Adam Alemayehu

1) a) $(1,1,1) \rightarrow (2,1,1)$ $L_x = L_y = L_z = L = 100\,\text{Å}$

$$E_{(1,1,1)} = \frac{\hbar^2\pi^2}{2mL^2}\left(1^2 + 1^2 + 1^2\right) = \frac{3\hbar^2\pi^2}{2mL^2}$$

$$E_{(2,1,1)} = \frac{\hbar^2\pi^2}{2mL^2}\left(2^2 + 1^2 + 1^2\right) = \frac{6\hbar^2\pi^2}{2mL^2}$$

$$\Delta E = E_{2,1,1} - E_{1,1,1} = \frac{3\hbar^2\pi^2}{2mL^2} = \frac{hc}{\lambda}$$

$$\lambda = \frac{2hcmL^2}{3\hbar^2\pi^2}$$

$$\boxed{\begin{array}{l} \lambda_1 = \cancel{2787\,nm} \\ 1{,}1 \cdot 10^{-4}\,m = \\ \hline 1{,}1 \cdot 10^{-6}\,m \\ \lambda_2 = 0{,}\cancel{2787\,nm} \end{array}}$$

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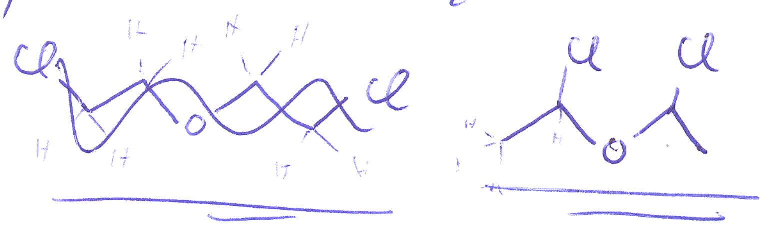
b) Energia prechodu je nepriamo úmerná druhej mocnine veľkosti krabice:

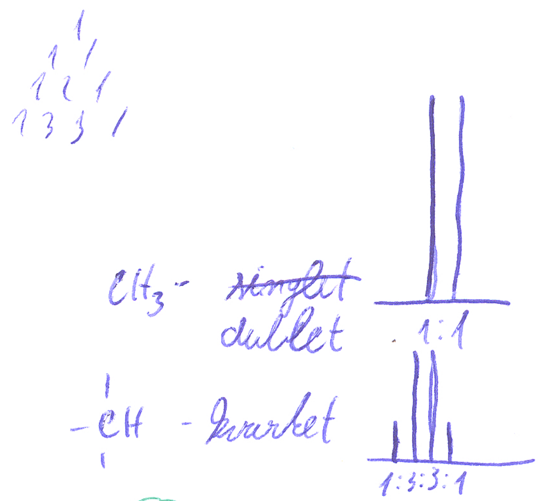
$$\Delta E = \frac{\hbar^2\pi^2}{2mL^2}\left(n_{x_2}^2 + n_{y_2}^2 + n_{z_2}^2 - n_{x_1}^2 - n_{y_1}^2 - n_{z_1}^2\right)$$

2) $C_4H_8Cl_2O$ $SU = \frac{8-8-2+2}{2} = 0$

a)



b)

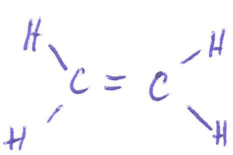


CH_3 - ~~singlet~~ dublet

-CH - kvartet

3

3.)



vib. módov $= 3N - 6 = 3 \cdot 6 - 6 = $ 12 vib. módov

$N = 6$

nemení sa dip. moment.

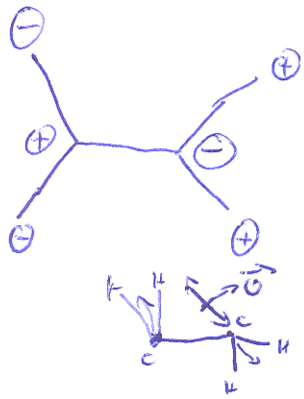
$\frac{d\mu}{dR} = 0 \Rightarrow$ nepozorujeme v IČ

$\frac{d\alpha}{dR} \neq 0 \Rightarrow$ pozorujeme v Ramanovom

$\frac{d\mu}{dR} \neq 0 \Rightarrow$ pozorovaní v IČ

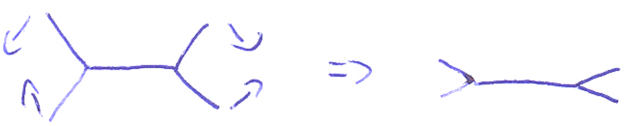
$\frac{d\alpha}{dR} = 0 \Rightarrow$ nepozorujeme v Ramanovom

mení sa ~~dip. mom.~~ dipólový moment



$\frac{d\mu}{dR} = 0 \Rightarrow$ nepozorujeme v IČ

$\frac{d\alpha}{dR} \neq 0 \Rightarrow$ pozorujeme v Ramanovej sp.



$\frac{d\mu}{dR} = 0 \Rightarrow$ nepozorujeme v IČ

$\frac{d\alpha}{dR} \neq 0 \Rightarrow$ pozorujeme v Ramanovom sp.

nedochádza k zmene μ

3

4.) $\tilde{\nu} = 19960{,}5\,cm^{-1}$

$\tilde{\nu}_{foton} = 17602{,}5\,cm^{-1}$

$\tilde{\nu}_{vib} = ?$

$k = ?$

$\tilde{\nu}_{vib} = \tilde{\nu} - \tilde{\nu}_{foton}$

$\tilde{\nu}_{vib} = 19960{,}5\,cm^{-1} - 17602{,}5\,cm^{-1}$

$\underline{\tilde{\nu}_{vib} = 2358\,cm^{-1}}$

"$N \equiv N$"

$$\tilde{\nu}_{vib} = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}}$$

$$\mu = \frac{m_N \cdot m_N}{m_N + m_N} = \frac{m_N}{2} = \frac{Ar_N}{2} \cdot m_u = \frac{14}{2} \cdot 1{,}66 \cdot 10^{-27}\,kg = 1{,}162 \cdot 10^{-26}\,kg$$

$$\tilde{\nu}_{vib}^2 = \frac{1}{4\pi^2 c^2}\frac{k}{\mu} \Rightarrow k = 4\pi^2 c^2 \tilde{\nu}_{vib}^2 \mu$$

$$k = 4 \cdot \pi^2 \cdot 9 \cdot 10^{16}\,m^2 s^{-2} \cdot 235800^2\,m^{-2} \cdot 1{,}162 \cdot 10^{-26}\,kg$$

$$\underline{k = 2293{,}3\,N\,m^{-1}}$$

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5.) $E_i = 3{,}44\cdot 10^{-18}\,J$

~~λ~~

$v = 1{,}03\cdot 10^{6}\,ms^{-1}$

$\tilde{\nu} = ?$

$$hc\tilde{\nu} = E_i + \frac{1}{2}mv^2$$

$$\tilde{\nu} = \frac{E_i + \frac{1}{2}mv^2}{hc}$$

$$\tilde{\nu} = \frac{3{,}44\cdot 10^{-18}J + \frac{1}{2}\cdot 9{,}1\cdot 10^{-31}kg\cdot (1{,}03\cdot 10^{6}ms^{-1})^2}{6{,}63\cdot 10^{-34}Js\cdot 3\cdot 10^{8}ms^{-1}}$$

$$\tilde{\nu} = 197220{,}2\,cm^{-1}$$

3

6.) a) $f(x) = \cos(kx)$ $\quad \hat{\Omega} = \frac{d^2}{dx^2}$

$\hat{\Omega} f(x) = \omega f(x)$

$$\hat{\Omega} f(x) = \frac{d}{dx}\left(\frac{d}{dx}\cos(kx)\right) = -k\frac{d}{dx}(\sin(kx)) = -k^2\cos(kx) =$$

$$= -k^2 f(x)$$ $\blacksquare$ $\quad \omega = -k^2$ -vlastná hodnota

b) $$\frac{w\cdot z}{w+z} = \frac{(1+2i)\cdot(-i)}{1+2i-i} = \frac{-i+2}{1+i} = \frac{2-i}{1+i}\cdot\frac{1-i}{1-i} = \frac{2-2i-i-1}{1+1} = \frac{1-3i}{2} = \frac{1}{2} - \frac{3}{2}i$$

$$\frac{w\cdot z}{w+z} = \frac{1}{2} - \frac{3}{2}i$$

3

7.) a) $[\hat{x},\hat{p}_x]\psi = \hat{x}\hat{p}_x\psi - \hat{p}_x\hat{x}\psi = x\left(-i\hbar\frac{\partial\psi}{\partial x}\right) - \left(-i\hbar\frac{\partial}{\partial x}\right)x\psi = \cancel{-i\hbar x\frac{\partial\psi}{\partial x}} + i\hbar\psi + \cancel{i\hbar x\frac{\partial\psi}{\partial x}} = i\hbar\psi$ ⇒ nekomutujú ⇒ veličiny x a p_x nie sú súčasne merateľné

b) $[\hat{x};\hat{p}_z]\psi = \hat{x}\hat{p}_z\psi - \hat{p}_z\hat{x}\psi = x\left(-i\hbar\frac{\partial\psi}{\partial z}\right) - \left(-i\hbar\frac{\partial}{\partial z}\right)x\psi = -i\hbar x\frac{\partial\psi}{\partial z} + i\hbar x\frac{\partial\psi}{\partial z} = 0$ ⇒

⇒ komutujú - x a p_z sú súčasne merateľné

c) $[\hat{L}_x, \hat{L}_y]\psi$

$$\hat{\vec{L}} = -i\hbar(\vec{r}\times\nabla) = -i\hbar \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x & y & z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z}\end{vmatrix} = -i\hbar\left[\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\vec{i} + \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\vec{j} + \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\vec{k}\right]$$

$$[\hat{L}_x, \hat{L}_y]\psi = \hat{L}_x\hat{L}_y\psi - \hat{L}_y\hat{L}_x\psi = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(-i\hbar\left(z\frac{\partial\psi}{\partial x} - x\frac{\partial\psi}{\partial z}\right)\right) + i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(-i\hbar\left(y\frac{\partial\psi}{\partial z} - z\frac{\partial\psi}{\partial y}\right)\right) = -\hbar^2\left[y\frac{\partial\psi}{\partial x} + yz\frac{\partial^2\psi}{\partial x\partial z} - yx\frac{\partial^2\psi}{\partial z^2} - z^2\frac{\partial^2\psi}{\partial x\partial z} - z\frac{\partial\psi}{\partial x} - z^2\frac{\partial^2\psi}{\partial x\partial y} + zx\frac{\partial^2\psi}{\partial z\partial y}\right]$$

$$+\hbar^2\left[zy\frac{\partial^2\psi}{\partial z\partial x} - z\frac{\partial\psi}{\partial y} - z^2\frac{\partial^2\psi}{\partial y\partial z} - xy\frac{\partial^2\psi}{\partial z\partial x} + x\frac{\partial\psi}{\partial y} + xz\frac{\partial^2\psi}{\partial z^2}\right] = \hat{L}_z\psi$$ - nekomutujú

nie sú súčasne merateľné

d) $[\hat{L}^2, \hat{L}_z] = 0 \Rightarrow$ komutujú $\Rightarrow$ sú súčasne merateľné

e) $[\hat{H}, \hat{L}^2] = 0 \rightarrow$ komutujú $\Rightarrow$ sú súčasne merateľné

3

8) ${}_1H{}_9F$: 10 elektrónov $Z_F = 9$ $Z_H = 1$

$$\hat{H}_{HF} = -\frac{\hbar^2}{2M_F}\nabla^2_{R_F} - \frac{\hbar^2}{2M_H}\nabla^2_{R_H} - \frac{\hbar^2}{2m_e}\sum_{i=1}^{10}\nabla^2_{r_i} - \frac{9e^2}{4\pi\varepsilon_0}\sum_{i=1}^{10}\frac{1}{|\vec{r}_i - \vec{R}_F|} - \frac{e^2}{4\pi\varepsilon_0}\sum_{i=1}^{10}\frac{1}{|\vec{r}_i - \vec{R}_H|} +$$

$$+ \frac{e^2}{4\pi\varepsilon_0}\sum_{i=1}^{10}\sum_{j=i+1}^{10}\frac{1}{|\vec{r}_i - \vec{r}_j|} + \frac{e^2}{4\pi\varepsilon_0}\sum_{I=1}^{2}\sum_{J=I+1}^{2}\frac{Z_I Z_J}{|\vec{R}_I - \vec{R}_J|}$$

$\vec{R}_H$ - poloha jadra vodíka, $\vec{R}_F$ - poloha jadra fluóru

M_F - hmotnosť jadra fluóru, M_H - hmotnosť jadra vodíka

m_e - hmotnosť elektrónu

$\vec{r}_i, \vec{r}_j$ - polohy elektrónov

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adam Alemayehu

9.) $\tilde{\nu} = ?$

$v = 5$

$k = 964\ Nm^{-1}$

$E_v = (\frac{1}{2} + v)\, h\nu_{vib}$

$\nu_{vib} = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$

$\nu_{vib} = 1{,}245 \cdot 10^{14}\ Hz$

$\mu = \frac{m_H \cdot m_F}{m_H + m_F} = \frac{1 \cdot 19}{1 + 19} \cdot m_u =$

$= 1{,}577 \cdot 10^{-27}\ kg$

$E_5 = \frac{11}{2} h\nu_{vib}$ $\quad E_0 = \frac{1}{2} h\nu_{vib}$

$\Delta E = 5 h\nu_{vib} = hc\tilde{\nu}$

$\tilde{\nu} = \frac{5\nu_{vib}}{c}$

$\tilde{\nu} = 20750\ cm^{-1}$

3

10.) $\tilde{\nu}_1 = 10cm^{-1}$

$\tilde{\nu}_2 = 100cm^{-1}$

$T = 298{,}15K$

$\frac{N_2}{N_1} = e^{-\frac{hc\tilde{\nu}}{k_B T}}$

$\left(\frac{N_2}{N_1}\right)_1 = e^{-\frac{6{,}63 \cdot 10^{-34} Js \cdot 3 \cdot 10^8 ms^{-1} \cdot 1000 m^{-1}}{1{,}38 \cdot 10^{-23} JK^{-1} \cdot 298{,}15K}}$

$\left(\frac{N_2}{N_1}\right)_1 = 0{,}953$

$\left(\frac{N_2}{N_1}\right)_2 = 0{,}617$

3

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