

Study of reactivity of E-4-methylcyclohexanol and 2-ethoxyethanol with the main atmospheric oxidants

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4-methylcyclohexanol and 2-ethoxyethanol are two saturated alcohols which are used as solvents for many organic liquids (1-2) and have been identified as diesel and diesel/biodiesel blends vehicle emissions (3). Its gas-phase reactivity is yet unknown, only data concerning the kinetic reactivity of 2-ethoxyethanol with OH (4-7) and NO₃ radicals and ozone have been studied (8). A product study of 2-ethoxyethanol with hydroxyl radicals has also been published (9).

In order to complete the study of the reactivity of these compounds in the atmosphere a set of experiments by employing a relative technique and FTIR and GC-TOFMS systems were carried out. The rate coefficients of E-4-methylcyclohexanol and 2-ethoxyethanol with the main atmospheric oxidants radicals were obtained at 700 Torr and ~ 298 K.

Except for the value of 2-ethoxyethanol with OH radicals, these are the first data reported and seem to be in good agreement with the expected values according to the gas phase reactivity. The value obtained for 2-ethoxyethanol with OH is close to the data reported in literature ($1.4\text{--}2.12 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) (4-7) and the one obtained for E- 4-methylcyclohexanol matches with the estimated value from the EPI suite program. The rate coefficients obtained for chlorine atoms are in the same order of other saturated alcohols.

The reaction product study also was done in order to establish the reaction mechanisms. Based on the products detected in this study and previous works for saturated alcohols an Hydrogen atom abstraction at CH₂ groups have been proposed as initial attack of radical (OH, NO₃ or Cl atoms).

References

- (1) Hentefrickel, K. *Eur. Polym. Paint Colour J.* **1994**, 184, 292-294.
- (2) Fisher, W.B.; VanPeppen, J.F.; *Kirk-Othmer Encyclopedia of Chemical Technology*. New York, NY. John Wiley & Sons, **2001**.
- (3) Lopes, M.; Serrano, L.; Ribeiro, I.; Cascao, P.; Pires, N.; et al., *Atmos. Environ.* **2014**, 84, 339-348.
- (4) Dagaut, P.; Liu, R.; Wallington, T. J. and Kurylo, M. J. *J. Phys. Chem.* **1989**, 93, 7838-7840.
- (5) Hartmann, D.; Gedra, A.; Rhäsa, D. and Zellner, R. *Proceedings of the European Symposium on Physico-Chemical Behaviour of Atmospheric Pollutants*; Riedel: Dordrecht, The Netherlands, **1987**.
- (6) Porter, E.; Wenger, J.; Treacy, J. and Sidebottom, H. *J. Phys. Chem.* **1997**, 101, 5770-5775.
- (7) Stemmler, K.; Kinnison, D. J. and Kerr, J. A. *J. Phys. Chem.* **1996**, 100, 2114-2116.
- (8) Aschmann, S.M. and Atkinson, R. *Int. J. Chem. Kinet.* **1998**, 30, 533-540.
- (9) Stemmler, K.; Kinnison, D. J. and Kerr, J. A. *Environ. Sci. Technol.* **1996**, 30, 3385-3391.