Kinetics Study of the Reactions of 4-Methyl-2-Pentanone and m-Ethyl Toluene with Hydroxyl Radical between 240-340 K and 1-8 Torr Using the Relative Rate/Discharge Flow/Mass Spectrometry Technique

Rachel Kaiser, John Hasenbein, and Zhuangjie Li*

Department of Chemistry and Biochemistry, California State University Fullerton, Fullerton, CA 92831

Supporting Information

Table 1S: List of relevant chemical reactions used in the chemical model simulation in assessing the contribution of atomic oxygen and hydrogen to the decay of styrene and reference compounds

Reaction[a]	k (cm^3 molecule^{-1} s^{-1})	Reference
$F + H_2O \rightarrow HF + OH$	1.4×10^{-11}	25
$OH + OH \rightarrow H_2O + O$	1.9×10^{-12}	25
OH + wall → product	10[b]	estimate[d]
$O + OH \rightarrow O_2 + H$	3.3×10^{-11}	25
H + wall → product	10[b]	estimate[d]
$H + OH + M \rightarrow H_2O + M$	2.3×10^{-31}[c]	33
$O + F_2 \rightarrow FO + F$	1.0×10^{-16}	34
$FO + OH \rightarrow O_2 + HF$	1.3×10^{-12}	estimate[e]
$H + F_2 \rightarrow HF + F$	1.38×10^{-12}	35
Target + OH → products	1.25×10^{-11}	this work[f]
Reference + OH → products	1.09×10^{-11}	27[g]
Target + O → products	4.52×10^{-12}	36-39[h]
Reference + O → products	3.50×10^{-11}	40-41[h]
Target + H → products	6.00×10^{-16}	36,38
Reference + H → products	4.37×10^{-15}	40-41[h]

[a]Initial concentrations are: $[F]_o = 1.0 \times 10^{13}$, $[H_2O]_o = 7.1 \times 10^{14}$, $[F_2]_o = 2.0 \times 10^{12}$, $[Target]_o = 4.3 \times 10^{13}$, $[Reference]_o = 7.9 \times 10^{13}$ molecules cm^{-3}, respectively. The initial concentrations of $[H]_o$ and $[O]_o$ are zero. [b]Units for the wall loss constant is s^{-1}, while the [c]units for the termination reaction of H + OH is cm^6 molecule^{-2} s^{-1}. [d]Estimate values were used on the basis from the OH wall loss. [e]Estimation was based on k(ClO + OH). [f]$k_{MIBK+OH} = 1.25 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1},

k_{MET+OH} = 2.07 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1}. [g]$k_{1,4\text{-}dioxane+OH}$ = 1.09 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1},[27] $k_{nonane+OH}$ = 1.13 × 10^{-11} cm^3 $molecule^{-1}$ s^{-1}.[28] [h]k_{MIBK+O} = 4.83 × 10^{-16} cm^3 $molecule^{-1}$ s^{-1}, and k_{MIBK+H} = 6.00 × 10^{-16} cm^3 $molecule^{-1}$ s^{-1} were estimated from O and H + acetone,[36] [h]k_{MET+O} = 3.98 × 10^{-13} cm^3 $molecule^{-1}$ s^{-1} was estimated from O + m-xylene,[37] k_{MET+H} = 1.82 × 10^{-13} cm^3 $molecule^{-1}$ s^{-1} was estimated from H + p-xylene,[38] $k_{1,4\text{-}dioxane+O}$ = $k_{1,4\text{-}dioxane+H}$ = 6.81 × 10^{-14} cm^3 $molecule^{-1}$ s^{-1} were estimated from O and H + 1,4-dioxane,[39] $k_{n\text{-}pentane+H}$ = 4.37 × 10^{-15} cm^3 $molecule^{-1}$ s^{-1} and $k_{nonane+O}$ = 1.70 × 10^{-13} cm^3 $molecule^{-1}$ s^{-1} was estimated from H and O + octane,[40,41] respectively.