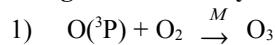


## Liite C. Reaktioyhtälöt ja niiden reaktionopeusvakiot

### Reaction

#### Inorganic Chemistry



#### Rate coefficient

( $s^{-1}$  for unimolecular reactions and  
 $cm^3 molecule^{-1} s^{-1}$  for others)

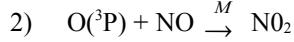
$$K_o O_2 = 6.2 \cdot 10^{-34} \cdot (T/300)^{-2.8} [O_2]$$

$$K_o N_2 = 5.6 \cdot 10^{-34} \cdot (T/300)^{-2.8} [N_2]$$

$$K_{INF} = 2.8 \cdot 10^{-12}$$

$$F_c = \exp(-T/696)$$

$$K_o O_2 = 8.6 \cdot 10^{-32} \cdot (T/300)^{-1.8} [O_2]$$



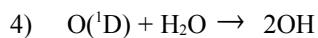
$$K_o N_2 = 1.0 \cdot 10^{-31} \cdot (T/300)^{-1.6} [N_2]$$

$$K_{INF} = 3.0 \cdot 10^{-11} \cdot (T/300)^{0.3}$$

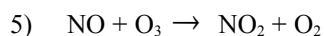
$$F_c = \exp(-T/1850)$$



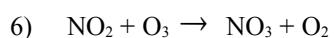
$$K(3) = 3.2 \cdot 10^{-11} \exp(67/T)$$



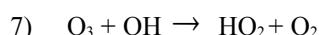
$$K(4) = 2.2 \cdot 10^{-10}$$



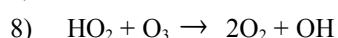
$$K(5) = 1.8 \cdot 10^{-12} \exp(-1370/T)$$



$$K(6) = 1.2 \cdot 10^{-13} \exp(-2450/T)$$



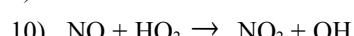
$$K(7) = 1.9 \cdot 10^{-12} \exp(-1000/T)$$



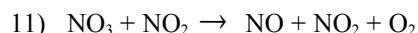
$$K(8) = 1.4 \cdot 10^{-14} \exp(-600/T)$$



$$K(9) = 1.8 \cdot 10^{-11} \exp(110/T)$$



$$K(10) = 3.7 \cdot 10^{-12} \exp(240/T)$$



$$K(11) = 2.3 \cdot 10^{-12} \exp(-1000/T)$$



$$K_o N_2 = 2.7 \cdot 10^{-30} (T/300)^{-3.4} [N_2]$$

$$K_{INF} = 2.0 \cdot 10^{-12} (T/300)^{0.2}$$

$$F_c = \exp(-T/250) + \exp(-1050/T)$$

$$K_o O_2 = 2.2 \cdot 10^{-30} (T/300)^{-2.9} [O_2]$$

$$K_o N_2 = 2.6 \cdot 10^{-30} (T/300)^{-2.9} [N_2]$$

$$K_{INF} = 5.2 \cdot 10^{-11}$$

$$F_c = \exp(-T/353)$$

$$K(14) = 4.1 \cdot 10^{-16}$$

$$K(15) = 8.5 \cdot 10^{-13} \exp(-2450/T)$$

$$K(16) = 1.3 \cdot 10^{-21}$$

$$K_o N_2 = 2.2 \cdot 10^3 (T/300)^{-4.4} \exp(-11080/T) [N_2]$$

$$K_{INF} = 9.7 \cdot 10^{14} (T/300)^{0.1} \exp(-11080/T)$$

$$F_c = \exp(-T/250) + \exp(-1050/T)$$

$$K(18) = 4.8 \cdot 10^{-11} \exp(250/T)$$

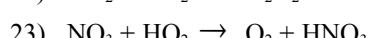
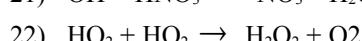
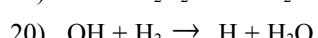
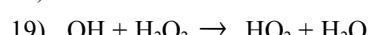
$$K(19) = 2.9 \cdot 10^{-12} \exp(-160/T)$$

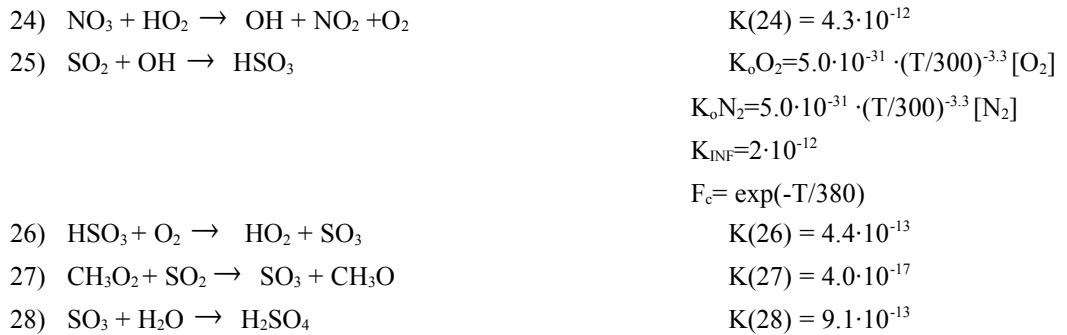
$$K(20) = 7.7 \cdot 10^{-12} \exp(-2100/T)$$

$$K(21) = 9.4 \cdot 10^{-15} \exp(778/T)$$

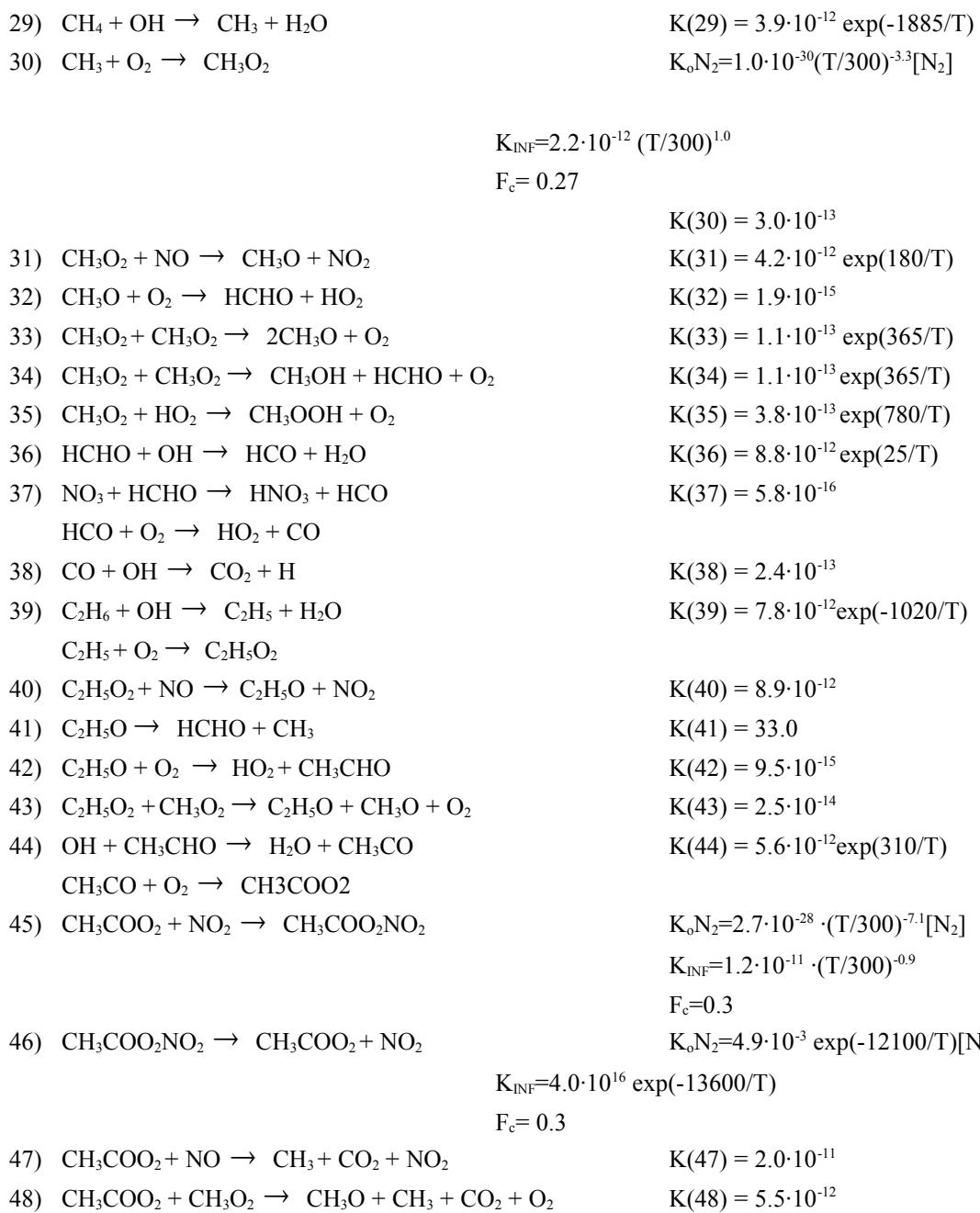
$$K(22) = 1.6 \cdot 10^{-12}$$

$$K(23) = 4.3 \cdot 10^{-12}$$





### Alkane Chemistry

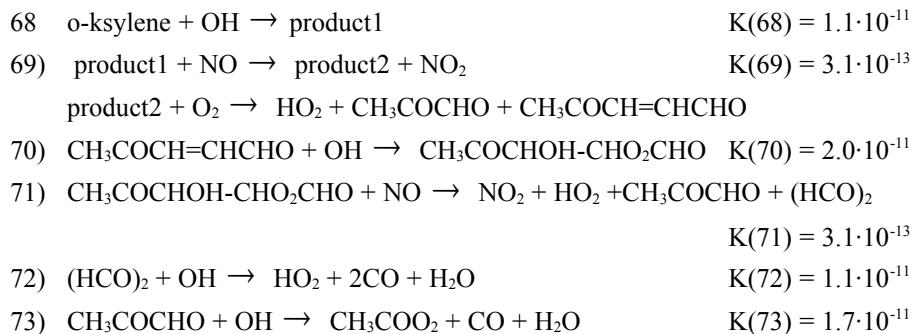


- 49)  $\text{C}_2\text{H}_5\text{O}_2 + \text{C}_2\text{H}_2\text{O}_2 \rightarrow 2\text{C}_2\text{H}_5\text{O} + \text{O}_2$   $K(49) = 9.8 \cdot 10^{-14} \exp(-110/T)$
- 50)  $2\text{CH}_3\text{COO}_2 \rightarrow 2\text{CH}_3 + \text{O}_2 + 2\text{CO}_2$   $K(50) = 2.8 \cdot 10^{-12} \exp(530/T)$
- 51)  $n\text{C}_4\text{H}_{10} + \text{OH} \rightarrow \text{secC}_4\text{H}_9 + \text{H}_2\text{O}$   $K(51) = 1.4 \cdot 10^{-11} \exp(-559/T)$   
 $\text{secC}_4\text{H}_9 + \text{O}_2 \rightarrow \text{secC}_4\text{H}_9\text{O}_2$
- 52)  $\text{secC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{secC}_4\text{H}_9\text{O} + \text{NO}_2$   $K(52) = 3.0 \cdot 10^{-12}$
- 53)  $\text{secC}_4\text{H}_9\text{O} + \text{O}_2 \rightarrow \text{HO}_2 + \text{CH}_3\text{COC}_2\text{H}_5$   $K(53) = 2.1 \cdot 10^{-16}$
- 54)  $\text{secC}_4\text{H}_9\text{O} \rightarrow \text{CH}_3\text{CHO} + \text{C}_2\text{H}_5$   $K(54) = 1.2 \cdot 10^3$
- 55)  $\text{secC}_4\text{H}_9\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{secC}_4\text{H}_9\text{O} + \text{HCHO} + \text{HO}_2$   $K(55) = 2.5 \cdot 10^{-14}$
- 56)  $\text{CH}_3\text{COC}_2\text{H}_5 + \text{OH} \rightarrow \text{CH}_3\text{COCHCH}_3 + \text{H}_2\text{O}$   $K(56) = 8.8 \cdot 10^{-13}$   
 $\text{CH}_3\text{COCHCH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{COCHO}_2\text{CH}_3$
- 57)  $\text{CH}_3\text{COCHO}_2\text{CH}_3 + \text{NO} \rightarrow \text{CH}_3\text{COCHOCH}_3 + \text{NO}_2$   $K(57) = 3.1 \cdot 10^{-13}$   
 $\text{CH}_3\text{COCHOCH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{COCOCH}_3 + \text{HO}_2$
- 58)  $\text{CH}_3\text{COCHO}_2\text{CH}_3 + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + 2\text{HO}_2 + \text{CH}_3\text{COCOCH}_3$   $K(58) = 2.5 \cdot 10^{-14}$

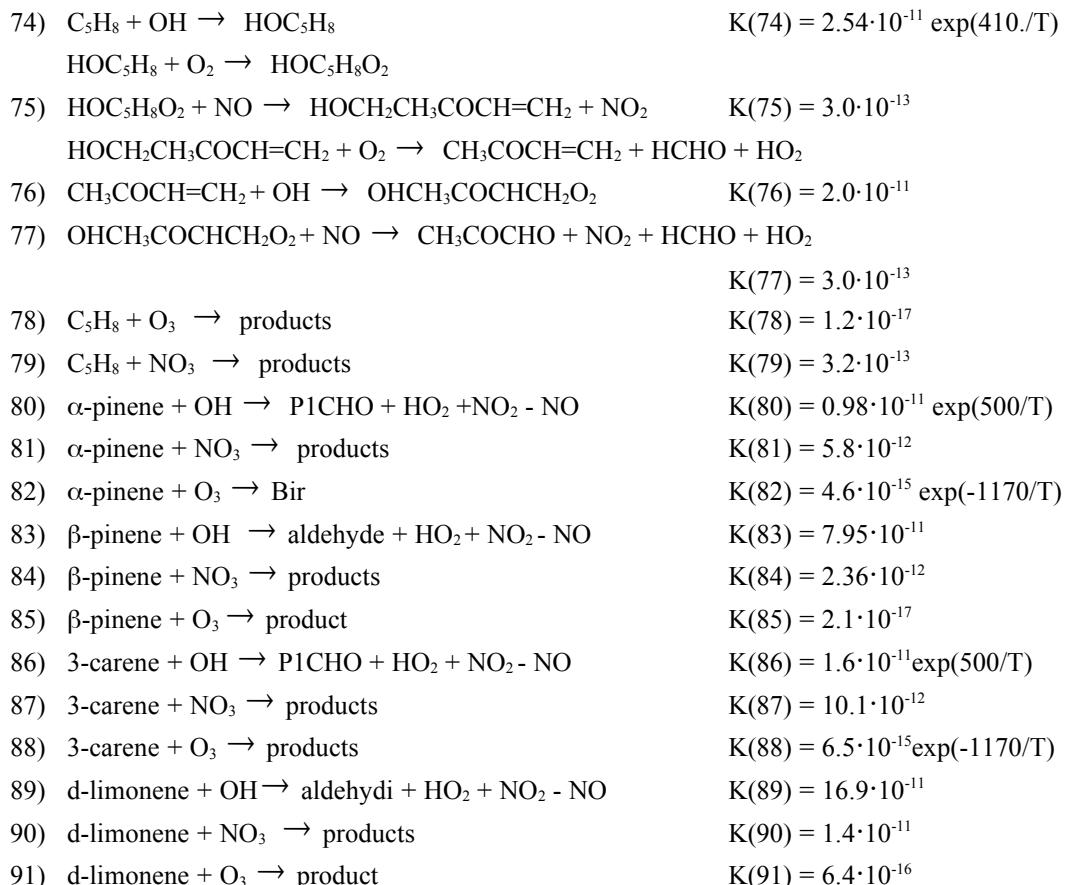
### Alkene chemistry

- 59)  $\text{C}_2\text{H}_4 + \text{OH} \xrightarrow{M} \text{CH}_2\text{CH}_2\text{OH}$   $K_o\text{O}_2 = 9.5 \cdot 10^{-29} \cdot (T/300)^{-3.1} [\text{O}_2]$   
 $K_o\text{N}_2 = 9.5 \cdot 10^{-29} \cdot (T/300)^{-3.1} [\text{N}_2]$   
 $K_{\text{INF}} = 9 \cdot 10^{-12}$   
 $F_c = \exp(-T/840)$   
 $\text{CH}_2\text{CH}_2\text{OH} + \text{O}_2 \rightarrow \text{CH}_2\text{O}_2\text{CH}_2\text{OH}$
- 60)  $\text{CH}_2\text{O}_2\text{CH}_2\text{OH} + \text{NO} \rightarrow \text{CH}_2\text{OCH}_2\text{OH} + \text{NO}_2$   $K(60) = 3.1 \cdot 10^{-13}$   
 $\text{CH}_2\text{OCH}_2\text{OH} + \text{O}_2 \rightarrow \text{HCHO} + \text{HCHO} + \text{HO}_2$
- 61)  $\text{CH}_2\text{O}_2\text{CH}_2\text{OH} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_2\text{OCH}_2\text{OH} + \text{CH}_3\text{O} + \text{O}_2$   $K(61) = 2.5 \cdot 10^{-14}$
- 62)  $\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow \text{HCHO} + \text{CH}_2\text{O}_2$   $K(62) = 1.2 \cdot 10^{-14} \cdot \exp(-2630/T)$   
 $\text{CH}_2\text{O}_2 + \text{O}_2 \rightarrow 0.42\text{CO} + 0.12\text{HO}_2 + 0.12\text{H}_2$
- 63)  $\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{CH}_3\text{CHO} + 0.42\text{CO} + 0.12\text{HO}_2 + 0.12\text{H}_2$   $K(63) = 6.5 \cdot 10^{-15} \cdot \exp(-1880/T)$
- 64)  $\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{HCHO} + 0.12\text{CH}_4 + 0.24\text{CO} + 0.29\text{HO}_2 + 0.19\text{OH} + 0.05\text{CH}_3\text{O} + 0.43\text{CH}_3\text{O}_2$   $K(64) = 6.5 \cdot 10^{-15} \cdot \exp(-1880/T)$
- 65)  $\text{C}_3\text{H}_6 + \text{OH} \xrightarrow{M} \text{CH}_3\text{CHCH}_2\text{OH}$   $K_o\text{O}_2 = 8 \cdot 10^{-27} \cdot (T/300)^{-3.5} [\text{O}_2]$   
 $K_o\text{N}_2 = 8 \cdot 10^{-27} \cdot (T/300)^{-3.5} [\text{N}_2]$   
 $K_{\text{INF}} = 3.0 \cdot 10^{-11}$   
 $F_c = \exp(-T/433)$   
 $\text{CH}_3\text{CHCH}_2\text{OH} + \text{O}_2 \rightarrow \text{CH}_3\text{CHO}_2\text{CH}_2\text{OH} (3.75)$
- 66)  $\text{CH}_3\text{CHO}_2\text{CH}_2\text{OH} + \text{NO} \rightarrow \text{CH}_2\text{CHOCH}_2\text{OH} + \text{NO}_2$   $K(66) = 3.1 \cdot 10^{-13}$   
 $\text{CH}_3\text{CHOCH}_2\text{OH} + \text{O}_2 \rightarrow \text{HCHO} + \text{CH}_3\text{CHO} + \text{HO}_2$
- 67)  $\text{CH}_3\text{CHO}_2\text{CH}_2\text{OH} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{CHOCH}_2\text{OH} + \text{CH}_3\text{O} + \text{O}_2$   
 $\text{CH}_3\text{CHOCH}_2\text{OH} + \text{O}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2$   $K(67) = 2.5 \cdot 10^{-14}$

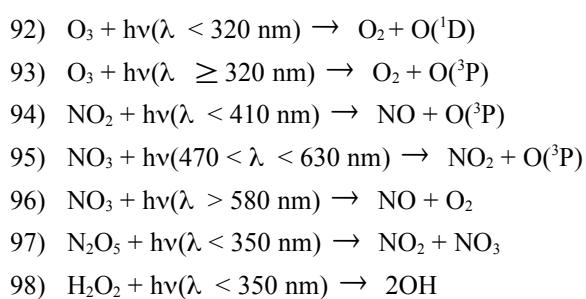
### Aromatic Chemistry



## Natural hydrocarbons



### Photochemical reactions



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