ASSESSING THE OH-INITIATED BREAKDOWN CHEMISTRY OF CAMPHENE AND 3-CARENE UNDER NO_X-FREE SIMULATED ATMOSPHERIC CONDITIONS

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ABSTRACT

Camphene and 3-carene are key atmospheric monoterpenes used in cosmetics, fragrances, and food flavouring. In order to assess their impacts on human health and the environment it is essential to have a thorough understanding of the degradation mechanisms involved in their reactivity. The present study aimed to investigate the OH radicals initiated atmospheric degradation of camphene and 3-carene under simulated NO_x-free conditions. The experiments were conducted using facilities provided by the 760 L Environmental Simulation Chamber made of Quartz (ESC-Q-UAIC) together with state-of-the-art instruments, including a proton-transfer-reaction time-of-flight mass spectrometer (PTR-ToF-MS, model 6000 X2, IONICON) coupled with an aerosol chemical composition analyzer (CHARON). In the present study, the rate constants of the reactions of camphene and 3-carene with OH radicals were determined to be $(7.81 \pm 0.95) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} and $(5.37 \pm 0.60) \times 10^{-11}$ cm^3 $molecule^{-1}$ s^{-1}, respectively. The obtained kinetic results, based on the relative rate technique with propene and 1,3,5-trimethylbenzene as reference compounds, are in agreement with the values reported in the literature. The measurements performed with the PTR-ToF-MS with CHARON particle inlet demonstrated that the photooxidation processes of camphene and 3-carene result in the formation of low-volatile species which play a significant role in the formation of secondary organic aerosols. Among the identified photooxidation products, camphenilone ($C_9H_{14}O$) and caronaldehyde ($C_{10}H_{16}O_2$) were assigned to the signals at the mass-to-charge ratio values of 139.112 Da and 169.122 Da, respectively, in both gas- and aerosol-phase measurements. The findings of this study will offer crucial insights to be incorporated into the Master Chemical Mechanism (MCM) for the detailed description of the gas-phase chemical processes involved in the tropospheric degradation of camphene and 3-carene, which are currently lacking.

Keywords: camphene, 3-carene, OH radicals, gas-phase reaction rate, gas-phase oxidation products, secondary organic aerosols, PTR-ToF-MS