

Product Study of the Reaction of OH Radicals with Isoprene

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Isoprene (2-methyl-1,3-butadiene) represents the dominant non-methane hydrocarbon emitted into the atmosphere by vegetation with a global emission rate of $\sim 5 \cdot 10^8$ tons per year. Atmospheric mixing ratios for isoprene span a range of 1 - 30 ppb [1]. The degradation process is governed by the initial attack of OH radicals at daytime resulting in a lifetime of ~ 1.5 h [2]. Chemical processes going on in the course of isoprene transformation and formed products are important issues in atmospheric chemistry. At the present time, new experimental findings from laboratory and field investigations [3] as well as results from quantum-chemical calculations [4] are discussed in the literature.

In the present laboratory study the reaction of OH radicals with isoprene was conducted under flow-tube conditions at 295 ± 2 K and a total pressure of 0.25 or 1.0 bar. OH radicals are formed via the reaction sequence $H + O_2 + M \rightarrow HO_2 + M$, $H + HO_2 \rightarrow 2 OH$ as well as via $NO + HO_2 \rightarrow OH + NO_2$ in the case of NO in the carrier gas. Analysis of reaction products has been performed by means of i) CI-MS using H_3O^+ and NO^+ as the reagent ions, ii) on-line coupled GC-MS with cryo-enrichment, iii) long-path FT-IR spectroscopy, and iii) long-path UV spectroscopy.

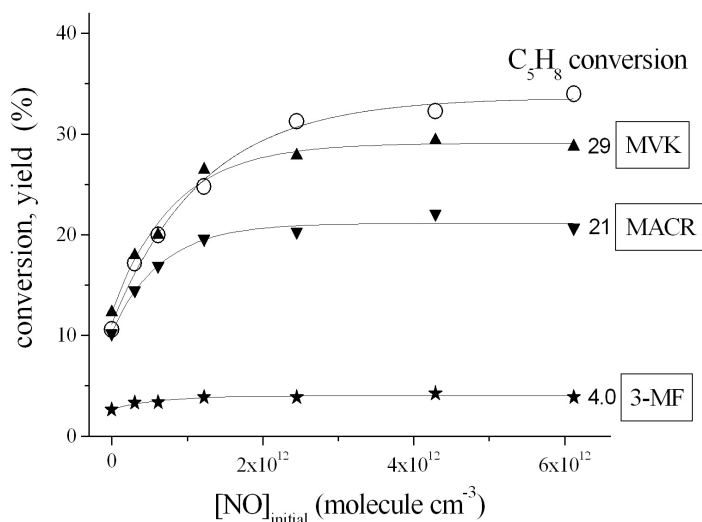


Fig. 1. Results from a measurement series at a pressure of 0.25 bar using on-line GC-MS analysis (MVK, MACR, 3-MF) and UV spectroscopy (C₅H₈); residence time of 1.7 sec.; [C₅H₈] = $2.0 \cdot 10^{12}$ molecule cm⁻³, [O₂] = $4.9 \cdot 10^{18}$ molecule cm⁻³. For initial NO concentrations $> 10^{12}$ molecule cm⁻³ 29 % methyl vinyl ketone (MVK), 21 % methacrolein (MACR) and 4.0 % 3-methylfuran are detected.

References

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