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On the oxidation of acetic acid isotopomers with the OH radical in the gas phase.

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The acetic acid is one of the most abundant carboxylic acids in the atmosphere [1]. Concentrations at the ppb level have been found in urban and rural areas as well as off the coasts [2]. For a better understanding of the OH- initiated reaction mechanism of this acid in the troposphere, kinetic and mechanistic investigations of this reaction have been undertaken in a Teflon simulation chamber equipped with an irradiation device in the UV range. The analyses of the reaction mixture were carried out by means of two complementary techniques:

- gas chromatography coupled to a detection by FTIR spectroscopy

- Cavity Ring-Down Spectroscopy (CRDS) in the near-infrared range.

Experiments aiming at determining the branching ratio $R = k_a/(k_a + k_b)$ between the two possible reaction pathways were carried out.

$OH + CH_3COOH$	$\rightarrow$	$CH_3 + CO_2 + H_2O$	(a)
	$\rightarrow$	$CH_2COOH + H_2O$	(b)

The quantification of the CO_2 formed in the channel (a) as a function of the acetic acid reacted allowed the measurement of this branching ratio.

For a better comprehension of the mechanism, experiments were performed with the 3 deuterated isotopes of the acetic acid (CD_3COOD, CD_3COOH, CH_3COOD). Prelim-

inary results tend to show that the substitution of the hydrogen atom by a deuterium one produces a strong isotopic effect on the kinetics of the reaction in agreement with previous studies [3,4].

References:

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