Gas-phase OH radical reaction of dimethyl phthalate

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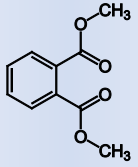
1. Introduction

- Phthalates are used as **plastiziers**.
- They have been detected indoors: **gas-phase**, **particulate matter** (PM), or **surfaces**. (1-4)
- They can negatively affect human health.

Dimethyl phthalate (DMP)



$$\text{DMP} + \text{OH} \xrightarrow{k_{OH}} \text{Prod.}$$

2. Experimental

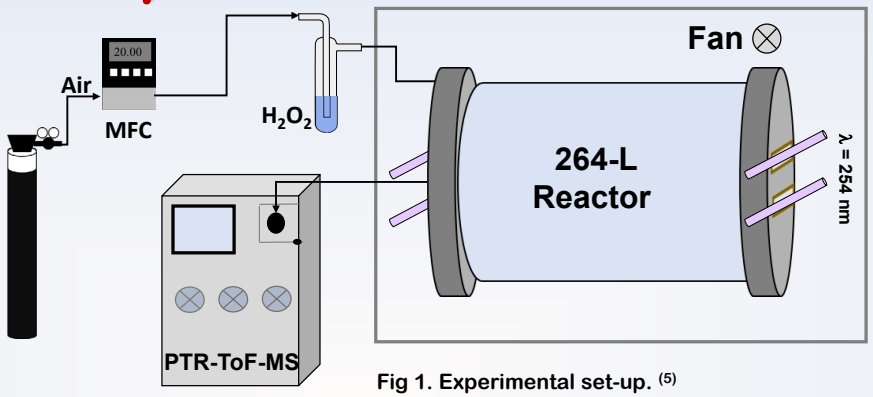


Fig 1. Experimental set-up. (5)

- DMP and reference compounds were measured by **PTR-ToF-MS**.
- The following peaks were used: **MH^+** for the reference compounds, and **$C_9H_7O_3^+$** (*m/z* = 163.03 and 164.042) and **$[C_{10}H_{10}O_4]H^+$** (*m/z* = 195.03)○
- Pseudo-first order **conditions were used: [OH] >> [DMP]**.
- OH radicals were gererated by **H_2O_2 photolysis** at 254 nm.

3. Results

A **relative method** has been used in the determination of k_{OH}:

$$\text{OH} + \text{DMP} \rightarrow \text{Products} \qquad (k_{OH})$$

$$\text{OH} + \text{R} \rightarrow \text{Products} \qquad (k_{Ref})$$

Several reference compounds (Ref) were used: **isoprene, ethanol, propene or α-pyrene**.

$$\ln\left(\frac{[DMP]_0}{[DMP]_t}\right) - k_{loss}t = \frac{k_{OH}}{k_{Ref}}\left\{\ln\left(\frac{[Ref]_0}{[Ref]_t}\right) - k_{Ref,loss}t\right\}$$

Due to the **low volatility** of DMP, a correction had to be done.

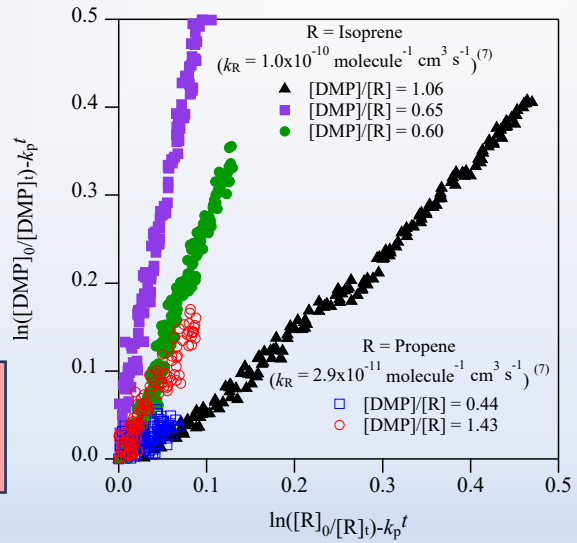


Fig 2. Examples of the decay of DMP and two reference compounds: isoprene and propene.

Preliminary results show a **great variability** depending on the reference compound and the ratio [DMP]/[Ref].

According to these results, k_{OH} could range between 1.6×10^{-11} and 5.3×10^{-10} cm^3 molecule^{-1} s^{-1}.

Further analysis is needed using other peaks of PTR-ToF mass spectra.

4. Conclusions

An estimation of τOH can be done from the preliminary results and $[OH]_{24h} = 1\times10^6$ radicals cm^{-3} (8): it can range **between 17 h and 31 min.**

5. References

(1) Bornehag et al. *Health Perspect.* **2005**, 113, 1399-404; (2) Rudel & Perovich *Atmos. Environ.* **2009**, 43, 170-181; (3) Fromme et al. *Indoor Air* **2004**, 14, 188-195; (4) Larsson et al. *Environ. Int.* **2017**, 102, 114-124; (5) Antiñolo et al. *Atmosphere* **2020**, 11, pp. 715(17); (6) Lacko et al. *Phys. Chem. Chem. Phys.* **2020**, 22, 16345-16352; (7) Atkinson et al. *Atmos. Chem. Phys.* **2006**, 6, 3625-4055.

Acknowledgements

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