Geophysical Research Abstracts,
Vol. 11, EGU2009-10242, 2009
EGU General Assembly 2009


# Analysis of High Mass Resolution PTR-TOF Spectra from 1,3,5-trimethylbenzene (TMB) Smog Chamber Experiments

M. Müller (1), M. Graus (1), A. Metzger (2,3), J. Dommer (3), A. Wisthaler (1), and A. Hansel (1)

(1) University of Innsbruck, Instutute of Ion Physics and Applied Physics, Innsbruck, AUSTRIA , (2) Ionicon Analytik Gesellschaft m.b.H, Innsbruck, AUSTRIA, (3) Paul Scherrer Institut, Villigen, SWITZERLAND

A series of 1,3,5-trimethylbenzene (TMB) photo-oxidation experiments was performed under various $NO_x$ conditions in the 27 $m^3$ Paul Scherrer Institute environmental chamber. Due to well-defined conditions under which smog chamber experiments can be performed, results are very valuable for the development and the evaluation of chemical mechanisms and to get a better understanding of processes leading to secondary organic aerosol (SOA) formation.

A prototype of a High Resolution Proton Transfer Reaction Time-of-Flight Mass Spectrometer (PTR-TOF) was applied for on-line VOC analysis. The soft PTR ionization technique hardly affects the structure of analyzed compounds during ionization. Therefore, a low amount of fragmentation with almost no loss of carbon and very little loss of oxygen into a neutral fragment occurs.

Using the PTR-TOF, 300 VOCs were found during TMB photo-oxidation experiments and corresponding time traces were recorded. About 100 VOCs were present with volume mixing ratios > 0.5 ppbv. Empirical formulas $C_nH_mN_pO_o$ were determined and VOCs were separated and grouped according to their C, O and N numbers. This allowed to determine photo-oxidation grade dependent values such as the O:C ratio and time traces of mono- and multi-oxygenated compounds. The results are compared with results predicted by the Master Chemical Mechanism (MCM).