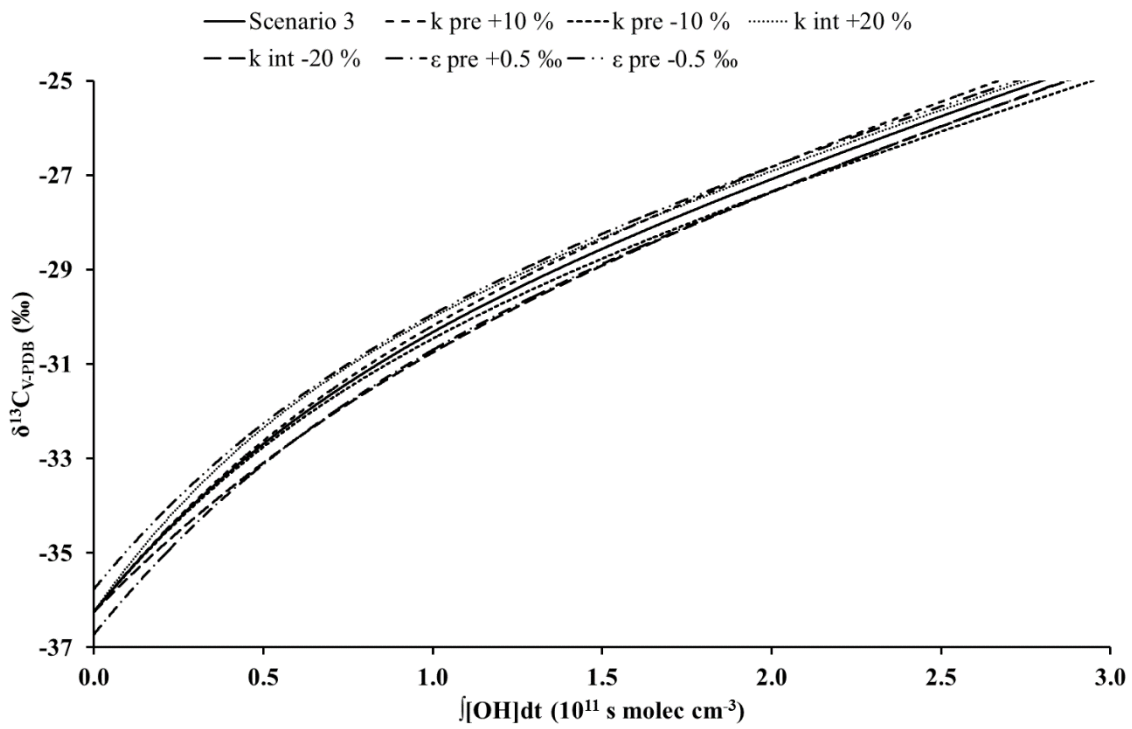

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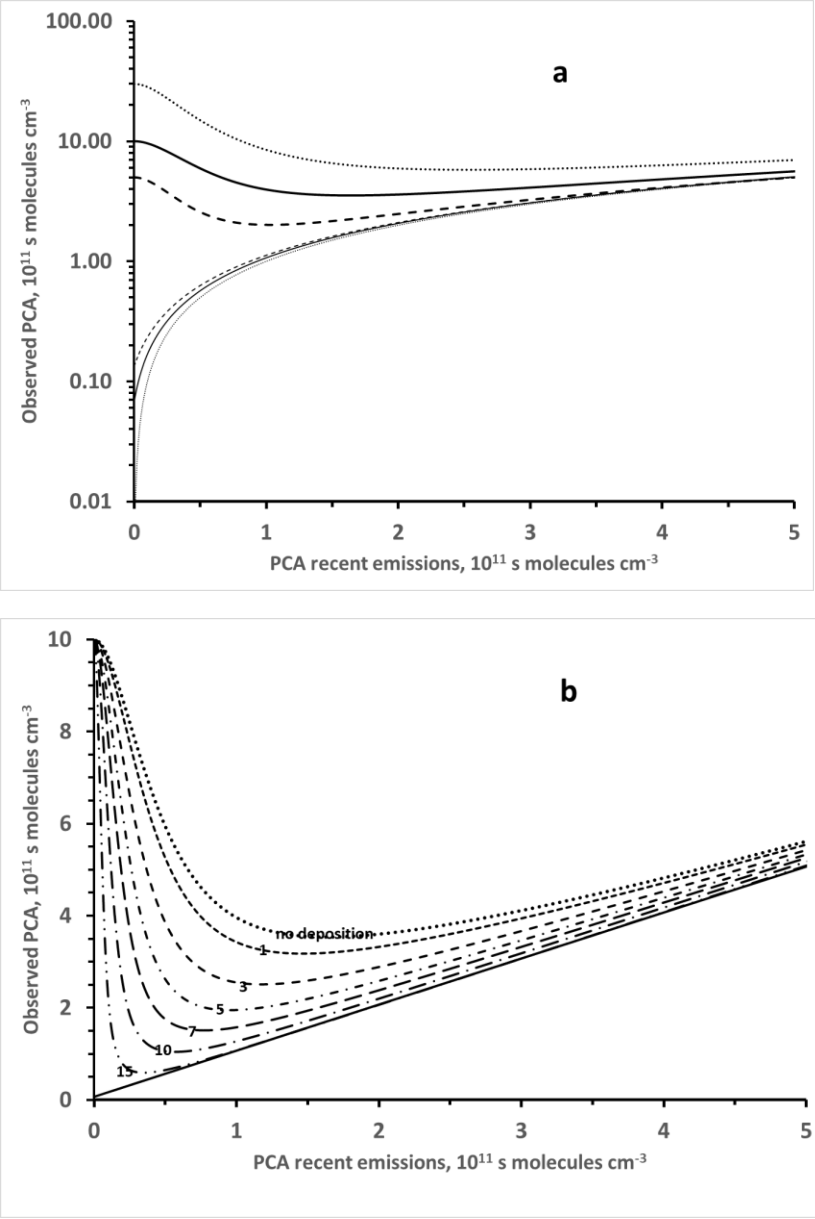

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