

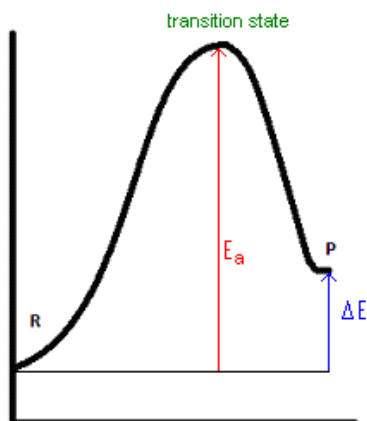
Collision Theory

1. What are three requirements for a reaction to proceed?
 - a. Particles must collide with each other.
 - b. Particles must be correctly orientated.
 - c. Particles must have enough energy to meet activation energy (E_a).

2. What is E_a ?

The energy required for reactants \rightarrow products.

3. Label



- a. Transition State
- b. Activation Energy
- c. ΔE

4. Write the Arrhenius Equation

$$k = A e^{\frac{-E_a}{RT}}$$

$$\ln(k) = \frac{-E_a}{R} \left(\frac{1}{T}\right) + \ln(A)$$

$$y = m x + b$$

k : rate constant

A : frequency factor

5. The activation energy for the decomposition of HI_(g) to H_{2(g)} and I_{2(g)} is 186 kJ/mol. The rate constant at 555K is 3.52 x 10⁻⁷ L/mol s. What is the rate constant at 645K?



$$E_a = 186 \text{ kJ/mol}$$

$$k_{555\text{K}} = 3.52 \times 10^{-7} \text{ M}^{-1} \text{ s}^{-1}$$

$$k_{645\text{K}} = ???$$

The first thing that we will need to do in this problem is determine the value of the frequency factor, A, using the information provided for k at 555K using:

$$k = A e^{\frac{-E_a}{RT}}$$

Once we have obtained that value, which assume to not be temperature dependent, we can then plug in and solve for the value of k at 645K.

$$3.52 \times 10^{-7} \text{ M}^{-1} \text{ s}^{-1} = A e^{\frac{186 \text{ kJ/mol}}{(8.314 \text{ J/mol K})(555\text{K})}}$$

Solving for A we get:

$$A = 1.129 \times 10^{11}$$

Now we can plug back into the same equation and solve for k at 645K.

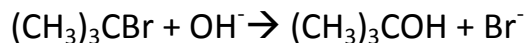
$$k = (1.129 \times 10^{11}) e^{\frac{-186000 \text{ J/mol}}{(8.314 \text{ J/mol K})(645 \text{ K})}}$$

Solving for k we get:

$$k = 9.75 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$$

This value makes sense as we expected a faster rate at a higher temperature.

6. The reaction



in a certain solvent is first order with respect to $(\text{CH}_3)_3\text{CBr}$ and zero order with respect to OH^- . A plot of $\ln(k)$ versus $1/T$ was constructed that resulted in a straight line with the slope of $-1.10 \times 10^4 \text{ K}$ and a y intercept of 33.5.

We will be using the following equation in the context of this problem:

$$\ln(k) = \frac{-E_a}{R} \left(\frac{1}{T} \right) + \ln(A)$$

$$y = m \quad x \quad + \quad b$$

a. Determine the E_a .

As you can see from the equation above, the slope is equal to $-E_a/R$.

So if we multiply the slope by -8.314 J/molK we will be able to determine the activation energy of this reaction.

$$\frac{-E_a}{R} = \text{slope} = -1.10 \times 10^4$$

$$E_a = -(8.314 \text{ J/molK})(-1.10 \times 10^4 \text{ K}) = 91454 \text{ J}$$

b. Determine A.

$$\ln(A) = \text{y-intercept} = 33.5$$

$$A = 3.54 \times 10^{14}$$

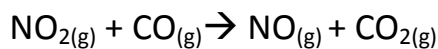
c. Calculate k at 298K.

$$k = A e^{\frac{-E_a}{RT}}$$

$$k = (3.54 \times 10^{14}) e^{\frac{-91454 \text{ J}}{8.314 \frac{\text{J}}{\text{molK}} (298 \text{ K})}}$$

$$k = 0.0330 \text{ s}^{-1}$$

7. Consider

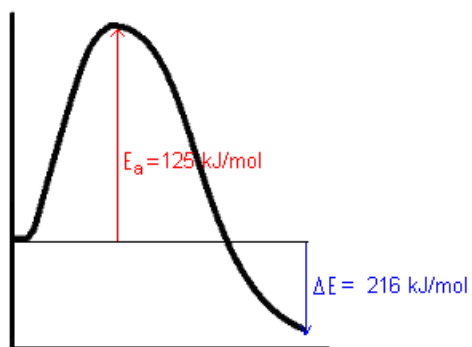


If the activation energy is 125 kJ/mol , and ΔE for the reaction is -216 kJ/mol . What is the activation energy for the reverse reaction?

$E_a = 125 \text{ kJ/mol}$ This is the amount of energy it takes to go from the reactant to the product.

$\Delta E = -216 \text{ kJ/mol}$ This value is the difference in energy between the products and reactants.

The negative ΔE tells us that the reaction is exothermic – I am going to just look at the magnitude of the value to determine the E_a for the reverse reaction.



So now, to determine the E_a for the reverse reaction you need to add the E_a of the forward reaction to the ΔE .

$$E_a(\text{reverse reaction}) = 125 + 216 = 341 \text{ kJ/mol}$$