Temperature dependence of nopinone partitioning coefficient in organic aerosol

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Secondary organic aerosol (SOA) represents a significant fraction of the total aerosol mass, thus strongly influencing aerosol properties. A detailed understanding of SOA formation from volatile organic compounds (VOCs) as well as the partitioning of the semi-volatile products between gas and particle phase is necessary to better predict the organic matter in the atmosphere. In this study, we present the experimentally determined partitioning coefficient of nopinone, a major oxidation product of β-pinene The observed temperature dependence of the partitioning coefficient is discussed.

Experiments studying the SOA formation from β-pinene ozonolysis were conducted in the temperature range between 243 K and 303 K at the AIDA chamber of the Karlsruhe Institute of Technology (KIT). During all β-pinene experiments, gas and particle phase concentration of the major reaction product, nopinone, was measured by combining an Aerosol Collection Module (ACM) with the high-resolution Proton Transfer Reaction-Time of Flight-Mass Spectrometer (PTR-ToF-MS). Alternate measurements of the nopinone concentration in gas phase only and particle phase only were used to calculate the partitioning coefficient of nopinone.

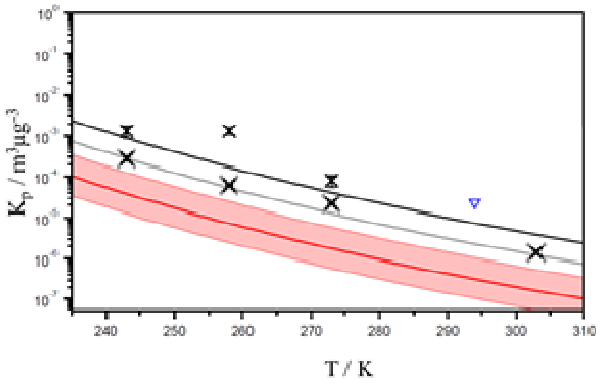

Figure 1: *Nopinone partitioning coefficient at different temperatures from measurements with PTR-ToF-MS and ACM (black crosses) as well as the temperature dependence fit (black line). Gray crosses mark the partitioning coefficient values derived from ACM measurements after additional nopinone injection. The gray line shows a fit to data points with added nopinone. The pink shaded area marks the range of theoretically determined partitioning coefficient following Jenkin, 2004. For this, an activity coefficient between 3 (lower limit) and 0.3 (upper limit of the pink area) is considered. The red line in the middle shows the partitioning coefficient temperature dependence for an activity coefficient of 1. The blue triangle shows the experimentally derived nopinone partitioning coefficient from Hohaus (2009).*

The partition coefficients experimentally determined at 243, 258, 273 and 303K , before and after an additional nopinone injection, are presented in Figure 1. Overall, the partitioning coefficient increases with decreasing temperatures. The experimental results are compared with calculations arising from studies on the gas-particle partitioning, based on the Pankow absorption model (Jenkin, 2004). These calculations were employed to fit the temperature dependence of nopinone partition coefficient to the experimental data sets. Using the activity coefficient as a free fitting parameter results in an activity coefficient of 0.042 ± 0.019. This is below the range of 0.3 - 3 that is typically assumed for activity coefficients in SOA formation (Seinfeld and Pankow, 2003).

The experimental partitioning coefficients determined in this study compare well with the value obtained by Hohaus (2009) and show a temperature dependence following the trend predicted by theory. Yet, they are up to two orders of magnitude higher than values calculated based on equilibrium partitioning assumptions. Possible reasons for this discrepancy will be discussed.

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