# Kinetic of the gas-phase reactions of a series of alcohols with $NO_3$ radical

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Alcohols are emitted into the atmosphere by a wide number of anthropogenic and natural processes (1). The BVOC that are emitted are mainly isoprene and monoterpenes, but a wide range of other compounds of biogenic origin, including oxygenated compounds, such as aldehydes and alcohols, have been found in the troposphere (2). The alcohols of interest in urban atmospheres are primarily methanol, ethanol and to a lesser extent the $C_3$ and $C_4$ species (3). Thus, alcohols have a potential to contribute to the adverse effects that are caused by anthropogenic organic air pollutants, photochemical oxidant formation and haze. The oxidation mechanisms of alcohols produce aldehydes, ketones and organic nitrates as major products (4) in urban areas. The main sources of saturated alcohols are due to their use as motor vehicle fuels, fuel additives and solvent in different industries.

The rate constant for the reaction of $NO_3$ radical with 2-butanol, 3-methyl-2-butanol and 2,3-dimethyl-2-butanol have been determined using relative kinetic technique in a 50 L glass pyrex photoreactor using in situ FT-IR spectroscopy under room temperature of (298± 2) K and in a range of pressure of 350-670 torr and 2-methyl-2-butanol with GC-MS at room temperature and atmospheric pressure. The rate constant measured (in units of $cm^3$ $molecule^{-1}$ $s^{-1}$) were (2.49±0.42) x $10^{-15}$, (3.04±0.51) x $10^{-15}$, (2.63±0.19) x $10^{-15}$ and (1.57±0.16) x $10^{-15}$, respectively. The main reaction channel should be an H-abstraction of the hydrocarbon chain. Thus, 3-methyl-2-butanol, with a $C_\alpha$-H, has the highest value of rate coefficient. 2-butanol and 2,3-dimethyl-2-butanol have similar rate coefficients and 2-methyl-2-butanol (containing -$CH_2$- groups) is the lowest reactive. The same trend in reactivity is observed for OH reactions with these alcohols.

The values are also compared with their homologues structural alkanes and discussed. Thus, the substitution of a $CH_3$ group by an OH group greatly enhances the reactivity of the resulting alcohol, in one magnitude order and a similar trend in reactivity that the observed with alcohols. The dominant atmospheric loss process for these alcohols is their daytime reaction with OH radicals since lifetime is in the range of a few hours. 2-methyl-2-butanol is the compound that remains in the atmosphere longer, and therefore, at night time, $NO_3$ radicals reaction with this compound should be a relevant process and it could contribute to GWP. MIR index calculations of these compounds indicate that 3-methyl-2-butanol is the most relevant source in ozone generation.

**References**

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