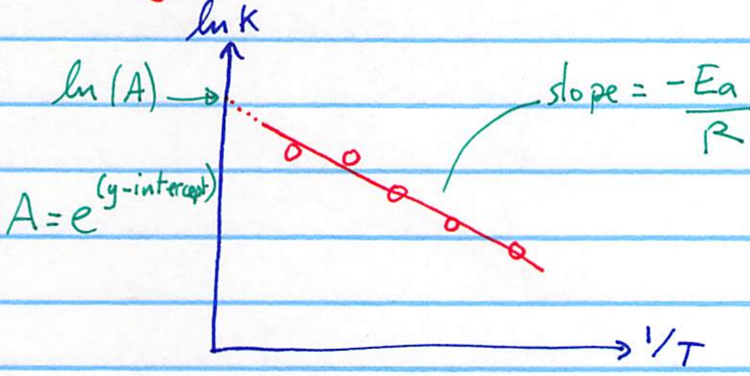
2/27/2019

$$k = Ae^{-E_a/RT}$$

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

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

Arrhenius plot



$\Rightarrow E_a = -R \times \text{slope}$

Data: $O_3 \rightarrow O_2 + O$ (from book).

slope of $\ln k$ vs $1/T$ was -1.12×10^4 K

$$E_a = -R \times \text{slope} = -8.3145 \ \text{J/mol·K} \times -1.12 \times 10^4 \ \text{K}$$

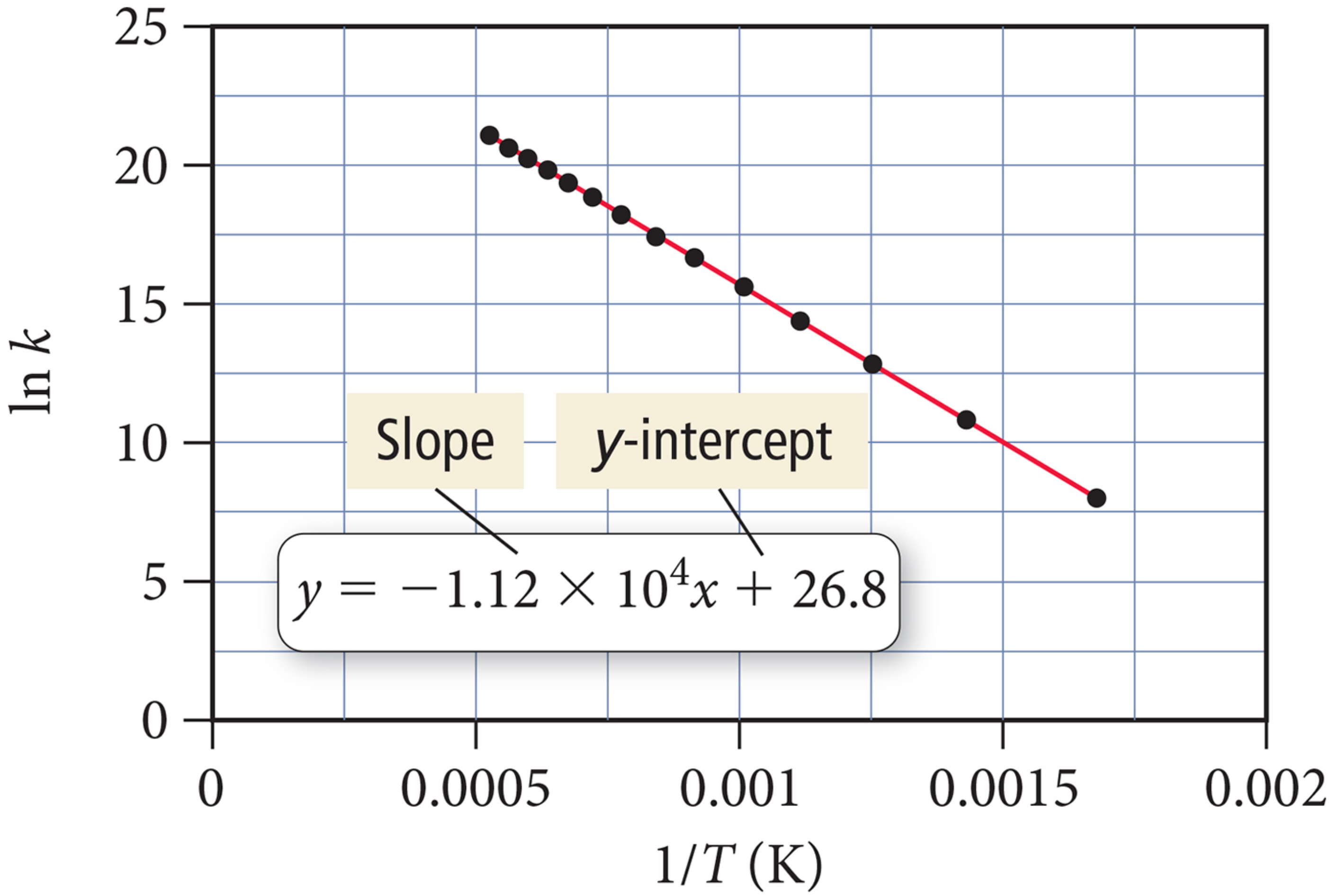
$$= 93{,}100 \ \text{J/mol}$$

$$= 93.1 \times 10^3 \ \text{J/mol} = 93.1 \ \text{kJ/mol}$$

A? $\ln A = \text{y-intercept} = 26.8 \Rightarrow A = e^{26.8} = 4.36 \times 10^{11}$

(has units: $M^{-1}s^{-1}$ ... read book)

Temperature (K)	Rate Constant ($M^{-1} \cdot s^{-1}$)	Temperature (K)	Rate Constant ($M^{-1} \cdot s^{-1}$)
600	3.37×10^3	1300	7.83×10^7
700	4.85×10^4	1400	1.45×10^8
800	3.58×10^5	1500	2.46×10^8
900	1.70×10^6	1600	3.93×10^8
1000	5.90×10^6	1700	5.93×10^8
1100	1.63×10^7	1800	8.55×10^8
1200	3.81×10^7	1900	1.19×10^9



25
20
15
10
5
0
ln k
0
0.0005
0.001
0.0015
0.002
1/T (K)
Slope
y-intercept
y = −1.12 × 10^4x + 26.8

Common to use a 2-point method to solve for E_a and A

$$K = A e^{-E_a/RT} \xrightarrow{\ln} \ln K = \ln A + \ln\left(e^{-E_a/RT}\right)$$

$$\Rightarrow \ln K_2 = \ln A - \left(\frac{E_a}{R}\right)\frac{1}{T_2}$$

K_1 @ T_1

K_2 @ T_2

$(-)$

$$\ln K_1 = \ln A - \left(\frac{E_a}{R}\right)\frac{1}{T_1}$$

$\ln A - \ln B = \ln \frac{A}{B}$

$$\ln K_2 - \ln K_1 = \left[\ln A - \left(\frac{E_a}{R}\right)\frac{1}{T_2}\right] - \left[\ln A - \left(\frac{E_a}{R}\right)\frac{1}{T_1}\right]$$

$$\ln\left(\frac{K_2}{K_1}\right) = -\left(\frac{E_a}{R}\right)\left[\frac{1}{T_2} - \frac{1}{T_1}\right]$$

OR:

$$\boxed{\ln\left(\frac{K_2}{K_1}\right) = \frac{E_a}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)}$$

$\frac{K_2}{K_1} = 2$ (exact)

ex: if rate constant for a rxn doubles as temp increases from 25°C to 29°C ~ What's E_a?

t_1 = 25°C, t_2 = 29°C

$T_1 = 25 + 273.15 = 298.15\,K$

$T_2 = 29 + 273.15 = 302.15\,K$

$$\frac{R \times \ln\left(\frac{K_2}{K_1}\right)}{\left(\frac{1}{T_1} - \frac{1}{T_2}\right)} = E_a = \frac{\left(8.3145\ J/mol\cdot K\right) \times \ln(2)}{\left(\frac{1}{298.15\,K} - \frac{1}{302.15\,K}\right)}$$

$= 130. \times 10^3\ J/mol = 130.\ kJ/mol$

(most E_a's are : 10's – 100's kJ/mol)