Za plinast HCl opazimo abs. sp. črte pri vrednostih $83{,}03\ cm^{-1}$, $103{,}73\ cm^{-1}$, $124{,}30\ cm^{-1}$, $145{,}03\ cm^{-1}$, $165{,}51\ cm^{-1}$, $185{,}86\ cm^{-1}$. So te črte posledica vibracijskih ali rotacijskih prehodov? Če so vibr., izračunaj konstanto k; če so rot., izračunaj razdaljo med H in Cl!

vibracije - HORMONSKI OSCILATOR :	$\Delta n = 1$	$E_n = \hbar\omega\left(n+\frac{1}{2}\right)$
rotacije - TOGI ROTATOR	$\Delta l = 1$	$E_l = \dfrac{\hbar^2 l(l+1)}{2I}$

$n \to n'$: $n \to n+1$ } absorpcija; $n \to n-1$ } emitacija

$$\Delta E = E_{n+1} - E_n = \hbar\omega\left(n+1+\tfrac{1}{2}\right) - \hbar\omega\left(n+\tfrac{1}{2}\right) = \hbar\omega\left(\cancel{n}+1+\cancel{\tfrac{1}{2}}-\cancel{n}-\cancel{\tfrac{1}{2}}\right) = \underline{\underline{\hbar\omega}}$$

– ena črta => rotacijski prehodi, ker vidimo 6 črt

$l \to l'$: $\underline{l \to l+1}$

$$\Delta E = E_{l+1} - E_l = \frac{\hbar^2 (l+1)(l+2)}{2I} - \frac{\hbar^2 l(l+1)}{2I} = \frac{\hbar^2 (l+1)(l+2) - l(l+1)}{2I} = \frac{\hbar^2 (l+1)\left((l+2)-l\right)}{2I} = \frac{2\hbar^2(l+1)}{2I} =$$

$$\underline{\underline{\Delta E = \frac{\hbar^2}{I}(l+1)}}$$

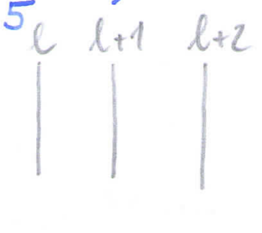
$$\boxed{\Delta E = \frac{hc}{\lambda}}$$

$$\frac{\Delta E_l}{\Delta E_{l+1}} = \frac{\frac{hc}{\lambda_1}}{\frac{hc}{\lambda_2}} = \frac{\lambda_2}{\lambda_1} = \boxed{\frac{\frac{1}{\lambda_1}}{\frac{1}{\lambda_2}}}$$

$$\frac{\frac{\hbar^2(l+1)}{I}}{\frac{\hbar^2(l+1+1)}{I}} = \boxed{\frac{\frac{1}{\lambda_1}}{\frac{1}{\lambda_2}}}$$

$$\frac{(l+1)}{(l+2)} = \frac{\frac{1}{\lambda_1}}{\frac{1}{\lambda_2}} = \frac{83{,}03}{103{,}73} = 0{,}8 = \frac{4}{5} \Rightarrow \underset{\sim}{l=3}$$

spekter:



VZTRAJNOSTNI MOMENT

$$\underline{I = \mu r^2}$$

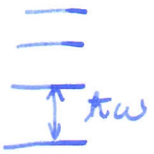
$$I = \frac{\hbar^2(l+1)}{\Delta E} = \frac{\hbar^2(l+1)\lambda_1}{hc} = \frac{\hbar^2(l+1)}{\frac{hc}{\lambda_1}} =$$

$$= \frac{\hbar^2\cdot 4}{hc\cdot\tilde{\nu}} = \frac{(1{,}055\cdot10^{-34}\,Js)^2\cdot 4 \quad \cancel{cm}\ 10^{-2}\,\cancel{m}}{6{,}63\cdot10^{-34}\,\cancel{J}\cdot 3\cdot10^{8}\,\cancel{m}\,s^{-1}\cdot 83{,}03}\ (kg\,m^2) = \underline{2{,}7\cdot10^{-47}\,kg\,m^2}$$

$$\mu = \frac{1\cdot 35{,}5}{36{,}5}\,u = 1{,}61\cdot10^{-27}\,kg$$

$$r = \sqrt{\frac{I}{\mu}} = \sqrt{\frac{2{,}7\cdot10^{-47}\,kg\,m^2}{1{,}61\cdot10^{-27}\,kg}} = 1{,}3\cdot10^{-10}\,m = \underline{1{,}3\,\text{Å}}$$

Razlaga:



$E_n = (n+\frac{1}{2})\hbar\omega$ → ENA ČRTA ~ HARMONSKI OSC. ⇒ vibracijski spekter

$\Delta E_l = \frac{\hbar^2}{I}(l+1)$ ~ razmeje 2 zaporednih črt

prehodi:

83,03 cm^{-1}	3 → 4	prehod iz $l \to l+1$
103,73	4 → 5	
124,30	5 → 6	
145,03	6 → 7	
165,51	7 → 8	
185,86	8 → 9	

Kakšna je degeneracija nivojev in energij za tridimenzionalni har. oscilator?

$$V(\vec{r}) = \frac{1}{2}kr^2 \qquad \hat{H}\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi + \frac{1}{2}k(x^2+y^2+z^2)\psi = E\psi$$

$$\boxed{\psi = XYZ}$$

$$\underbrace{-\frac{\hbar^2}{2m}\frac{\ddot{X}}{X} + \frac{1}{2}kx^2}_{\text{HAR. OSCILATOR v smeri } x} - \frac{\hbar^2}{2m}\frac{\ddot{Y}}{Y} + \frac{1}{2}ky^2 - \frac{\hbar^2}{2m}\frac{\ddot{Z}}{Z} + \frac{1}{2}kz^2 = E$$

$$E_{nx} = \hbar\omega\left(n_x + \frac{1}{2}\right)$$

$$\boxed{E = E_{nx} + E_{ny} + E_{nz}}$$

$$E = \hbar\omega\left(n_x + \frac{1}{2} + n_y + \frac{1}{2} + n_z + \frac{1}{2}\right) =$$
$$= \hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right)$$

pri har. oscilatorju je n vrednost (najmanjša) = 0 !!

n_x	n_y	n_z	E	deg
0	0	0	$\frac{3}{2}\hbar\omega$	1
1	0	0	$\frac{5}{2}\hbar\omega$	3
0	1	0		
0	0	1		
1	1	0	$\frac{7}{2}\hbar\omega$	6
1	0	1		
0	1	1		
2	0	0		
0	2	0		
0	0	2		
1	2	0	$\frac{9}{2}\hbar\omega$	10
2	1	0		
1	0	2		
2	0	1		
0	2	1		
0	1	2		
1	1	1		
3	0	0		
0	3	0		
0	0	3		