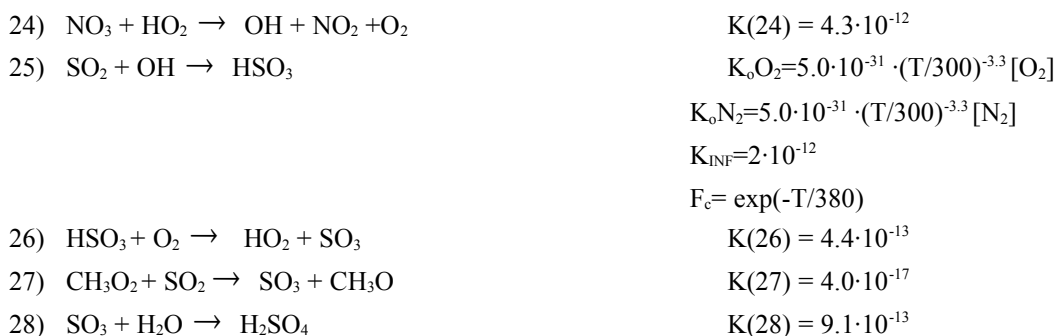


Liite C. Reaktioyhtälöt ja niiden reaktionopeusvakiot

Reaction	Rate coefficient
Inorganic Chemistry	
1) $O(^3P) + O_2 \xrightarrow{M} O_3$	$K_oO_2=6.2 \cdot 10^{-34} \cdot (T/300)^{-2.8} [O_2]$
	$K_oN_2=5.6 \cdot 10^{-34} \cdot (T/300)^{-2.8} [N_2]$
	$K_{INF}=2.8 \cdot 10^{-12}$
	$F_c=\exp(-T/696)$
2) $O(^3P) + NO \xrightarrow{M} NO_2$	$K_oO_2=8.6 \cdot 10^{-32} \cdot (T/300)^{-1.8} [O_2]$
	$K_oN_2=1.0 \cdot 10^{-31} \cdot (T/300)^{-1.6} [N_2]$
	$K_{INF}=3.0 \cdot 10^{-11} \cdot (T/300)^{0.3}$
	$F_c=\exp(-T/1850)$
3) $O(^1D) + M \rightarrow O(^3P) + M$	$K(3) = 3.2 \cdot 10^{-11} \exp(67/T)$
4) $O(^1D) + H_2O \rightarrow 2OH$	$K(4) = 2.2 \cdot 10^{-10}$
5) $NO + O_3 \rightarrow NO_2 + O_2$	$K(5) = 1.8 \cdot 10^{-12} \exp(-1370/T)$
6) $NO_2 + O_3 \rightarrow NO_3 + O_2$	$K(6) = 1.2 \cdot 10^{-13} \exp(-2450/T)$
7) $O_3 + OH \rightarrow HO_2 + O_2$	$K(7) = 1.9 \cdot 10^{-12} \exp(-1000/T)$
8) $HO_2 + O_3 \rightarrow 2O_2 + OH$	$K(8) = 1.4 \cdot 10^{-14} \exp(-600/T)$
9) $NO_3 + NO \rightarrow 2NO_2$	$K(9) = 1.8 \cdot 10^{-11} \exp(110/T)$
10) $NO + HO_2 \rightarrow NO_2 + OH$	$K(10) = 3.7 \cdot 10^{-12} \exp(240/T)$
11) $NO_3 + NO_2 \rightarrow NO + NO_2 + O_2$	$K(11) = 2.3 \cdot 10^{-12} \exp(-1000/T)$
12) $NO_3 + NO_2 \rightarrow N_2O_5$	$K_oN_2=2.7 \cdot 10^{-30} (T/300)^{-3.4} [N_2]$
	$K_{INF}=2.0 \cdot 10^{-12} (T/300)^{0.2}$
	$F_c=\exp(-T/250)+\exp(-1050/T)$
13) $NO_2 + OH \rightarrow HNO_3$	$K_oO_2=2.2 \cdot 10^{-30} (T/300)^{-2.9} [O_2]$
	$K_oN_2=2.6 \cdot 10^{-30} (T/300)^{-2.9} [N_2]$
	$K_{INF}=5.2 \cdot 10^{-11}$
	$F_c=\exp(-T/353)$
14) $NO_3 + H_2O_2 \rightarrow HNO_3 + HO_2$	$K(14) = 4.1 \cdot 10^{-16}$
15) $NO_3 + NO_3 \rightarrow 2NO_2 + O_2$	$K(15) = 8.5 \cdot 10^{-13} \exp(-2450/T)$
16) $N_2O_5 + H_2O \rightarrow 2HNO_3$	$K(16) = 1.3 \cdot 10^{-21}$
17) $N_2O_5 \rightarrow NO_3 + NO_2$	$K_oN_2=2.2 \cdot 10^3 (T/300)^{-4.4} \exp(-11080/T) [N_2]$
	$K_{INF}=9.7 \cdot 10^{14} (T/300)^{0.1} \exp(-11080/T)$
	$F_c=\exp(-T/250)+\exp(-1050/T)$
18) $OH + HO_2 \rightarrow H_2O + O_2$	$K(18) = 4.8 \cdot 10^{-11} \exp(250/T)$
19) $OH + H_2O_2 \rightarrow HO_2 + H_2O$	$K(19) = 2.9 \cdot 10^{-12} \exp(-160/T)$
20) $OH + H_2 \rightarrow H + H_2O$	$K(20) = 7.7 \cdot 10^{-12} \exp(-2100/T)$
21) $OH + HNO_3 \rightarrow NO_3 + H_2O$	$K(21) = 9.4 \cdot 10^{-15} \exp(778/T)$
22) $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	$K(22) = 1.6 \cdot 10^{-12}$
23) $NO_3 + HO_2 \rightarrow O_2 + HNO_3$	$K(23) = 4.3 \cdot 10^{-12}$

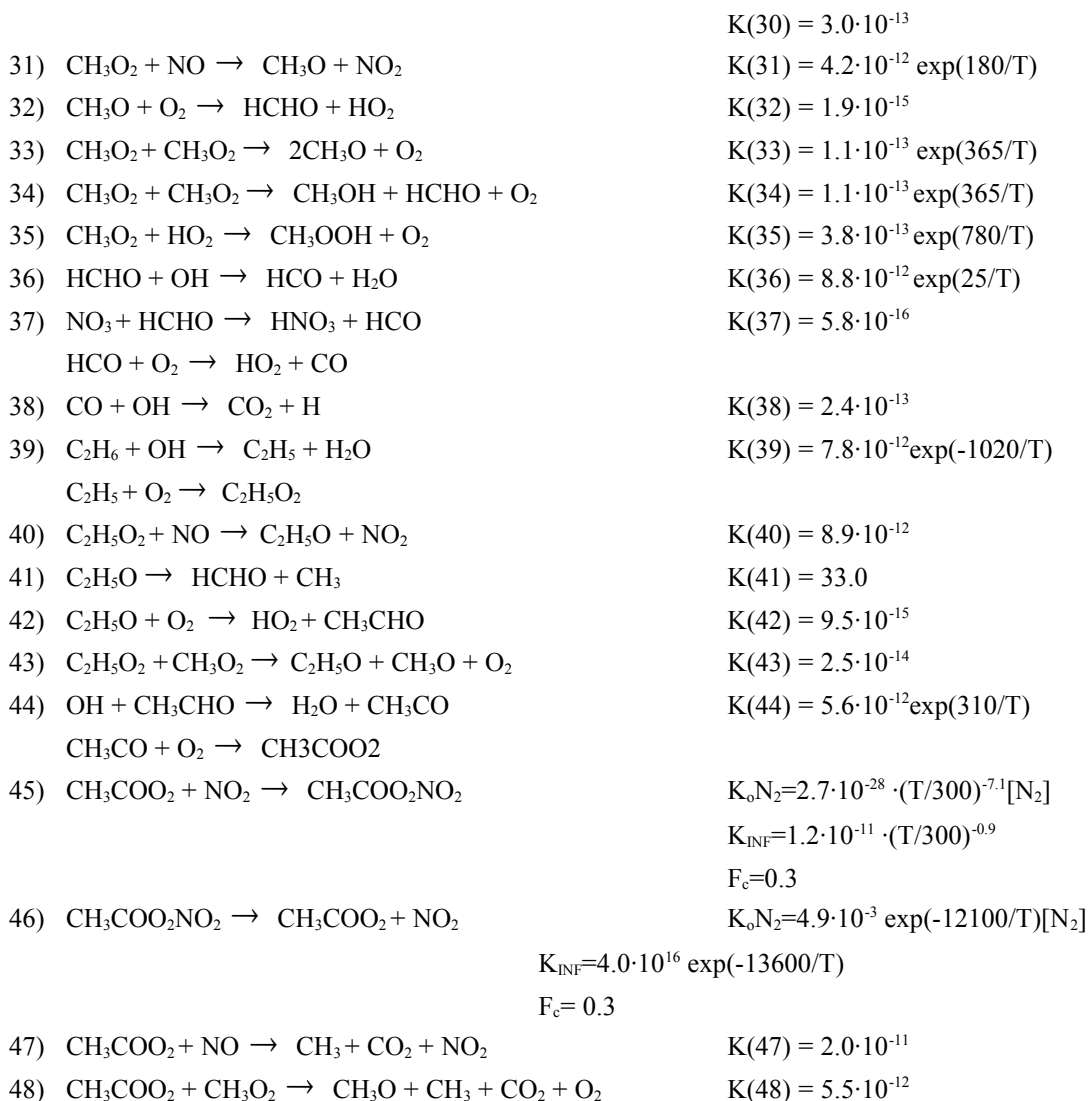


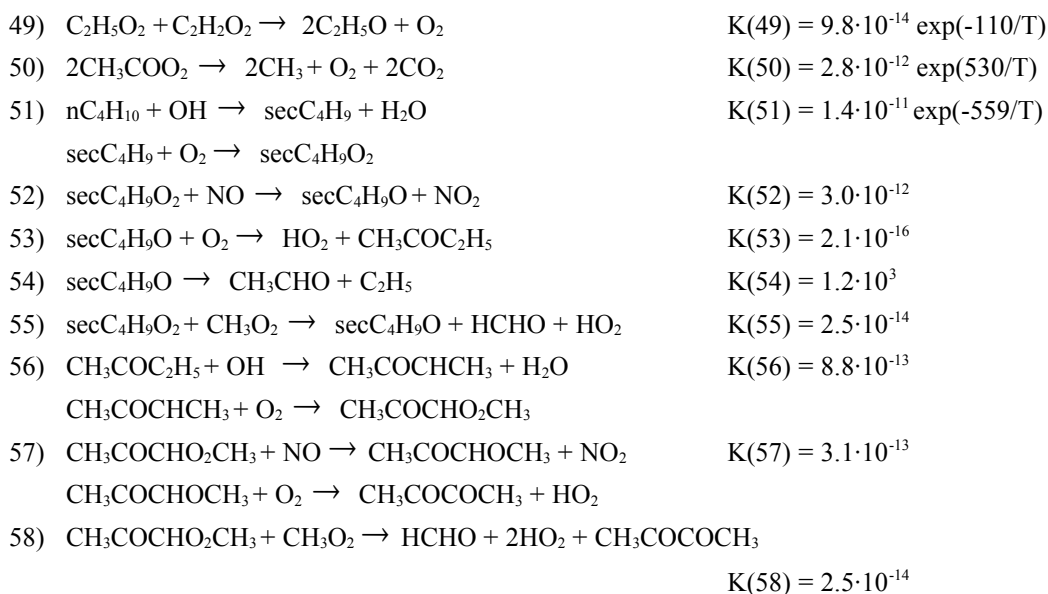
Alkane Chemistry



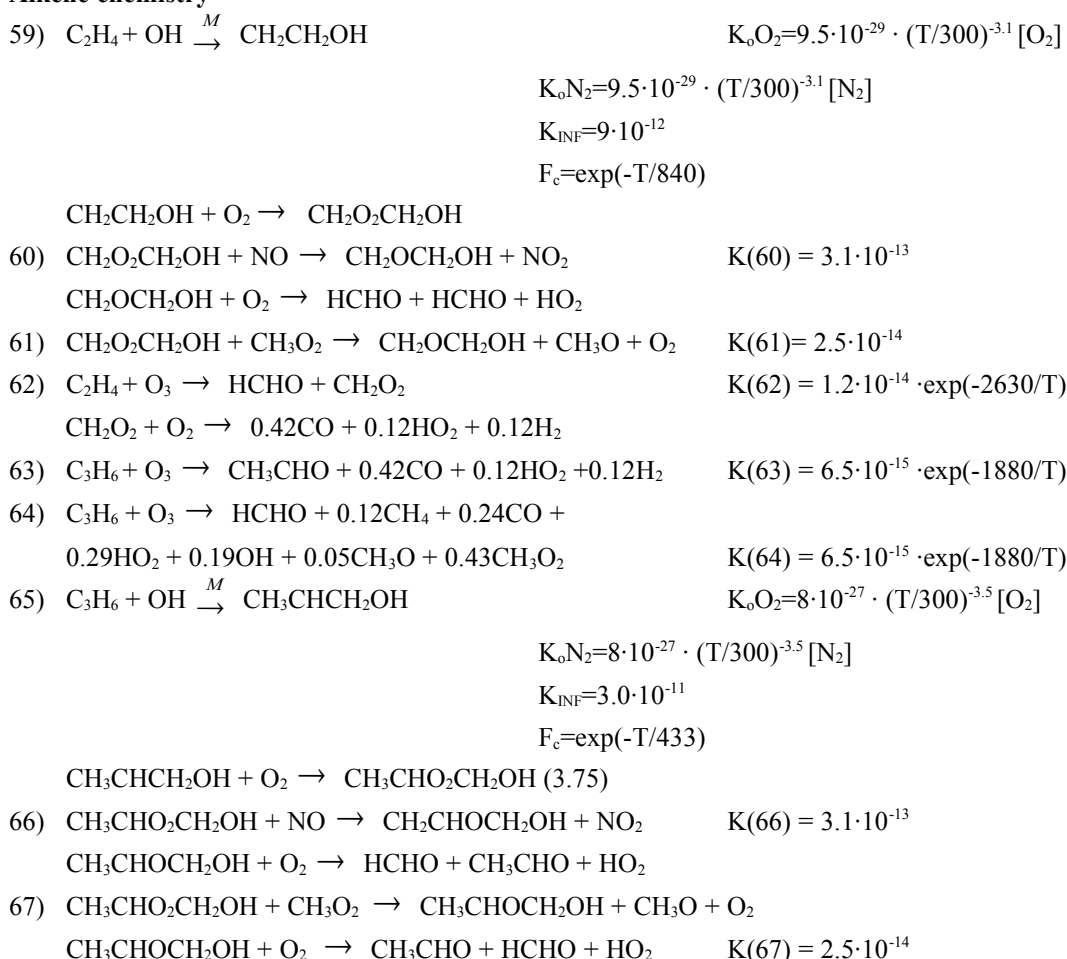
$$K_{\text{INF}} = 2.2 \cdot 10^{-12} (T/300)^{1.0}$$

$$F_c = 0.27$$

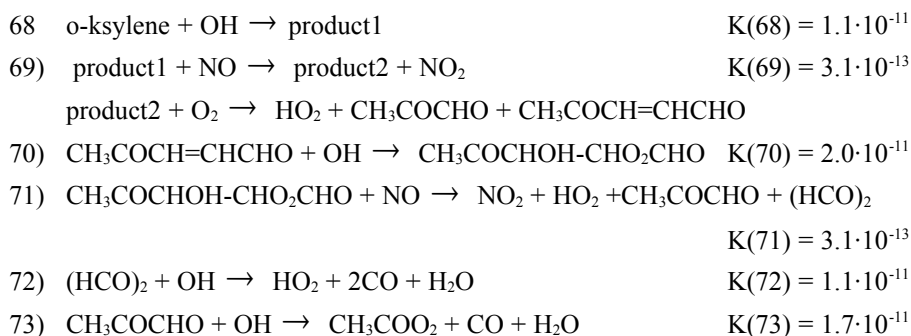




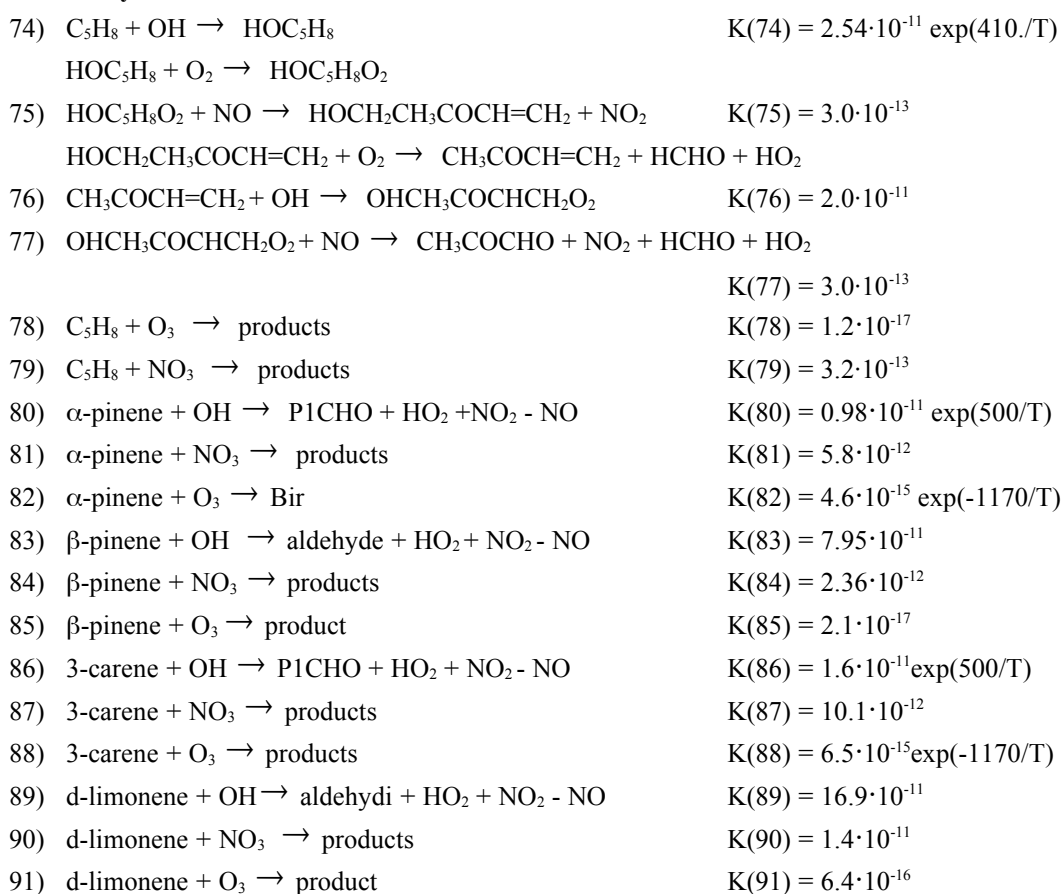
Alkene chemistry



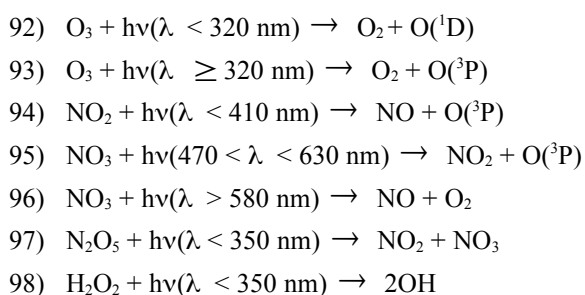
Aromatic Chemistry



Natural hydrocarbons



Photochemical reactions



- 99) $\text{HNO}_3 + h\nu(\lambda < 320 \text{ nm}) \rightarrow \text{NO}_2 + \text{OH}$
100) $\text{HCHO} + h\nu(\lambda < 370 \text{ nm}) \rightarrow \text{HCO} + \text{H}$
101) $\text{HCHO} + h\nu(\lambda < 370 \text{ nm}) \rightarrow \text{CO} + \text{H}_2$
102) $\text{CH}_3\text{CHO} + h\nu(\lambda < 325 \text{ nm}) \rightarrow \text{CH}_3\text{O}_2 + \text{HO}_2 + \text{CO}$
103) $\text{CH}_3\text{COC}_2\text{H}_5 + h\nu \rightarrow \text{CH}_3\text{COO}_2 + \text{C}_2\text{H}_5\text{O}_2$
104) $\text{CH}_3\text{COCOCH}_3 + h\nu \rightarrow 2\text{CH}_3\text{COO}_2$
105) $\text{HCOCHO} + h\nu(\lambda < 470 \text{ nm}) \rightarrow \text{CO} + \text{HCHO}$
106) $\text{CH}_3\text{OOH} + h\nu(\lambda < 350 \text{ nm}) \rightarrow \text{CH}_3\text{O} + \text{OH}$
107) $\text{CH}_3\text{COCHO} + h\nu(\lambda < 470 \text{ nm}) \rightarrow \text{CH}_3\text{CO} + \text{CO} + \text{HO}_2$