

# Autooxidation reaction study of photolyzed iodoalkanes under atmospheric conditions

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Keywords: gas phase autooxidation mechanism, secondary aerosol formation, mass spectrometry, aeroFAPA  
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A large amount of volatile organic compounds are emitted by trees. These compounds get oxidized in the atmosphere where the low volatile organic compounds (LVOC) form the secondary organic aerosol (SOA). The SOA plays an important role in our ecological system because it has influencing effects on the earth's climate and human's health. The monitored amount of SOA can't be completely explained with the generation of SOA by LVOCs.

A recent study has shown that extreme low-volatile organic compounds (ELVOC) might close the gap between theoretic models and reality (Ehn *et al.*, 2014). Especially highly oxidized compounds (HOM) could have an extreme low vapour pressure that causes an irreversible condensation onto aerosol particles or even lead to particle formation. So it is important to get the knowledge how the high oxidation grade is reached. One way could be a gas phase autooxidation mechanism which leads via H-shift reactions to hydroperoxides (Crouse *et al.*, 2013). Because biogenic compounds can form very complex oxidation products, it is useful to find an easier model system.

A former study used the photolysis of 1-iodooctane to examine the radicalic autooxidation process (Kalafut-Pettibone *et al.*, 2013). Filter samples were analyzed by HPLC-MS.

In this study the photolysis of 1-iodononane, 5-iodononane and 2-iodo-2,6-dimethylheptane is used to investigate the mechanism and to get informations about the preferred H-shift (e.g. 1,5H; 1,6H, 1,7H). The reactions are performed in a 70 L cylindric glass chamber with a built in UV-Lamp to photolyze the iodoalkane compounds. An online measurement method using a soft ionisation source called aeroFAPA (Brüggemann *et al.*, 2015) allows direct analysis of the chamber content via iontrap mass spectrometry (LCQ DECA XP Plus, Thermo Scientific).

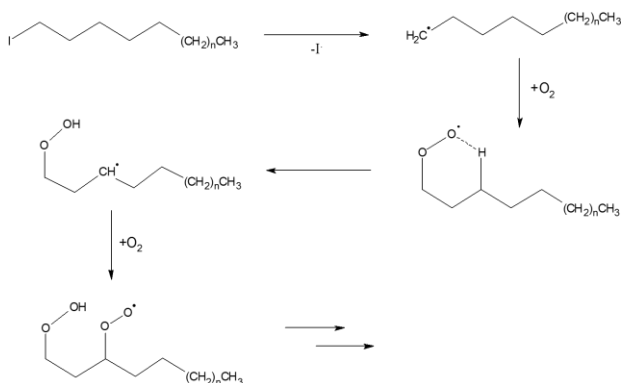


Fig. 1: Proposed autooxidation mechanism for iodoalkane (5-H shift) (Ehn *et al.*, 2014).

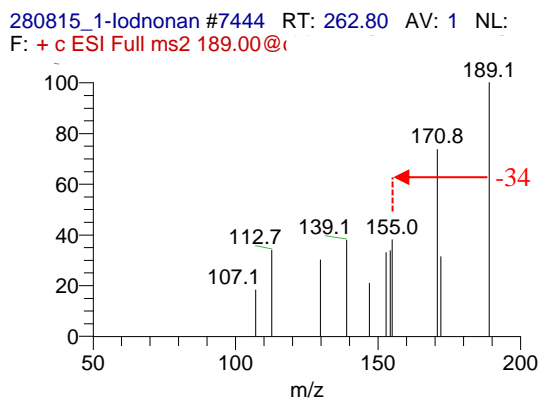


Figure 2: MS<sup>2</sup> for  $m/z$  189 [M+H] found during chamber experiment with (fragment  $m/z$  155 after H<sub>2</sub>O<sub>2</sub> loss).

During the recent experiments several interesting  $m/z$  were found. For example, the MS/MS spectrum of  $m/z$  189, found during a chamber experiment with 1-iodononane, shows the loss of H<sub>2</sub>O<sub>2</sub> (M=34 amu) and CO (M=28 amu). As well, the  $m/z$  175 and 161 showed possible H<sub>2</sub>O<sub>2</sub> losses. Similar results could be observed during the experiments with the other mentioned iodononane-isomers.

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