Atmos. Chem. Phys. Discuss., 15, C9539–C9541, 2015
www.atmos-chem-phys-discuss.net/15/C9539/2015/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Secondary formation of nitrated phenols: insights from observations during the Uintah Basin Winter Ozone Study (UBWOS) 2014" *by* B. Yuan et al.

Anonymous Referee #1

Received and published: 19 November 2015

In this work, the authors used a new analytical technique that allows for high time resolution and sensitive measurements of nitrated phenols in the gas phase. The measurement technique is based on time of flight chemical ionization mass spectrometry (ToF-CIMS) with acetate as the reagent ion. The sampling was conducted in winter of 2014 at the Horse Pool site in the Uintah Basin. The authors combined the measured diurnal profile of nitrophenols with box model simulations to provide insight into the generation and removal pathways of the nitrophenols. Overall, this is a nice manuscript that demonstrates the ability of the techniques to measure low level of nitrated VOCs and improve our understanding of their evolution in the atmosphere. The manuscript is recommended for publication. More detailed comments follow below:

P15, L2 Different vapor pressures for 2,4-dinitrophenol and 4-nitrophenol were reported in the literature (Mackay et al., 2006) with values ca. 2 orders of magnitude lower than in Schwarzenbach et al. (1988), this might explain the difference in the calculated fraction of nitrophenols in the particle phase in this work and the experimental data for 4-NP (Cecinato et al., 2005) and DNP (Morville et al., 2006).

P11 L25 Which hydrocarbons were measured and used for the simulation. It would be nice to show a table in the supplement with characteristic concentrations. P12 L10. What was the assumption with respect to an emission rate of benzene? P13 L25 Vinylfuran was detected in biomass burning (Stockwell et al., 2015), but very low BB influence was claimed in this study. What is the source of vinyilfuran and why is it not present in the daytime? Perhaps the online GC-MS used in this study can give some insight on the interference at mass 138. The C3H4F2OH+ ion that overlaps with the phenol peak (Fig. 2d) looks a little unusual. Does it come from the heated Teflon inlet? It would be useful to show the zero air signal with this ion to demonstrate this. Figure S2a, b, c show a large number of radical species measured. Since the acetate ionization technique is a soft method, some explanation is necessary about the source of these radicals. Is it because of the strong voltage used in the declustering region? It would be useful to show the peaks at m/z 137 along with the peaks at m/z 138 in figure 2a in order to show that the peaks at 138 are not the C13 isotopes. According to P8 L26 the error in peak fitting was 0-10%, according to figure S2 the DNP peak area account for about 3% of the whole peak area at m/z 183 (DNP peak height 10% from the total peak height and peak width about 1/3 of the total peak width), therefore the area of the DNP peak is below the accuracy of the peak fitting. Some additional explanation about the accuracy of the peak fitting is needed. Figure 7 shows that the measured DNP concentration sometimes has a negative value, is it an artifact from the peak fitting procedure or background subtraction? Does the DNP peak area correlate with the area of the C8H7O5- peak? P7 L6 What was the length of the short inlet? Technical: P36 fig 5 What is the line for the G/P partitioning using 4-NP?

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15, C9539–C9541, 2015

Reference

Mackay, D., Shiu, W.-Y., Ma, K.-C. and Lee, S. C.: Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Second Edition, CRC Press., 2006. âĂČ

Interactive comment on Atmos. Chem. Phys. Discuss., 15, 28659, 2015.