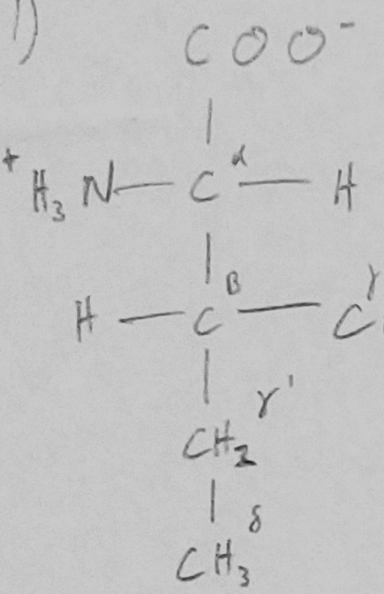
Arthur Zhou
10/3/24

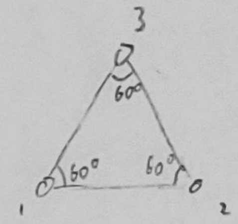
BioE 100 Hw 1

1)



d) $\boxed{\text{Rotamer}}$

e)



$$\phi_{LJ} = -\beta \frac{1}{r^6} + \delta \frac{1}{r^{12}}$$

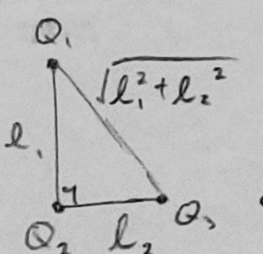
$\boxed{\text{Decrease}}$ since β has a "-" sign. As all β increases it'll reduce overall PE.

f) Covalent bonds aren't broken during the minimization procedures

2) $\boxed{\text{Equilibrium}}$, since we are investigating the final status of the water after a long time. Kinetic phenomenon analyze the rate of change / gradient and we are only looking at final state.

3) $\boxed{\text{Gln , Gl}}$

4)



$$PE = \phi_{12} + \phi_{13} + \phi_{23}$$

$$\phi_e = k\frac{Q_1 Q_2}{r}$$

$$\phi_{LJ} = -\beta \frac{1}{r^6} + \delta \frac{1}{r^{12}}$$

$$\boxed{\begin{aligned}\phi_{12}&\left\{ = k\frac{Q_1 Q_2}{l_1} - \beta_{12}\frac{1}{l_1^6} + \delta_{12}\frac{1}{l_1^{12}}\right.\\ \phi_{13}&\left\{ + k\frac{Q_1 Q_3}{\sqrt{l_1^2+l_2^2}} - \beta_{13}\frac{1}{(\sqrt{l_1^2+l_2^2})^6} + \delta_{13}\frac{1}{(\sqrt{l_1^2+l_2^2})^{12}}\right.\\ \phi_{23}&\left\{ + k\frac{Q_2 Q_3}{l_2} - \beta_{23}\frac{1}{l_2^6} + \delta_{23}\frac{1}{l_2^{12}}\right.\end{aligned}}$$

5)

a) Internal energy comprises of translational, rotational, & kinetic energy of the molecules. Bonds such as covalent bonds also store energy as well as other inter/intramolecular interactions.

b) $\boxed{\text{Equilibrium}}$, since we are only looking at the steady / final state

c) $\vec{F}_e = -\vec\nabla \phi_e$ $\qquad \phi_{LJ} = -\beta\frac{1}{r^6} + \underbrace{\delta\frac{1}{r^{12}}}_{\text{excluded volume}} = \delta\frac{1}{r^{12}}$

Since spherical $\frac{\partial \phi_e}{\partial \theta} = \frac{\partial \phi_e}{\partial \phi} = 0$ $\qquad \boxed{\vec{F}_e(l) = 12\delta r^{-13}\hat{r}}$

$$\vec{F}_e = -\vec\nabla \phi_e = \frac{-d}{dr}\left(\delta\frac{1}{r^{12}}\hat{r}\right) = +12\delta r^{-13}\hat{r}$$

6) $P = 2r^{\frac{1}{2}} + 5\theta^2\phi^3$

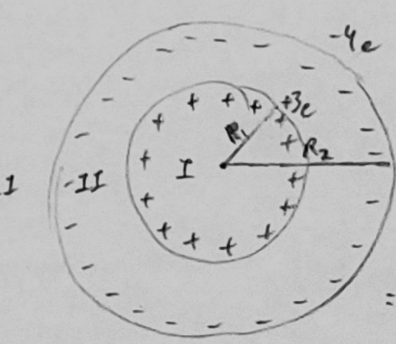
$$\vec{F} = -\vec\nabla P = -\left(\frac{\partial P}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial P}{\partial \theta}\hat\theta + \frac{1}{r\sin\theta}\frac{\partial \phi}{\partial \theta}\hat\phi\right)$$

$$= -\left[\frac{\partial}{\partial r}(2r^{\frac12} + 5\theta^2\phi^3)\hat{r} + \frac{1}{r}\frac{\partial}{\partial\theta}(2r^{\frac12} + 5\theta^2\phi^3)\hat\theta + \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}(2r^{\frac12} + 5\theta^2\phi^3)\hat\phi\right]$$

$$= -\left[r^{-\frac12}\hat{r} + \frac{1}{r}\cdot 10\theta\phi^3\hat\theta + \frac{1}{r\sin\theta}\cdot 15\theta^2\phi^2\hat\phi\right]$$

$$\boxed{= -r^{-\frac12}\hat{r} - \frac{10\theta\phi^3}{r}\hat\theta - \frac{15\theta^2\phi^2}{r\sin\theta}\hat\phi}$$

7)



$r = R_1^+$: $\varepsilon_{II}\oint \vec{E}\cdot d\vec{s} = \frac{Q}{\varepsilon_0}$

$$\Rightarrow \oint\left[-\frac{d\varphi}{dr}\Big|_{R_1^+}\hat{r}\right]ds(\hat{r}) = \frac{Q}{\varepsilon_0\varepsilon_{II}}$$

$$\Rightarrow -\frac{d\varphi}{dr}\Big|_{R_1^+}\oint \hat{r}\cdot\hat{r}\,ds = \frac{Q}{\varepsilon_0\varepsilon_{II}}$$

$$\Rightarrow \boxed{\frac{d\varphi}{dr}\Big|_{R_1^+} = \frac{-3e}{4\pi R_1^2\varepsilon_0\varepsilon_{II}}}$$

$r = R_2^+$: $\varepsilon_{III}\oint \vec{E}\cdot d\vec{s} = \frac{Q}{\varepsilon_0}$

$$\Rightarrow \oint\left[-\frac{d\varphi}{dr}\Big|_{R_2^+}\hat{r}\right]ds(\hat{r}) = \frac{-e}{\varepsilon_{III}\varepsilon_0}$$

$Q = -4e + 3e = -e$

$$\Rightarrow -\frac{d\varphi}{dr}\Big|_{R_2^+}\oint \hat{r}\cdot\hat{r}\,ds = \frac{-e}{\varepsilon_{III}\varepsilon_0}$$

$$\Rightarrow -\frac{d\varphi}{dr}\Big|_{R_2^+}\cdot 4\pi R_2^2 = \text{"}$$

$$\Rightarrow \boxed{\frac{d\varphi}{dr}\Big|_{R_2^+} = \frac{+e}{4\pi R_2^2\varepsilon_{III}\varepsilon_0}}$$

8) $\phi_{tot} = \phi_{12} + \phi_{13} + \phi_{14} + \phi_{23} + \phi_{24} + \phi_{34}$

$$\begin{cases} = -\beta_{12}\frac{1}{\ell_1^6} + \delta_{12}\frac{1}{\ell_1^{12}} - \beta_{13}\frac{1}{(\ell_1^2+\ell_2^2)^3} + \delta_{13}\frac{1}{(\ell_1^2+\ell_2^2)^6} \\ -\beta_{14}\frac{1}{\ell_2^6} + \delta_{14}\frac{1}{\ell_2^{12}} - \beta_{23}\frac{1}{\ell_2^6} + \delta_{13}\frac{1}{\ell_2^{12}} \\ -\beta_{24}\frac{1}{(\ell_1^2+\ell_2^2)^3} + \delta_{34}\frac{1}{(\ell_1^2+\ell_2^2)^6} - \beta_{34}\frac{1}{\ell_1^6} + \delta_{34}\frac{1}{\ell_1^{12}} \end{cases}$$

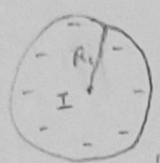
9) $\oint \vec{E}\cdot d\vec{s} = \frac{-3e}{\varepsilon_{II}\,\varepsilon_0}$

$\Rightarrow \oint -\frac{\partial\psi}{\partial r}\Big|_{R_1^+}\hat{r}\cdot ds(\hat{r}) = \frac{-3e}{\varepsilon_{II}\,\varepsilon_0}$

$\Rightarrow -\frac{\partial\psi}{\partial r}\Big|_{R_1^+}\oint \hat{r}/\hat{r}\, ds = {}''$

$\Rightarrow -\frac{\partial\psi}{\partial r}\Big|_{R_1^+}\oint ds = \frac{\partial\psi}{\partial r}\Big|_{R_1^+} 2\pi R_1 L = {}''$

$\Rightarrow +\frac{\partial\psi}{\partial r}\Big|_{R_1^+} = \frac{+3e}{2\pi R_1 L\,\varepsilon_{II}\,\varepsilon_0}$



cylindrical:

$\nabla\psi = \frac{\partial\psi}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial\psi}{\partial\theta}\hat{\theta} + \frac{\partial\psi}{\partial z}\hat{z}$

$\vec{E} = -\vec{\nabla}\phi = \frac{\partial\psi}{\partial r}\hat{r}$

Inward, since $\hat{r}$ is NEGATIVE!

$$\boxed{\vec{E}\Big|_{R_1^+} = -\frac{\partial\psi}{\partial r}\Big|_{R_1^+}\hat{r} = \frac{-3e}{2\pi R_1 L\,\varepsilon_{II}\,\varepsilon_0}\hat{r}}$$

10) $\boxed{\text{Lys, K}}$

1) REMINDER: $\frac{\partial\psi}{\partial\theta} = \frac{\partial\psi}{\partial\phi} = 0$

$\vec{\nabla}\phi = \frac{\partial\psi}{\partial r}\hat{r}$, $\vec{F} = -\vec{\nabla}\phi$

$\phi_{13} = \frac{-\beta_{13}}{(\ell_1^2+\ell_2^2)^3} + \frac{\delta_{13}}{(\ell_1^2+\ell_2^2)^6}$

$\vec{F} = -\vec{\nabla}\phi = -\frac{\partial}{\partial r}(\quad)\hat{r}$

$$\boxed{= \left(-6\frac{\beta_{13}}{(\ell_1^2+\ell_2^2)^{3.5}} + 12\frac{\delta_{13}}{(\ell_1^2+\ell_2^2)^{6.5}}\right)\hat{r}}$$

12)

a) $\boxed{\text{Yes}}$, covalent bonds store potential energy

b) $\boxed{\text{London}}$

c) Phenylalanine, Tyrosine, Tryptophan

d) Translational, rotational, kinetic energy
Covalent bonds potential energy
Energy within inter & intramolecular reactions

13)

a) $\boxed{1.4\text{A}}$

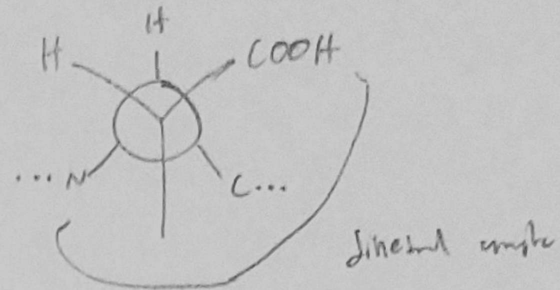
b) $\boxed{\text{Equilibrium}}$, since you are only looking at state of final result

c) The $\boxed{\text{electrons}}$

d) $\boxed{\text{True}}$

e) $\boxed{\text{Red}}$

f) $\boxed{\text{Aspartic Acid}}$



14) $\frac{\partial\phi}{\partial\theta} = \frac{\partial\phi}{\partial\phi} = 0 \longrightarrow \nabla\phi = \frac{\partial\phi}{\partial r}$

$\vec{E} = -\nabla\phi = -\frac{\partial\phi}{\partial r}$

$\varepsilon_{II}\oint \vec{E}\cdot d\vec{s} = \frac{5e}{\varepsilon_0}$

$\Rightarrow -\oint\left[\frac{\partial\psi}{\partial r}\Big|_{R_1^+}\hat{r}\right]ds(\hat{r}) = \frac{5e}{\varepsilon_{II}\,\varepsilon_0}$

$\Rightarrow -\frac{\partial\phi}{\partial r}\Big|_{R_1^+}\oint \hat{r}/\hat{r}\,ds = \frac{5e}{\varepsilon_{II}\,\varepsilon_0}$

$$\Rightarrow \boxed{+\frac{\partial\psi}{\partial r}\Big|_{R_1^+} = \frac{-5e}{4\pi R_1^2\,\varepsilon_{II}\,\varepsilon_0}}$$

15)

a) $\boxed{\text{KINETIC}}$

b) $\boxed{\text{BOTH}}$