

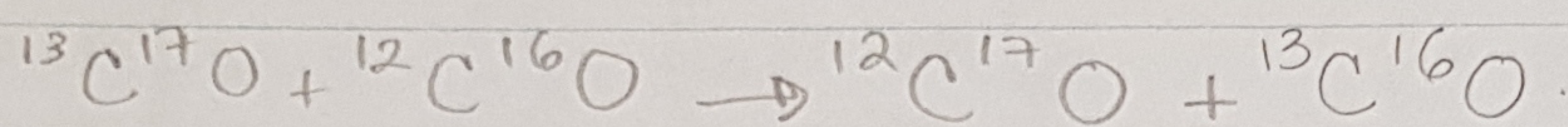
Assignment (21)

① $E_J = \frac{\hbar^2 J(J+1)}{2\mu r_e^2}$, $\mu_{^{12}_6\text{C}-^{16}_8\text{O}} < \mu_{^{14}_6\text{C}-^{18}_8\text{O}} \rightarrow \Delta E_{J, ^{12}_6\text{C}-^{16}_8\text{O}} > \Delta E_{J, ^{14}_6\text{C}-^{18}_8\text{O}}$.

The rotational levels of $^{12}_6\text{C}-^{16}_8\text{O}$ have a bigger spacing between the energy levels.

② The trial function has the exact right form of the solutions for the harmonic oscillator, so its ground state energy is given by $E_0 = \frac{1}{2} \hbar \nu_0 = \frac{1}{2} (6.026 \times 10^{-34} \text{ J}\cdot\text{s}) (6.42 \times 10^{13} \text{ Hz}) = 2.127 \times 10^{-20} \text{ J}$.

③ $r_e = 113.1 \text{ pm}$
 $k = 1902 \text{ N/m}$



$\Delta H^\circ ?$

$E_{\text{vib}} = \frac{1}{2} \hbar \omega_0 = \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}}$

$\mu(^{13}\text{C}^{17}\text{O}) = \frac{13 \cdot 17}{13+17} = 7.3667 \text{ amu}$

$\rightarrow E_{\text{vib}}(^{13}\text{C}^{17}\text{O}) = \frac{1}{2} \hbar \sqrt{\frac{1902 \text{ N/m}}{(7.3667)(1.66 \times 10^{-27} \text{ kg})}} = 1.188 \times 10^{-19} \text{ J}$

$\mu(^{12}\text{C}^{16}\text{O}) = \frac{12 \cdot 16}{12+16} = 6.8571 \text{ amu}$

$\rightarrow E_{\text{vib}}(^{12}\text{C}^{16}\text{O}) = 1.232 \times 10^{-19} \text{ J}$

$\mu(^{12}\text{C}^{17}\text{O}) = \frac{12 \cdot 17}{12+17} = 7.0345 \text{ amu}$

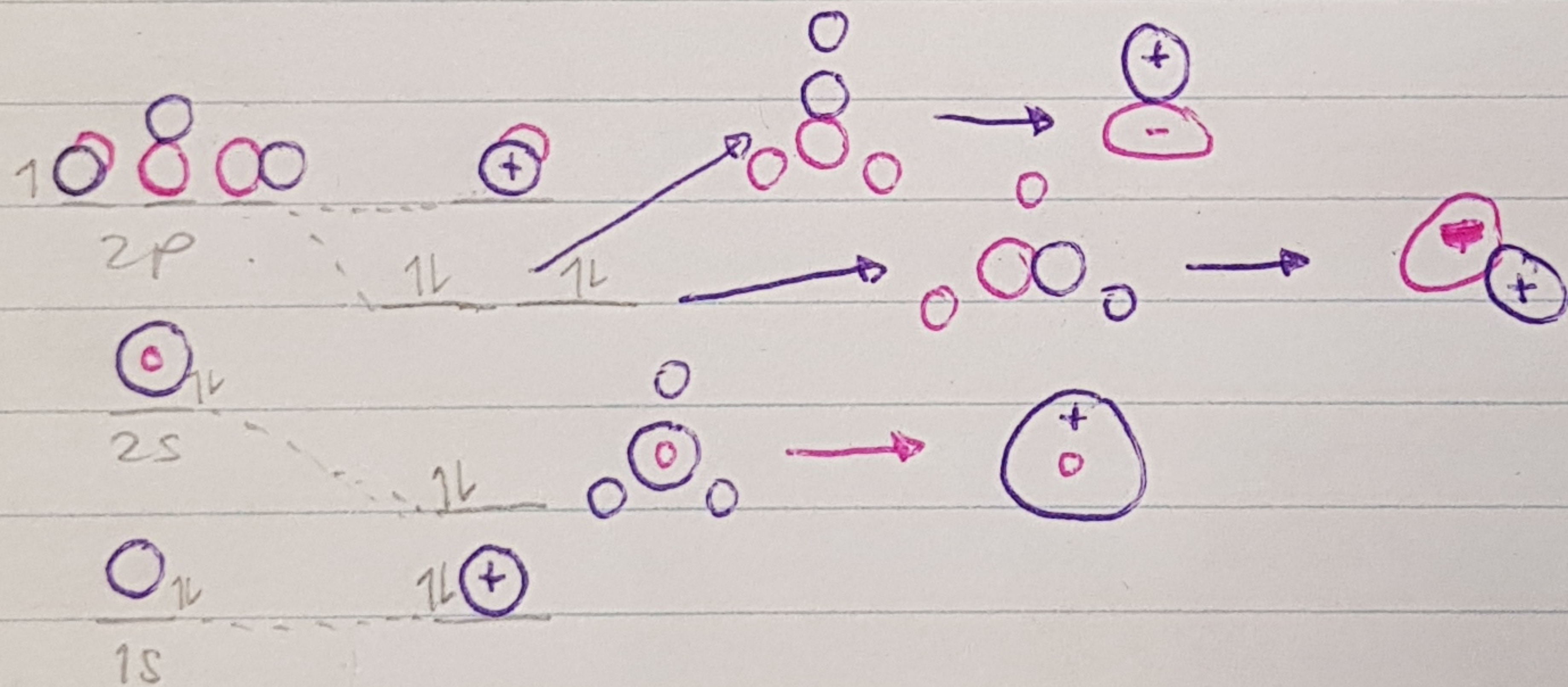
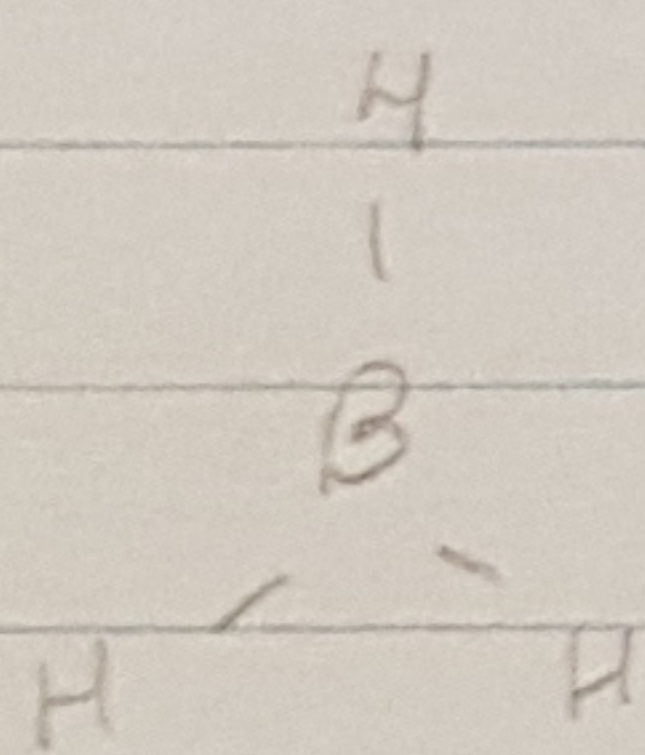
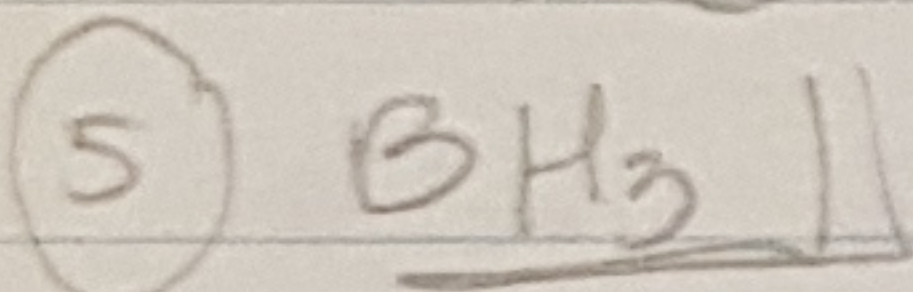
$\rightarrow E_{\text{vib}}(^{12}\text{C}^{17}\text{O}) = 1.216 \times 10^{-19} \text{ J}$

$\mu(^{13}\text{C}^{16}\text{O}) = \frac{13 \cdot 16}{13+16} = 7.1724 \text{ amu}$

$\rightarrow E_{\text{vib}}(^{13}\text{C}^{16}\text{O}) = 1.204 \times 10^{-19} \text{ J}$

$\Delta H^\circ = E_{\text{vib}}(^{12}\text{C}^{17}\text{O}) + E_{\text{vib}}(^{13}\text{C}^{16}\text{O}) - E_{\text{vib}}(^{13}\text{C}^{17}\text{O}) - E_{\text{vib}}(^{12}\text{C}^{16}\text{O})$
 $= 0 \text{ J}$

- ④ a) P
b) A
c) S
d) O



⑥ $1s^1 2s^1 2p^1$

$L = 1$

$S = \frac{3}{2}$

$J = M_J = \frac{5}{2}$

$M_J = \frac{5}{2} \rightarrow M_J = M_L + M_S$

M_L can only be +1, $M_S = \frac{3}{2} \rightarrow$ all electrons are alpha

$|\Psi_{1s2s2p}\rangle = \frac{1}{\sqrt{3!}} \begin{bmatrix} \psi_{1s}(\vec{r}_1) \alpha(1) & \psi_{2s}(\vec{r}_1) \alpha(1) & \psi_{2p}(\vec{r}_1) \alpha(1) \\ \psi_{1s}(\vec{r}_2) \alpha(2) & \psi_{2s}(\vec{r}_2) \alpha(2) & \psi_{2p}(\vec{r}_2) \alpha(2) \\ \psi_{1s}(\vec{r}_3) \alpha(3) & \psi_{2s}(\vec{r}_3) \alpha(3) & \psi_{2p}(\vec{r}_3) \alpha(3) \end{bmatrix}$