III 3) Pri težjih atomih, rentgenskih spektrih (prehodi notranjih e^-) in jedrskih spektrih pride v poštev J-J sklopitev. V tem režimu bo prispevek posameznega elektrona prevladal nad elektrostatskoo en. in se sešteje najprej v $j_1 = l_1 + s_1$ in ločeno v $j_2 = l_2 + s_2$, nato v $J = j_1 + j_2$. Na koncu je $\Delta H_{es} \propto \Delta H_{j_1} + \Delta H_{j_2} \propto \frac{\hbar^2}{2}\left(j(j+1) - l(l+1) - s(s+1)\right)_1 + 1 \leftrightarrow 2$

$l_1 = 1$, $s_1 = \frac{1}{2}$

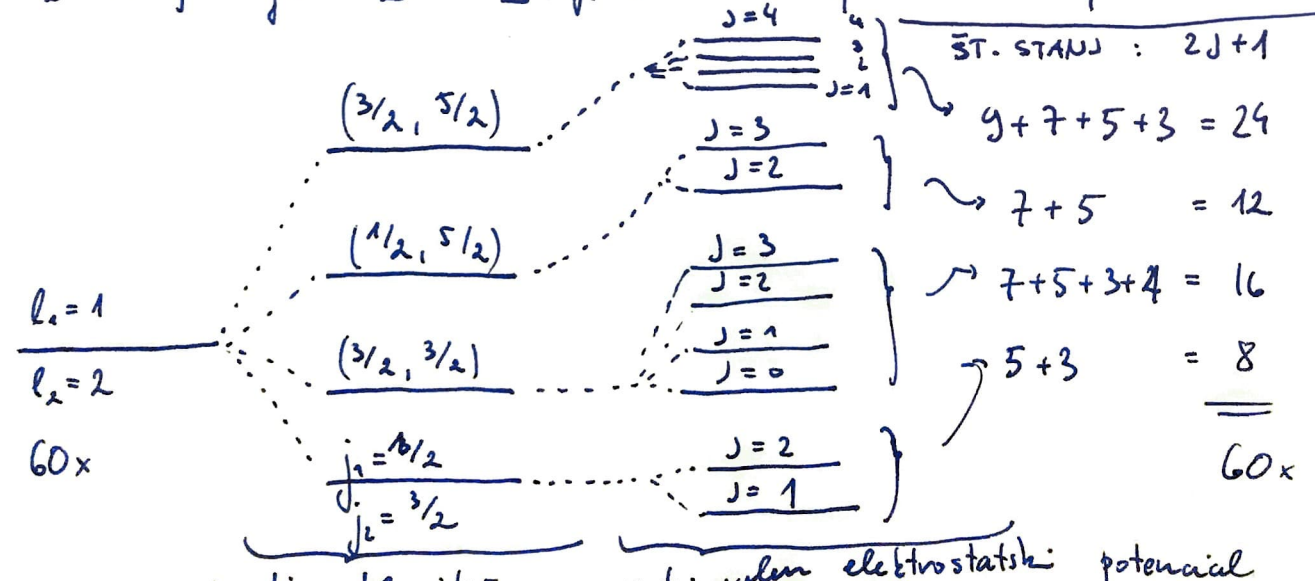
$j_1^{max} = \frac{3}{2}$: $\Delta H_{j_1 = 3/2} \propto \frac{3 \cdot 5}{4} - 2 - \frac{3}{4} = \frac{15-8-3}{4} = 1$

$j_1^{min} = \frac{1}{2}$: $\Delta H_{j_1 = 1/2} \propto \frac{3}{4} - 2 - \frac{3}{4} = -2$

$l_2 = 2$, $s_2 = \frac{1}{2}$

$j_2 = \frac{5}{2}$: $\Delta H_{j_2 = 5/2} \propto \frac{5 \cdot 7}{4} - 6 - \frac{3}{4} = \frac{35-24-3}{4} = 2$

$j_2 = \frac{3}{2}$: $\Delta H_{j_2 = 3/2} \propto \frac{15-24-3}{4} = -\frac{12}{4} = -3$



III./14 Razcep črte $^3P_1 \to {}^3D_2$ pri atomu ogljika v magnetnem polju $B = 0{,}05\ T$ = šibko magnetno polje.

$\Downarrow$ Landéjev faktor

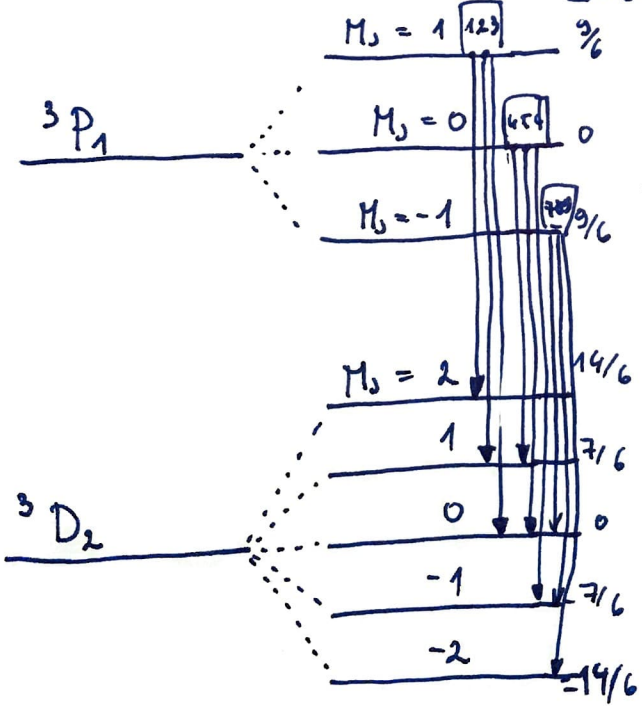
$\boxed{{}^{2S+1}L_J}$

$^3P_1 : S=1,\ L=1,\ J=1$

$^3D_2 : S=1,\ L=2,\ J=2$

a) Razcep energijskih nivojev $\Delta E_B = g_J M_J \mu_B B$, $E_0 = \frac{e\hbar}{2m_e}$

$$g_J = \frac{3}{2} - \frac{L(L+1)-S(S+1)}{2J(J+1)} = \begin{cases} \frac{3}{2} - \frac{2-2}{2\cdot 2} = \frac{3}{2} \\ \frac{3}{2} - \frac{6-2}{2\cdot 6} = \frac{9-2}{6} = \frac{7}{6} \end{cases}$$



$E_4 = -\frac{7}{6}E_0$, $E_7 = -\frac{9}{6}E_0$

$E_5 = 0$, $E_8 = -\frac{2}{6}E_0$

$E_6 = +\frac{7}{6}E_0$, $E_9 = \frac{5}{6}E_0$

b) Sevalni prehodi $\Rightarrow$ 9 črt

$\Delta L = \pm 1,\ \Delta J = \pm 1, 0$ (ok)

$\Delta S = 0,\ \Delta M_S = 0$

$\Delta M_J = \pm 1, 0$

c) Spekter fotonov $E_\gamma = \Delta E$

$E_1 = \frac{9-14}{6}E_0 = -\frac{5}{6}E_0$

$E_2 = \frac{9-7}{6}E_0 = \frac{2}{6}E_0$

$E_3 = \frac{9-0}{6}E_0 = \frac{9}{6}E_0$

$$\Delta E = \left(\pm 9, \pm 7, \pm 5, \pm 2, 0\right)\frac{E_0}{6} \rightsquigarrow \frac{e\hbar B}{2m} = \frac{E_0}{6}$$

III/39 Vezavna energija molekule Na^+Cl^-

$$V_{odb} = \frac{C}{r^{35}}, \quad W_{ion} = 5{,}14\,eV, \quad W_{af} = 3{,}81\,eV$$

$$r_0 = 0{,}89\, r_0^{\text{kristal NaCl}}, \quad M^{Na} = 23\,kg, \quad M^{Cl} = 35\,kg, \quad \rho^{NaCl} = 2160\ \frac{kg}{m^3}$$

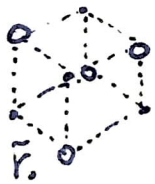
Celotna vezavna energija

$$W_{ver} = W_{ion} - W_{af} - \frac{\alpha\, hc}{r_0} + \frac{C}{r_0^{35}}$$

a) Določimo C iz $\left.\frac{dW}{dr}\right|_{r_0} = 0 = + \frac{\alpha\, hc}{r_0^2} - \frac{35\,C}{r_0^{36}} = 0$

$$\Rightarrow C = \frac{\alpha\, hc}{35} \cdot r_0^{34}$$

b) Izračunajmo $r_0^{\text{kristal NaCl}} = \tilde{r}_0$



$$\rho = \frac{\Sigma m}{V} = \frac{\frac{1}{8}(4 m_{Cl} + 4 m_{Na})}{r_0^3} = \frac{\frac{1}{2}(35+23)}{\tilde{r}_0^3} = \frac{29 m_p}{\tilde{r}_0^3}$$

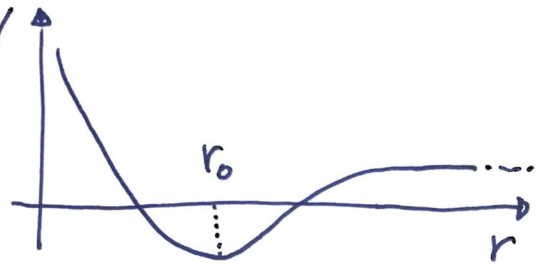
$V = \tilde{r}_0^3 \Rightarrow \tilde{r}_0 = \sqrt[3]{\frac{29 m_p}{\rho}} = \sqrt[3]{\frac{29 \cdot 2 \cdot 10^{-27}\,kg}{2{,}2 \cdot 10^3\,kg/(10^9\,m)^3}} = \underline{0{,}28\,nm}$

c) Vezavna energija

$$W_{ver}^{\circ} = W_{ion} - W_{af} - \frac{\alpha\, hc}{r_0}\left(1 - \frac{1}{35}\right)$$

$$= W_{ion} - W_{af} - 1.11\ \frac{\alpha\, hc}{\tilde{r}_0}\ \frac{34}{35} = \underline{-4{,}16\,eV}.$$

d) Na^+ mmm Cl^- Molekül nimmt Abstand r_0



$$V \sim V_0 + \underbrace{\frac{dV}{dr}\Big|_{r_0}}_{=0}(r-r_0) + \frac{1}{2}\underbrace{\frac{d^2V}{dr^2}\Big|_{r_0}}_{m\omega^2}(r-r_0)^2 + \dots$$

$$\frac{1}{m} = \frac{1}{m_{Na}} + \frac{1}{m_{Cl}}$$

$$\frac{\alpha\hbar c}{35} r_0^{34} = C$$

$$\frac{d^2V}{dr^2} = -2\frac{\alpha\hbar c}{r_0^3} + 35\cdot 36\,\frac{C}{r_0^{37}} = \frac{\alpha\hbar c}{r_0^3}(-2+36) = 34\,\frac{\alpha\hbar c}{r_0^5} = m\omega^2$$

$$\Rightarrow E_{min} = \hbar\omega\left(\underbrace{n}_{0}+\frac{1}{2}\right) = \frac{1}{2}\hbar\omega = \frac{1}{2}\hbar\sqrt{\frac{34\,\alpha\hbar c}{m r_0^3}}$$

$$\frac{1}{m} = \left(\frac{1}{23}+\frac{1}{35}\right)\frac{1}{m_p} \Rightarrow m = \frac{23\cdot 35}{58}m_p$$

$\Rightarrow E_{min} = 0{,}047\,eV$ in $W_{rot} = W_{rot}^{0} + E_{min}$

$= (-4{,}16 + 0{,}05)\,eV$

$= -4{,}11\,eV$

III / 38 $V = V_0 \left(e^{-2(r-r_0)/a} - 2 e^{-(r-r_0)/a} \right)$

$V_0 = 3\,eV$

$a = 0{,}12\,nm$

$M = 16$

$\frac{1}{m} = \frac{1}{m_1} + \frac{1}{m_2} = \frac{2}{16 m_p} \quad 8$

$m = 8 m_p$

• pri $r \sim r_0$ razvijemo potencial za majhne odmike

$e^x \sim 1 + x + \frac{x^2}{2} + \dots$

$V = V_0 \left(1 - \frac{2(r-r_0)}{a} + \frac{1}{2} \frac{(2(r-r_0))^2}{a^2} - 2 + 2\frac{(r-r_0)}{a} - \frac{1}{2} 2 \left(\frac{r-r_0}{a}\right)^2 + \dots \right)$

$= -V_0 + \frac{1}{2} \underbrace{\frac{2V_0}{a^2}}_{\frac{1}{2} m \omega^2} \underbrace{(r-r_0)^2}_{x^2} + \dots$, $E_n = \hbar\omega \left(n + \frac{1}{2}\right)$

$n = 0 : E_0 = \hbar\omega/2$

$n = 1 : E_1 = \hbar\omega\, 3/2$

$\hbar\omega = \hbar \sqrt{\frac{2V_0}{m a^2}} = \frac{\hbar c}{2a} \sqrt{\frac{V_0}{m_p c^2}} = \frac{200\,eV\,nm}{2 \cdot 0{,}12\,nm} \sqrt{\frac{3\,eV \cdot 10}{10^3\,eV \cdot 10}}$

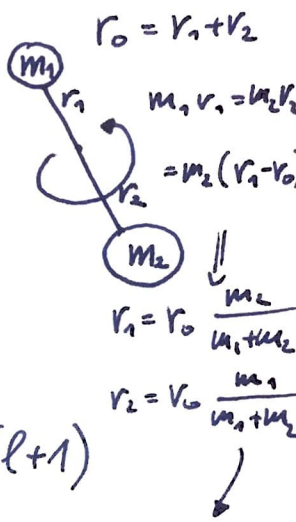
$m = 8 m_p$

$= \frac{100\sqrt{30}}{0{,}12 \cdot 10^5}\,eV = 46\,meV.$

Osnovno stanje : $E_0 = \frac{42}{2}\,meV = 23\,meV,$

1. vzbujeno stanje : $E_1 = 3 \cdot E_0 = 69\,meV.$

III 130 Rotacijski spekter molekule



$r_0 = 0{,}074\,nm$

H_2, HD, D_2

$$E_{rot} = \frac{J^2}{2J} \Rightarrow \langle E \rangle_{rot} = \frac{\langle \ell^2 \rangle}{2J} = \frac{\hbar^2}{2J}\ell(\ell+1)$$

- vztrajnostni moment: $J = J_1 + J_2 = m_1 r_1^2 + m_2 r_2^2$

$$= m r_0^2, \quad m = \frac{m_1 m_2}{m_1 + m_2}$$

$$r_0 = r_1 + r_2$$

- Rotacijski prispevki za H_2, HD, D_2

$$E_r^{H_2} = \frac{\hbar^2 c^2}{2 m r_0^2 c^2} = \frac{(200\,eV\,nm)^2}{\underbrace{2 \cdot \frac{1}{2} m_p}_{1\,GeV} (0{,}07\,nm)^2} = \underline{7{,}6\,meV}$$

$$E_r^{DH} = \frac{(\hbar c)^2}{\lambda \left(\frac{2}{3} m_p c^2\right) r_0^2} = \frac{3}{4} E_r^{H_2} = 5{,}6\,meV$$

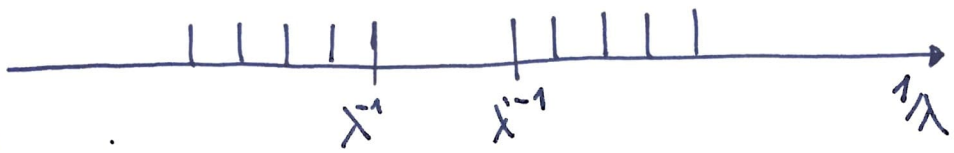
$$E_r^{D_2} = \frac{1}{2} E_r^{H_2} = 3{,}8\,meV$$

	$E_r^{H_2}$	E_r^{HD}	$E_r^{D_2}$	$2\ell+1$ = Degeneracija
0	0	0	0	1x
1	15	11	7,5	3x
2	45	33	23	5x
3	90	66	45	7x
⋮			⋮	⋮

III/135. Vibracijsko – rotacijski spekter molekul

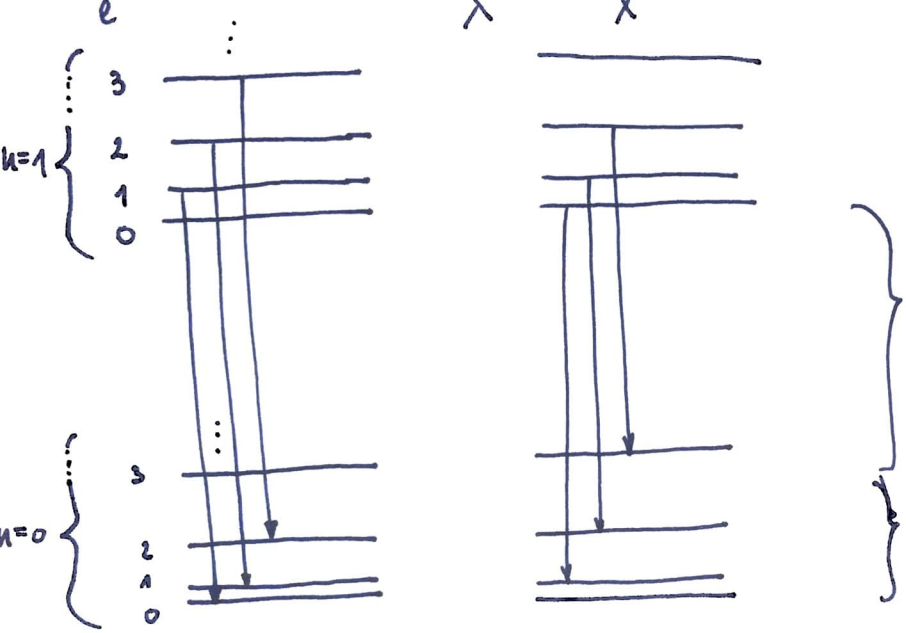
$$E = E_{ee} + \underbrace{\hbar\omega\left(n+\tfrac{1}{2}\right)}_{E_{vib}} + \underbrace{\frac{\hbar^2}{2J}\ell(\ell+1)}_{E_{rot}}$$

$\Delta n = \pm 1$ $\qquad$ $\Delta \ell = \pm 1$



$\lambda'^{-1} = 0{,}2907\,\mu m^{-1}$

$\lambda = 0{,}2866\,\mu m^{-1}$



nihajni načini

rotacijski načini

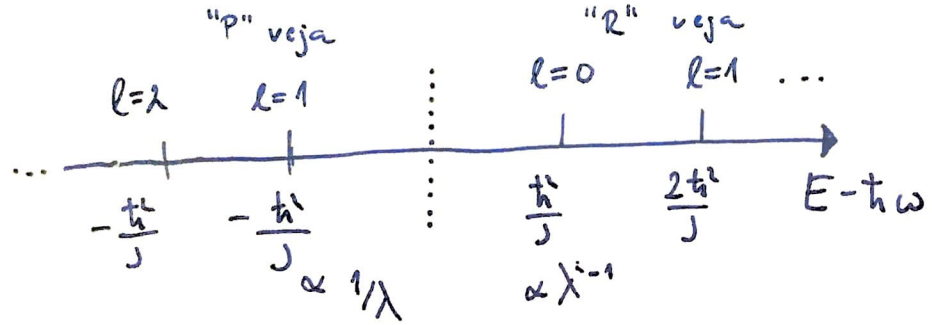
$\ell+1 \to \ell$ $\qquad$ $\ell \to \ell-1$

"R"-veja $\qquad$ "P" veja

$\ell = 0, 1, 1, \ldots$

$$\Delta E_R = \hbar\omega + \frac{\hbar^2}{2J}\left((\ell+1)(\ell+2) - \ell(\ell+1)\right) = \hbar\omega + \frac{\hbar^2}{2J}(\ell+1)\cdot 2$$

$$\Delta E_P = \hbar\omega + \frac{\hbar^2}{2J}\left(-\ell(\ell+1) + (\ell-1)\ell\right) = \hbar\omega - \frac{\hbar^2}{J}\ell \quad , \quad \ell = 1, 2, \ldots$$



$$E_R = 2\pi\hbar c\,\lambda'^{-1} = \hbar\omega + \frac{\hbar^2}{J}$$

$$E_P = 2\pi\hbar c\,\frac{1}{\lambda} = \hbar\omega - \frac{\hbar^2}{J}$$

* $E_R - E_P = \frac{2\hbar^2}{J} = \frac{2\hbar^2}{m r_0^2}$, $m = \frac{m_H m_{Ce}}{m_H + m_{Ce}} = \frac{35}{36} m_p$

$\Downarrow$

$\boxed{r_0}$

$$r_0^2 = \frac{2\hbar^2}{2\pi \hbar c \, \Delta\lambda^{-1} m}$$

$$r_0 = \sqrt{\frac{36\ \hbar c}{35\ m_p c^2 \pi \Delta\lambda^{-1}}} = 0{,}13\ \mu m$$

$\boxed{k}$

$\Uparrow$

* $E_R + E_P = 2\hbar\omega = 2\hbar\sqrt{\frac{k}{m}} = 2\pi \hbar c \, \Sigma\lambda^{-1}$

$$\frac{k}{m} = \pi^2 c^2 (\Sigma\lambda^{-1})^2 \Rightarrow k = \frac{35}{36} m_p c^2 \pi^2 (\Sigma\lambda^{-1})^2$$

$$= 3\ \frac{keV}{hm^2} = 481\ \frac{N}{m}$$