# A Survey of Reactions of Alkyl-naphthalenes with the OH Radical

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Naphthalene and its alkyl- derivatives, the methylnaphthalenes (MNs), ethylnaphthalenes (ENs) and dimethylnaphthalenes (DMNs), are present in the atmosphere from both natural and anthropogenic sources, with vehicle exhaust being an important one. They are semivolatile and kinetic studies show that the major atmospheric loss process for them is by gas-phase reaction with hydroxyl (OH) radicals. Studies done in this lab also indicate that the major products from the OH radical–initiated reaction of gas-phase naphthalene are ring cleavage species, including 2-formyl-cinnamaldehyde and phthalicdicarboxaldehyde. However, products from the OH radical-initiated reactions with alkyl-substituted naphthalenes have not been identified and the reaction pathways remain to be elucidated.

In this study, we have used in-situ direct air sampling atmospheric pressure ionization mass spectrometry (API-MS) as well as gas chromatography-mass spectrometry (GC-MS) techniques to investigate the products of the gas-phase reactions of OH radicals with a series of alkyl-substituted naphthalenes and with the corresponding deuterium-substituted analogues when available. The major reaction products are a ring-opened dicarbonyl product that is 32 mass units higher in molecular weight than the parent compound, one or more ring-opened dicarbonyls of lower molecular weight that may be secondary products from the initial dicarbonyls, and a ring-containing compound which has hydroxyl, epoxide, and ketone-carbonyl groups. Other products observed were alkylnaphthalene-quinones and hydroxy- and nitro- alkylnaphthalenes. The position of alkyl-substitution on the naphthalene ring is a key factor deciding the ring cleavage site and the isomeric product distribution. Based on the time-resolved monitoring of species during the reaction, a reaction scheme is proposed to explain the formation of the products observed.