

# Atmospheric reactivity of biomass burning emitted compounds: methoxyphenols OH rate constants and Secondary Organic Aerosol formation

A. Lauraguais<sup>1,2</sup>, C. Coeur-Tourneur<sup>1,2</sup>, A. Cassez<sup>1,2</sup>, J.C. Wenger<sup>3</sup>, A. Seydi<sup>4</sup>, K. Deboudt<sup>1,2</sup>, M. Fourmentin<sup>1,2</sup>, and M. Choël<sup>1,5</sup>

<sup>1</sup> Université Lille Nord de FRANCE, Lille, Nord-Pas-de-Calais, 59000, France

<sup>2</sup> Laboratoire de Physico-Chimie de l'Atmosphère, Université du Littoral Côte d'Opale, Wimereux, 62930, France

<sup>3</sup> Department of Chemistry and Environmental Research Institute, University College Cork, Cork, Ireland

<sup>4</sup> University of Cheikh Anta Diop, Dakar, Sénégal

<sup>5</sup> Laboratoire de Spectrochimie Infrarouge et Raman, UMR CNRS 8516, Université Lille 1, Villeneuve d'Ascq Cedex, Nord-Pas-de-Calais, 59655, France.

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Presenting author email: amelie.lauraguais@univ-littoral.fr

Methoxyphenols are low molecular weight semi-volatile polar aromatic compounds produced from the pyrolysis of wood lignin.

The atmospheric reactivity of methoxyphenols (2-methoxyphenol or guaiacol, 3-methoxyphenol, 4-methoxyphenol, 2-methoxy-4-methylphenol and 2,6-dimethoxyphenol or syringol) with hydroxyl radical has been studied in a simulation chamber (8 m<sup>3</sup>) at 294 ± 2 K, atmospheric pressure and dry conditions (RH < 1%).

Their OH rate coefficients, determined using the relative kinetic method, are summarized in table 1 together with their atmospheric lifetime. The atmospheric lifetime of methoxyphenols is around 2 hours, indicating that they are too reactive to be considered as stable tracers for wood smoke emissions.

In the discussion, the reactivity of methoxyphenols will be compared with other substituted aromatics and interpreted in relation to the type, number, and positions of the different substituents on the aromatic ring.

Table 1. Rate coefficients for methoxyphenol reaction with OH radicals (at 294 ± 2 K) and associated atmospheric lifetimes.

Compound	$k_{OH}^a$	$\tau_{OH}^b$	Reference
2-methoxyphenol (guaiacol)	7.53 ± 0.41	2.3	Coeur <i>et al.</i> (2010)
3-methoxyphenol	9.80 ± 0.46	1.8	Coeur <i>et al.</i> (2010)
4-methoxyphenol	9.50 ± 0.55	1.8	Coeur <i>et al.</i> (2010)
2-methoxy-4-methylphenol	9.45 ± 0.59	1.8	Coeur <i>et al.</i> (2010)
2,6-dimethoxyphenol (syringol)	9.66 ± 1.11	1.8	Lauraguais <i>et al.</i> (2012)

<sup>a</sup> Units of 10<sup>-11</sup> cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup>.

<sup>b</sup> Units of hour.  $\tau_{OH} = 1/k_{OH}[OH]$ , where 12 hour daily average [OH] = 1.6 × 10<sup>6</sup> molecule cm<sup>-3</sup>.

Secondary organic aerosol formation from the OH reaction with guaiacol and syringol was also investigated under high NO<sub>x</sub> conditions. The aerosol production was monitored using a SMPS (Scanning Mobility Particle Sizer). The SOA yields (Y) were determined as the ratio of the suspended aerosol mass

corrected for wall losses (M<sub>0</sub>) to the total reacted methoxyphenol concentration assuming a particle density of 1.4 g cm<sup>-3</sup>. For guaiacol and syringol, particle formation was observed in the first few minutes of the reaction, with a very fast increase in the particle number concentration followed by a gradual decrease over the course of the experiment (Fig. 1).

The SOA yields were in the range 0.10-0.36 and 0.003-0.87 for syringol and guaiacol, respectively. Syringol SOA yields were lower than those of guaiacol, likely due to novel methoxy group chemistry that leads to early fragmentation in the gas-phase photooxidation (Yee *et al.*, 2013).

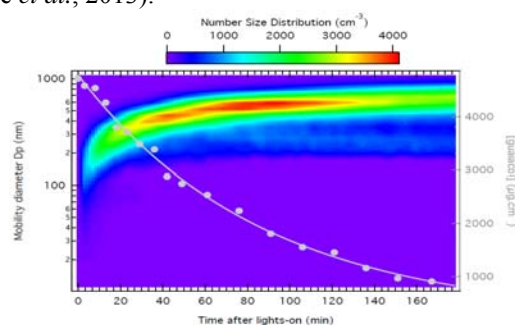


Figure 1. Typical concentration-time profiles for guaiacol and SOA (number-weighted size distribution) from a guaiacol/OH experiment.

SOA formed from the OH reaction with guaiacol have been characterized: 4-nitroguaiacol and 5-nitroguaiacol were clearly identified by GC/MS (Gas Chromatography/Mass Spectrometry), indicating that these compounds may be used as biomass burning aerosol tracers. Complementary analyses were also performed by Transmission (TEM) and Scanning (SEM) Electronic Microscopy: the corresponding pictures show that SOA are in an amorphous state which suggests the formation of oligomers.

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