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Temperature dependence of carbon kinetic isotope effect for the oxidation reaction of ethane by OH radicals under atmospherically relevant conditions

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Modeling of the global distribution of atmospheric ethane sources and sinks by using the ^{13}C isotopic composition requires accurate knowledge of the carbon kinetic isotope effect (KIE) of its atmospheric removal reactions. The quantum mechanical prediction implies the necessity to elucidate the temperature dependence of KIE within atmospherically relevant temperature range by experiment. In this study, the KIE and its temperature dependence for ethane oxidation by OH radicals was investigated at ambient pressure in a temperature range of 243 K to 303 K. The chemical reactions were carried out in a 15 L PFE reaction chamber, suspended in a thermally controlled oven. The isotope ratios of the gas phase components during the course of the reactions were measured by Thermal Desorption – Gas Chromatography – Isotope Ratio Mass Spectrometry (TD-GC-IRMS). For each temperature, the KIE was derived from the temporal evolution of the concentration and stable carbon isotope ratio ($\delta^{13}\text{C}$) of ethane using a method adapted from the relative reaction rate concept. The room temperature KIE of the ethane reaction with OH radicals was found to be $6.85 \pm 0.32 \text{ ‰}$. This value is in agreement with the previously reported value of $8.57 \pm 1.95 \text{ ‰}$ [Anderson et al. 2004] but has a substantially lower uncertainty. The experimental results will be discussed with the KIE temperature dependence predicted by quantum mechanical calculations.

Reference: Rebecca S. Anderson, Lin Huang, Richard Iannone, Alexandra E. Thompson, and Jochen Rudolph (2004), Carbon Kinetic Isotope Effects in the Gas Phase Reactions of Light Alkanes and Ethene with the OH Radical at $296 \pm 4 \text{ K}$, *J. Phys. Chem. A*, 108, 11537–11544