CHEMICAL KINETICS:-

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Ex. 1 calculate frequency factor (A) for the unimolecular decomposition of an organic substance at 285°c The value entropy of activation (ΔS^*) is 13.15 cal. mol^{-1} deg^{-1}. (e.u.)

Ans:

અહીં $\Delta S^* = 13.15\ cal\ mol^{-1}\ deg^{-1}$ e.u.

$T = 285°c = 285 + 273 = 558\ K$

$k = 1.38 \times 10^{-16}$ ergs $molecule^{-1}$ or ergs

$h = 6.626 \times 10^{-27}$ ergs.sec ~~[illegible]~~

$R = 1.987$ cal. ~~[illegible]~~ mol^{-1}, deg^{-1}

OR

cal K^{-1}, M^{-1}

frequency factor (A) = (?)

$$A = \frac{kT}{h} \exp \frac{\Delta S^*}{R}$$

$$= \frac{1.38 \times 10^{-16} \times 558}{6.626 \times 10^{-27}} \times \exp \frac{13.15}{1.987}$$

$$= \frac{1.38 \times 10^{-16} \times 558}{6.626 \times 10^{-27}} \exp (6.618017111)$$

$$= \frac{1.38 \times 10^{-16} \times 558}{6.626 \times 10^{-27}} \times (748.4595126)$$

$$= 86982.15561 \times 10^{11}$$

$$= 8.69 \times 10^{15}$$

$$A = 8.7 \times 10^{15}\ \text{સેકંડ}^{-1}$$

Ex:2 calculate frequency factor (A) for the decomposition of N_2O_5 at 25°c. The value entropy of activation (ΔS^*) is 4.354 cal. mole^{-1} deg^{-1} (e.u.)

2021 2014

Ans:

$\Delta S^* = 4.354$ cal mole^{-1} deg^{-1} (e.u.)

$K = 1.38 \times 10^{-16}$ ergs

$h = 6.626 \times 10^{-27}$ ergs. sec

$T = 25 + 273 = 298K$

$R = 1.987$ cal K^{-1}, M^{-1}

$A = (?)$

$$A = \frac{KT}{h} \exp^{\Delta S^*/R}$$

$$= \frac{1.38 \times 10^{-16} \times 298}{6.626 \times 10^{-27}} \times \exp \frac{4.354}{1.987}$$

$$= \frac{1.38 \times 10^{-16} \times 298}{6.626 \times 10^{-27}} \times \exp (2.19124308)$$

$$= \frac{1.38 \times 10^{-16} \times 298}{6.626 \times 10^{-27}} \times 8.946327206$$

$$= 555.250 \times 10^{11}$$

$$A = 5.55 \times 10^{13} \text{ સેકન્ડ}^{-1}$$

Ex:3 Calculate the entropy of activation (ΔS^*) for a reaction

2013 2010

$$H_2 + I_2 \rightleftharpoons 2HI$$

at 575 °K The value of frequency factor (A) is 7.94×10^{10} sec^{-1}

Ans:

અહીં $A = 7.94 \times 10^{10}$ સેકન્ડ$^{-1}$

$T = 575°K$

$k = 1.38 \times 10^{-16}$ ergs

$h = 6.626 \times 10^{-27}$ ergs sec

$\Delta S^* = ??$

$R = 1.987$ cal. K^{-1}, M^{-1}

$$A = \frac{KT}{h} \exp^{\Delta S^*/R}$$

અહીં $k = R/N$

$$A = \frac{RT}{Nh} \exp^{\Delta S^*/R}$$

$$\therefore e^{\Delta S^*/R} = \frac{A \times N \times h}{R \times T}$$

$$= \frac{7.94 \times 10^{10} \times 6.02 \times 10^{23} \times 6.626 \times 10^{-27}}{1.987 \times 575}$$

$$e^{\Delta S^*/R} = 0.2772 \times 10^{6}$$

$$\therefore e^{\Delta S^*/R} = 2.772 \times 10^{5}$$

$$\therefore \ln e^{\Delta S^*/R} = \ln (2.772 \times 10^{5})$$

$$\therefore \frac{\Delta S^*}{R} = 2.303 \times \log 2.772 \times 10^{5}$$

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$$\Delta S^* = 2.303 \times R \times \log(2.772 \times 10^5)$$

$$\Delta S^* = 2.303 \times 1.987 \times 5.4427$$

$$\Delta S^* = 24.906 \text{ cal mol}^{-1} \text{deg}^{-1} \text{ (e.u)}$$

Ex:4 Calculate the frequency factor (A) for the unimolecular decomposition of $(CH_3CO)_2$ at 285°c. The value of entropy of Activation (ΔS^*) is 13.15 cal mol^{-1} deg^{-1} (e.u)

2010 2018

Ans:-

Same → example:-1

Ex:-5 Calculate frequency factor (A) for a reaction $\frac{1}{2}Cl_2 + H_2 \rightleftharpoons HCl + \frac{1}{2}H_2$ at 450°K. The value of entropy of activation (ΔS^*) is 12.74 cal mol^{-1} deg^{-1} (e.u).

2011

Ans:-

$$A = \frac{KT}{h} \exp^{\Delta S^*/R}$$

$$= \frac{1.38 \times 10^{-16} \times 450}{6.626 \times 10^{-27}} e^{12.74/1.987}$$

$$= \frac{1.38 \times 10^{-16} \times 450}{6.626 \times 10^{-27}} e^{(6.411675893)}$$

$$= 93.72170238 \times 608.9133 \times 10^{11}$$

$$= 57068.39 \times 10^{11}$$

$$A = 5.7 \times 10^{15} \text{ cal.mol}^{-1} \text{deg}^{-1} \text{ (e.u)}$$

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Ex:6 Calculate the entropy of activation (ΔS^*) for a reaction $H_2 + I_2 \rightleftharpoons 2HI$ at 473°K. The value of frequency factor is 8.0×10^{10} sec^{-1}

2011 2018

Ans:-

$$A = \frac{KT}{h} \exp^{\Delta S^*/R}$$

$$A = \frac{RT}{Nh} \exp^{\Delta S^*/R}$$

$$\therefore \exp^{\Delta S^*/R} = \frac{A \times N \times h}{R \times T}$$

$$= \frac{8.0 \times 10^{10} \times 6.02 \times 10^{23} \times 6.626 \times 10^{-27}}{1.987 \times 473}$$

$$\exp^{\Delta S^*/R} = 0.3395 \times 10^6$$

$$= 3.395 \times 10^5$$

$$\ln_e \exp^{\Delta S^*/R} = \ln 3.395 \times 10^5$$

$$\therefore \Delta S^*/R = 2.303 \times \log 3.395 \times 10^5$$

$$\Delta S^* = 2.303 \times R \times \log 3.395 \times 10^5$$

$$\Delta S^* = 2.303 \times 1.987 \times 5.530839779$$

$$\Delta S^* = 25.309 \text{ cal mol}^{-1} \text{deg}^{-1} \text{ (e.u)}$$

EX:7 At 290°c the frequency factor of the unimolecular decomposition of $(CH_3CO)_2$ is found to be 8.5×10^{15} sec^{-1}. calculate entropy of activation (ΔS^*) for reaction.

2012

Ans:

$$A = \frac{KT}{h} \exp^{\Delta S^*/R}$$

$$\exp^{\Delta S^*/R} = \frac{A \times h}{KT}$$

$$= \frac{8.5 \times 10^{15} \times 6.626 \times 10^{-27}}{1.38 \times 10^{-16} \times 563}$$

$$= 0.072490 \times 10^{4}$$

$$\exp^{\Delta S^*/R} = 724.90 \text{ OR } 7.2490 \times 10^{2}$$

$$\ln_e \exp^{\Delta S^*/R} = \ln 7.249 \times 10^2 \text{ OR } 724.90$$

$$\Delta S^*/R = 2.303 \log 724.90$$

$$\Delta S^* = 2.303 \times 1.987 \times 2.8602781$$

$$\Delta S^* = 13.08 \text{ cal mol}^{-1} \text{deg}^{-1} \text{ (e.u)}$$

EX:7 ~~Calculate the frequency factor (A) for the decomposition of $(CH_3CO)_2$ is found to be 8.5×10^{15} sec^{-1}. calculate of entropy activation (ΔS^*).~~

EX:8 Calculate the frequency factor (A) for decomposition of organic substance at 300°K. The value entropy of activation (ΔS^*) is 6.48 cal. mole^{-1} deg^{-1} (e.u)

2012

Ans:

$$A = \frac{KT}{h} \exp^{\Delta S^*/R}$$

$$= \frac{1.38 \times 10^{-16} \times 300}{6.626 \times 10^{-27}} \exp^{6.48/1.987}$$

$$= \frac{1.38 \times 10^{-16} \times 300}{6.626 \times 10^{-27}} \times \exp(3.26119778)$$

$$= \frac{1.38 \times 300 \times 10^{-16}}{6.626 \times 10^{-27}} \times 26.08075761$$

$$= 1629.55 \times 10^{11}$$

$$A = 1.629 \times 10^{14} \text{ Sec}^{-1}$$

Ex. 9 At 350°K, the frequency factor (A) has value of 1.20×10^{10} sec^{-1} for reaction.

2013

$$1/2\, Cl_2 + H_2 \rightleftharpoons HCl + 1/2\, H_2$$

calculate the entropy of Activation (ΔS^*)

$$A = \frac{KT}{h} \exp^{\Delta S^*/R}$$

$$\exp^{\Delta S^*/R} = \frac{Ah}{KT}$$

$$= \frac{1.2 \times 10^{10} \times 6.626 \times 10^{-27}}{1.38 \times 10^{-16} \times 350}$$

$$= 0.01646 \times 10^{-1}$$

$$\ln \exp^{\Delta S^*/R} = \ln 1.646 \times 10^{-3}$$

$$\therefore \Delta S^*/R = \ln 1.646 \times 10^{-3}$$

$$\Delta S^* = 1.987 \times 2.303 \times \log 0.001646$$

$$= 1.987 \times 2.303 \times (-2.7835)$$

$$\Delta S^* = -12.73 \text{ cal mol}^{-1} \text{deg}^{-1} \text{(e.u)}$$

Ex. 10 At 558°K the frequency factor (A) for a reaction is found to be 8.7×10^{15} sec^{-1}. calculate the entropy of activation (ΔS^*) Reaction.

2014

Ans:-

$$A = \frac{KT}{h} \exp^{+\Delta S^*/R}$$

$$\therefore \exp^{\Delta S^*/R} = \frac{Ah}{KT}$$

$$= \frac{8.7 \times 10^{15} \times 6.626 \times 10^{-27}}{1.38 \times 10^{-16} \times 558}$$

$$= 0.07486 \times 10^{4}$$

$$= 7.486 \times 10^{2}$$

$$\ln_e \exp^{\Delta S^*/R} = \ln 748.6$$

$$\frac{\Delta S^*}{R} = 2.303 \log 748.6$$

$$\Delta S^* = 2.303 \times 1.987 \times 2.874249823$$

$$\Delta S^* = 13.15 \text{ cal mol}^{-1} \text{deg}^{-1} \text{(e.u)}$$

Ex. 11 If the activation energy of reaction is 80.9 KJ mol^{-1}, calculate the fraction of molecules at 400°c which have energy products.

2015

2017

Q:-13 The energy of activation for the decomposition of N_2O_5 into NO_2, O_2 is 24.7 Kcal mol^{-1}. If the rate constant is 4.0×10^{-5} sec^{-1} at 27°C, calculate the frequency factor A in Arrhenius equation R = 1.987 cal deg^{-1} mole^{-1}

Ans:-

$$K = A\, e^{-E/RT}$$

$$\log k = \log A - \frac{E}{2.303\,RT}$$

$$\therefore \log A = \log k + \frac{E}{2.303\,RT}$$

$$= \log 4.0\times10^{-5} + \frac{24700}{2.303\times1.987\times300}$$

$$= -4.3979 + 17.9921$$

$$\log A = 13.5942$$

$$\therefore A = \text{Antilog}\ (13.5942)$$

$$= 3.928\times10^{13}$$

Ex:14 2018 The energy of activation for the decomposition of N_2O_5 into NO_2 and O_2 is 25.7 K cal. mole^{-1} if the rate constant is 5×10^{-5} sec^{-1} and 27°c calculate the frequency factor (A) In Arrhenius equation. $R = 1.987$ liter atm mol^{-1} deg^{-1}.

Ans:

$$K = A\,e^{-E/RT}$$

$$\log k = \log A - \frac{E}{2.303\,RT}$$

$$\therefore \log A = \log k + \frac{E}{2.303\,RT}$$

$$\therefore\ = \log 5\times10^{-5} + \frac{25700}{2.303\times1.987\times300}$$

$$= -4.3010 + 18.7206$$

$$\log A = 14.4196$$

$$A = \text{Antilog}\ (14.4196)$$

$$A = 2.6278\times10^{14}$$

Ex: 15 calculate the entropy of activation (ΔS^*) for a reaction $H_2 + I_2 \rightleftharpoons 2HI$ at 470°k. The value of frequency (A) is 9×10^{10} sec^{-1}.

Ans:

$$A = \frac{KT}{h}\exp^{\Delta S^*/R}$$

$$\therefore \exp^{\Delta S^*/R} = \frac{AhN}{RT}$$

$$= \frac{9 \times 10^{10} \times 6.626 \times 10^{-27} \times 6.02 \times 10^{23}}{1.987 \times 470}$$

$$= 0.3844 \times 10^{6}$$

$$= 3.844 \times 10^{5}$$

$$\Delta S^{*}/R = 2.303 \times \log 3.844 \times 10^{5}$$

$$\Delta S^{*} = 2.303 \times 1.987 \times \log (384400)$$

$$\Delta S^{*} = 25.55 \text{ cal mol}^{-1} \text{deg}^{-1}$$