Chemical Kinetics Assignment 2
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Q1) Given reaction

$$E + S \underset{k_a'}{\overset{k_a}{\rightleftharpoons}} ES \underset{k_b'}{\overset{k_b}{\rightleftharpoons}} P + E$$

at steady state

$$\frac{d[ES]}{dt} = 0 \Rightarrow -k_b[ES] + k_b'[P][E] + k_a[E][S] - k_a'[ES] = 0$$

$$\therefore \boxed{[ES] = \frac{k_b'[E][P]}{k_b + k_a'} + \frac{k_a[E][S]}{k_b + k_a'}}$$

also $[ES] + [E] = [E]_0$ (total mass remains same only changes form)

$$\therefore [E]_0 - [E] = [E]\left[\frac{k_b'[P]}{k_b + k_a'} + \frac{k_a[S]}{k_b + k_a'}\right]$$

$$\Rightarrow \boxed{[E] = [E]_0\left(\frac{k_b + k_a'}{k_b'[P] + k_a[S] + k_b + k_a'}\right)}$$

$$\text{rate} = v = \frac{d[P]}{dt} = k_b[ES] - k_b'[P][E]$$

$$v = \frac{k_b k_b'}{k_a' + k_b}[E][P] + \frac{k_b k_a}{k_b + k_a'}[E][S] - k_b'[P][E]$$

$$v = \frac{+k_b k_a}{k_b + k_a'}[E][S] - \frac{k_a' k_b'[P][E]}{k_b + k_a'}$$

$$= \frac{k_b[E]}{k_b + k_a'}\left[-k_a'[P] + k_a[S]\right)$$

$$v = \frac{(k_b)[E_0])(k_a[S] - k_a'[P])}{(k_b'[P] + k_a[S] + k_b + k_a')}$$

$$V = \frac{V_{max}\left(1 - \frac{K_a'[P]}{K_a[S]}\right)}{\frac{K_b'[P]}{K_a[S]} + K_a + \left(\frac{K_b + K_a'}{[S]}\right)}$$

$\therefore$ $V = V_{max}$ given $[S] >> [P]$

or $[P]/[S] \to 0$.

$$V = \frac{V_{max}(1-0)}{1 + \frac{K_m}{[S]}} \rightarrow$$ Michaelis Menten equation

where $K_m = \dfrac{K_b + K_a'}{K_a}$.

Q2) For one photon $E = hc/\lambda$

given $\lambda = 207$ nm.

$$\therefore E = \frac{6.626\times10^{-34} \times (3\times10^{8})}{(207)\times10^{-9}} J.$$

$\boxed{E = 9.6\times10^{-19} J}$ → for one photon

↳ No. of photons for 1 J = $1/9.6\times10^{-19}$

$= \boxed{10.4\times10^{17}}$

Molar mass of HI = 254.8 g

$\therefore$ No. of molecules of HI in 440×10^{-6} g

$$= \frac{440\times10^{-6}}{254.8} \times 6.022\times10^{23}$$

$= \boxed{10.4\times10^{17}}$

$\therefore$ we can say that one photon decomposes 1 molecule of HI

$$2HI + 2h\nu \rightarrow H_2 + I_2$$

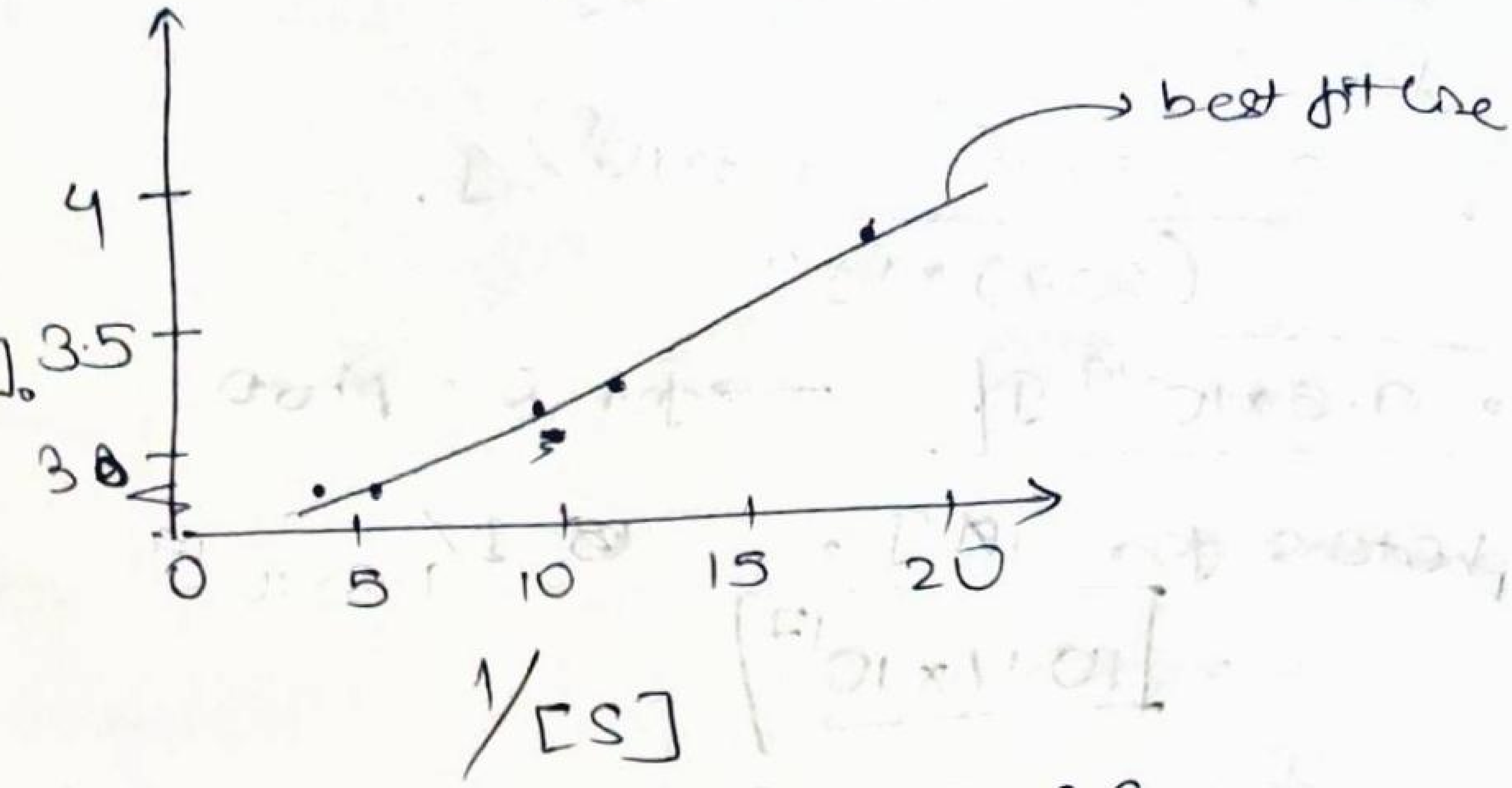
A possible mechanism is:

$$HI + h\nu \rightarrow H^+ + I^-$$
$$HI + h\nu \rightarrow H^+ + I^-$$
$$H^+ + H^+ \rightarrow H_2$$
$$I^- + I^- \rightarrow I_2$$

Q3) In michaelis menten kinetics, in the absence of an inhibitor

$$\frac{1}{V} = \frac{1}{V_{max}} + \left(\frac{K_m}{V_{max}}\right)\frac{1}{[S]}$$

On plotting the data, we get:



intercept = $1/v_{max}$ = 2.188

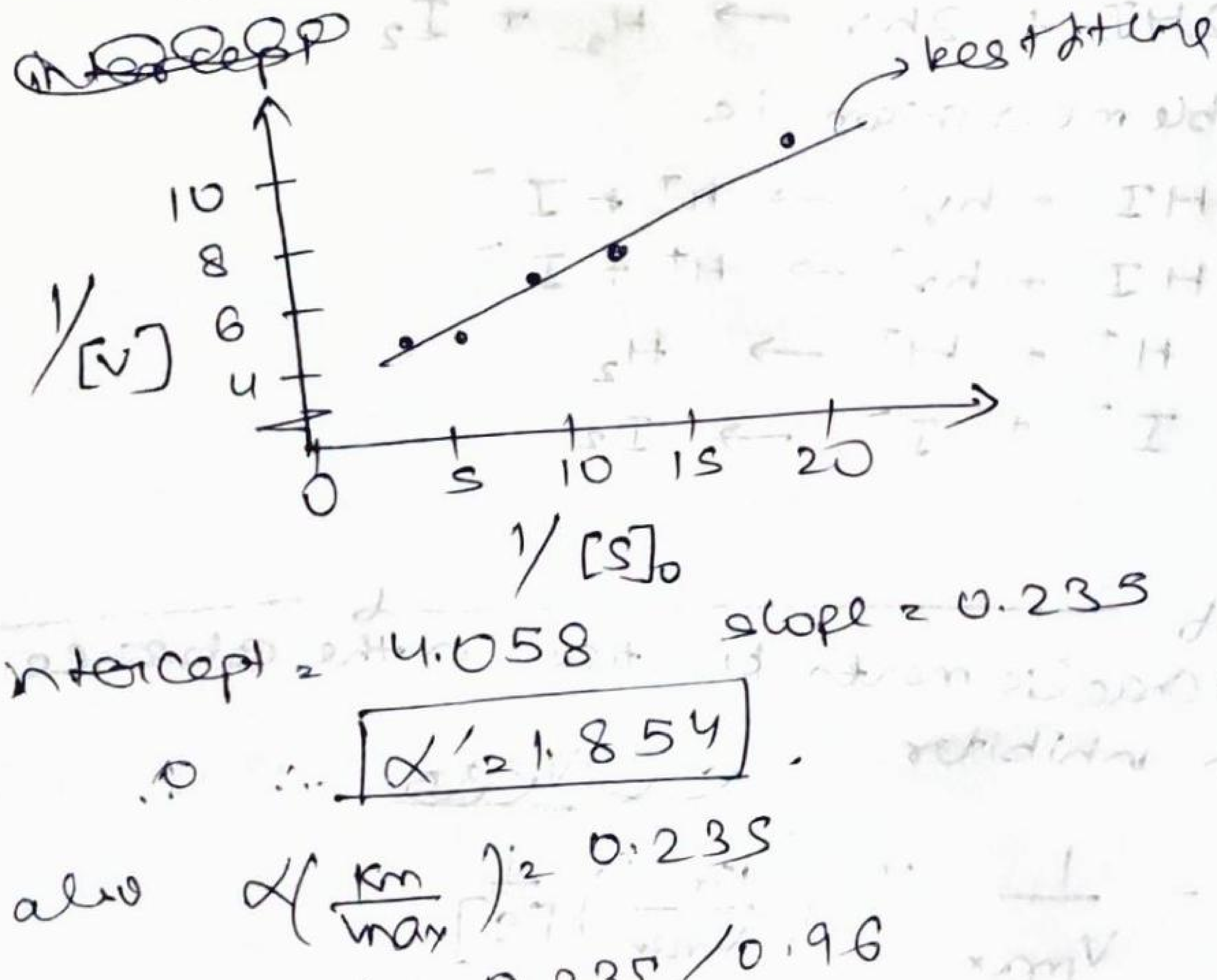
$\therefore$ $\boxed{v_{max} = 0.457 \text{ mol } l^{-1} s^{-1}}$

slope = $\frac{K_m}{v_{max}}$ = 0.096

$\therefore$ $\boxed{K_{max} = 0.044 \text{ mol } l^{-1}}$

b) Doing the same for 2M Urea

~~intercept~~



intercept = 4.058 slope = 0.235

$\therefore$ $\boxed{\alpha' = 1.854}$

also $\alpha\left(\frac{K_m}{v_{max}}\right) = 0.235$

$\therefore$ $\alpha = 0.235/0.96$

$\boxed{\alpha = 0.2448}$

as both α' & $\alpha > 1$ therefore we can conclude that Urea is a non competitive inhibitor

Q4) a) $E_{photon} = \frac{hc}{\lambda} = \frac{6.626 \times 10^{-34} \times 3 \times 10^{8}}{680 \times 10^{-9}}$

$E = 2.923 \times 10^{-19}$ J. ~~/~~ photon

$= 2.923 \times 10^{-19} \times 6.022 \times 10^{23}$ J / Einstein

$\boxed{E = 17.602 \times 10^{4} \text{ J/ einstein}}$

b) $\Delta H_r = 116$ Kcal/mol

$= 116 \times 4184$ J/mol

$= 48.53 \times 10^{4}$ J/mol.

$\therefore$ Minimum no. of einsteins of radiation required for 1mol

$\frac{48.53}{17.602} \times \frac{\cancel{10^4}}{\cancel{10^4}} = 2.76$

but integer $\therefore$ $\boxed{3}$

c) Quantum yield ϕ

$= \frac{\text{No. of reactant formed}}{\text{No. of photons absorbed.}}$

$\frac{\cancel{N_A}}{9(\cancel{N_A})} \leq \phi \leq \frac{\cancel{N_A}}{8(\cancel{N_A})}$

$= \boxed{0.11 \leq \phi \leq 0.125}$

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