

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

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A series of 1,3,5-trimethylbenzene (TMB) photo-oxidation experiments was performed under various NO<sub>x</sub> levels in the 27 m<sup>3</sup> Paul Scherrer Institute environmental chamber.

A prototype High Resolution Proton Transfer Reaction Time-of-Flight Mass Spectrometer (HR PTR-TOF) was deployed for on-line VOC analysis. The HR PTR-TOFMS combines the advantages of soft ionization via proton transfer reactions from hydronium ions with the analytical power of a state-of-the-art time-of-flight mass spectrometer. A mass resolution of ~ 5000 (FWHM) combined with a 5-to-10 ppm mass accuracy allows for exact mass determination and identification of empirical sum formulas. VOCs are quantitatively detected with a detection limit of ~ 20 ppt.

HR PTR-TOF mass spectra showed ~ 300 peaks being formed during TMB photo-oxidation. About 100 peaks were present at intensities equivalent to volume mixing ratios > 0.5 ppbv. We determined their empirical sum formulas (C<sub>n</sub>H<sub>m</sub>N<sub>p</sub>O<sub>o</sub>) and grouped the products according to their C, O and N numbers. This allowed us to determine photo-oxidation grade dependent values such as the O:C ratio and to derive the time evolution of mono- and multi-oxygenated species. The experimental results were compared with results predicted by the Master Chemical Mechanism (MCM).