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ES 292

**Homework #8: 10.2, 10.3 for NO**

**10.2**

When T = 298 K and pd = 1013 hPa, calculate the first-order rate coefficient for

Repeat for T = 288 K. Discuss temperature effects on the reaction rate coefficient.

This is the nonelementary form of a bimolecular decomposition reaction, dependent on temperature.

10.20 :

10.30 :

From table B.4, k~0, T~ = 1.00 x 10 -3 (300/T)3.5 x e^ -11000/T^ cm6 molec. -2 s-1 k~inf, T~ = 9.70 x 1014(300/T)-0.1 x e-11080/T cm3 molec. -1 s-1 Fc = 0.33

pd <- 1013 #hPa  
T1 <- 298 #K  
T2 <- 288 #K  
kb <- 1.380658 \* 10^(-19) # cm3 hPa K-1 molec -1  
Fc <- .33  
  
  
rt\_coef <- function(t, p){  
 M <- p / (kb \* t)  
 k0t <- (1.00 \* (10^-3)) \* (((300/t)^(3.5)) \* exp(-11000/t))  
 kinf <- (9.7 \* (10^14)) \* (((300/t)^(-.1)) \* exp(-11080/t))  
 kr <- ((kinf \* k0t \* M)/(kinf + k0t\*M)) \* (Fc ^ ((1 + (log10((k0t \* M)/kinf))^2)^-1))  
 print(M)  
 print(k0t)  
 print(kinf)  
 print(kr)  
}  
  
rt\_coef(298,1013)

## [1] 2.462108e+19  
## [1] 9.531541e-20  
## [1] 0.06900614  
## [1] 0.04812731

rt\_coef(288,1013)

## [1] 2.547598e+19  
## [1] 2.981359e-20  
## [1] 0.01891146  
## [1] 0.01352878

The rate coefficient at T = 298K is 0.04812731 cm3 s-1 while at T = 288K, the coefficient is 0.01352878 cm3s-1. At a lower temperature, with pressure held equal, the rate of change of concentration decreases. Reactions are temperature dependent, or more accurately, collisional dependent. At higher temperatures, atoms and molecules are moving more than at lower temperatures, affording more possibilities for collisions, and thus reactions, to occur.

**10.3 for NO**

Estimate the e-folding lifetimes of CO, **NO**, O3 , SO2 , HNO3 , ISOP (iso- prene), and HO2 against loss by OH if [OH] = 1.0 × 106 molec. cm^{−3}, T = 288 K, and pd = 1010 hPa. The rate coefficients are listed in Appendix Table B.4. Order the species from shortest to longest lifetimes. Which species will most likely reach the stratosphere if only OH reaction is considered?

An e-folding lifetime is the time required for a species ( in this case, NO) to decrease to 1/e its original value.

In a bimolecular reaction, the e folding lifetime is

10.49:

ks <- 7.4 \* (10^-31) \* (300/288)^(2.4) #cm3 s-1

In the reaction ,

= 8.161702510^{-31}, from appendix B.4 and [B], the initial quantity of OH, is 1.0 × 106 molec. cm^{−3} Thus,

bb <- 1.0 \* (10^6) #molec. cm-3  
ta2 <- 1 / ks \* (bb) #seconds

The e-folding lifetime of NO is 1.2252346 x 1036 seconds. This time period (on the order of days) should allow NO to reach the stratosphere, which is only 50-60 km.