Investigation of SOA Composition from the Photolysis of 1-Nitronaphthalene using Single Particle Mass Spectrometry

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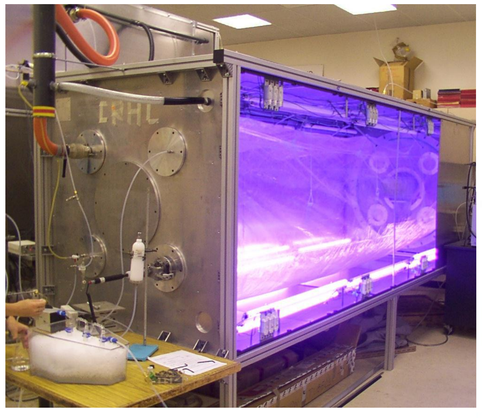
Why 1-nitronaphthalene (1NN)?

Nitrated Polyclyclic Aromatic Hydrocarbons (nitro-PAHs) are of concern from a health perspective due to their known mutagenic and carcinogenic effects.[1] The most abundant gas phase nitro-PAHs are 1- and 2-nitronaphthalene.[2] Photolysis is known to be the major degradation pathway for 1NN in the troposphere,[3] however the gas and particle phase products, and the SOA-forming potential of this reaction have received relatively little attention.

Experimental setup: online



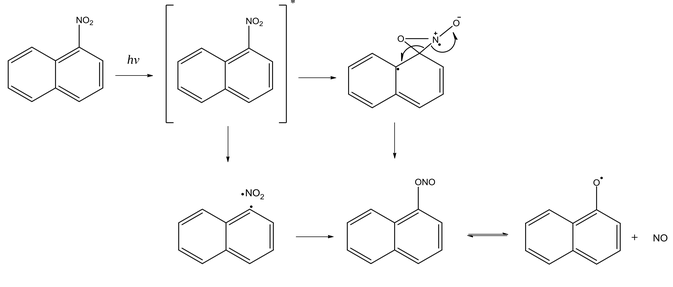
- 3910 L Simulation Chamber

- Aerosol Time-of-Flight Mass Spectrometer (ATOFMS, TSI 3800)

- Scanning Mobility Particle Sizer (SMPS, TSI 3081)

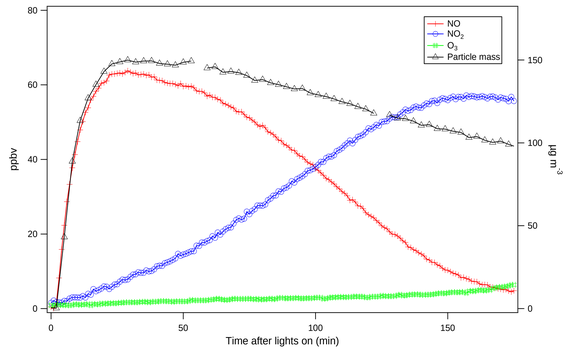
- Trace gas analyzers (Thermo 49*i*, 42*i*)

1NN photolysis mechanism



Photolysis of 1NN resulting in the formation of a **naphthoxy radical** and **NO**.

Rapid NO production supports mechanism

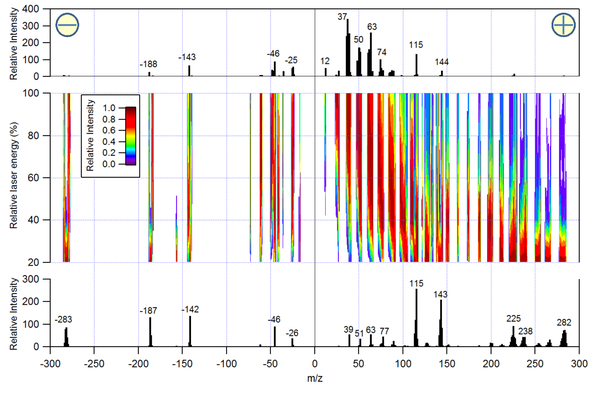


NO increases with particle mass. NO_2 increases much later through oxidation of NO

Rapid SOA formation

After lamps are switched on, SOA forms within time taken for first SMPS scan (<3 min)

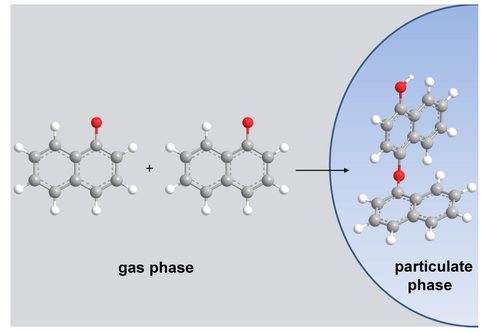
Optimizing ATOFMS operating conditions



Laser energy reduced in 0.2 mJ steps. Optimum laser pulse energy = 0.2 mJ pulse^{-1}

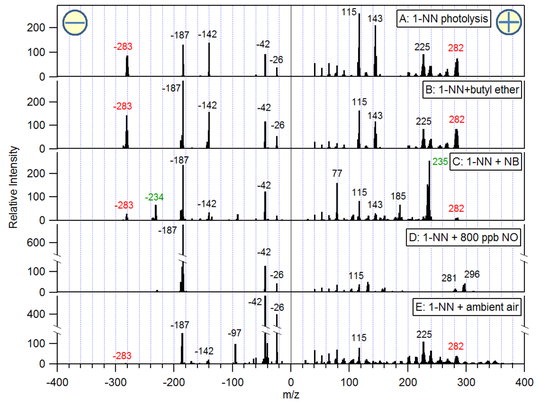
Cluster of ions at *m/z* > 280 suggests a high MW product- **dimer formation**?

Dimer formation



Identified products: (i) a newly identified naphthoxy dimer formed through **naphthoxy radical self-reaction** and (ii) nitronaphthol. The identities of these products were confirmed using off-line ultrahigh resolution Orbitrap MS

Dimer formation under different conditions



A: Standard experiment. **B:** Naphthoxy dimers formed in the presence of an OH scavenger. **C:** Naphthoxy-phenoxy dimers formed in the presence of nitrobenzene. **D:** Excess NO_x suppressed dimer formation and led to a higher nitronaphthol yield. **E:** Dimers formed in the presence of ambient air/particles

Acknowledgements and References

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2 Dimashki M., Harrad S., Harrison R. M. Atmos. Environ. ***2000****, 34 (15), 2459-2469.*

3 Atkinson R., Aschmann S. M., Arey J., Barbara Z., Schuetzle D. Atmos. Environ. ***1989****, 23 (12), 2679-2690.*