PROBLEMA 1

STATO ECCITATO $1s\,2p$

STATO FONDAMENTALE $1s\,1s$

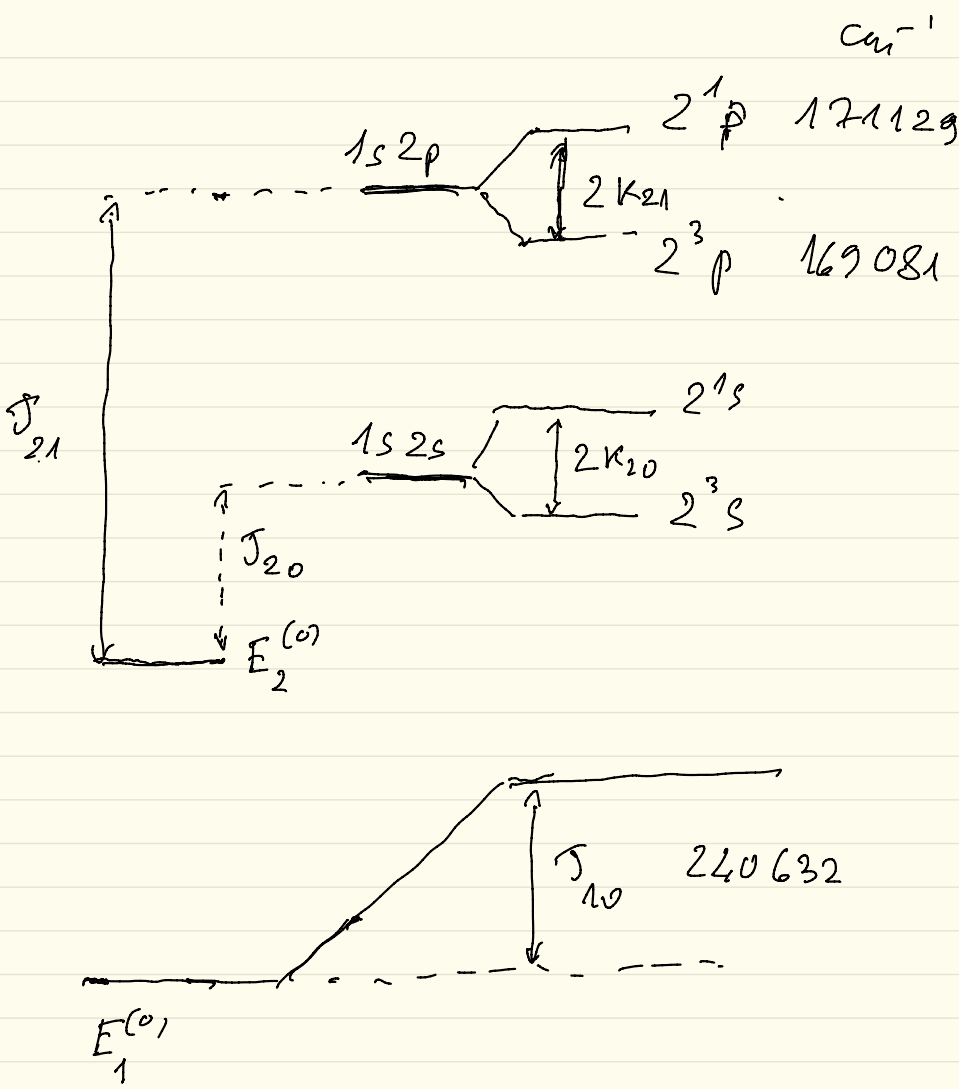
$$E = E_n^{(0)} + J_{nl} \pm K_{nl}$$

$$E_n^{(0)} = -\frac{Z^2}{2}\left(1 + \frac{1}{n^2}\right) \quad \text{a.u.}$$

$$J_{nl} > 0 \qquad K_{nl} > 0$$

$+K_{nl}$ con $S = 0$

$-K_{nl}$ con $S = 1$



$$2K_{21} = E(2^1P) - E(2^3P)$$

$$K_{21} = 1024 \text{ cm}^{-1}$$

$$E_1^{(0)} = -2RZ^2 = -377896 \text{ cm}^{-1}$$

$$E_1^{(0)} + T_{10} = -637264 \text{ cm}^{-1}$$

$$E(1s2p) = E(2^1p) - K_{21} = 170105 \text{ cm}^{-1}$$

$$E(1s2p) = E_2^{(0)} + T_{21} - \left(E_1^{(0)} + T_{10}\right)$$

quindi con

$$E_2^{(0)} = -548685 \text{ cm}^{-1}$$

$$T_{21} = E(1s2p) + \left(E_1^{(0)} + T_{10}\right) - E_2^{(0)}$$

$$T_{21} = (170105 - 637264 + 548685) \text{ cm}^{-1}$$

$$T_{21} = 81526 \text{ cm}^{-1}$$

EFFETTO ZEEMAN

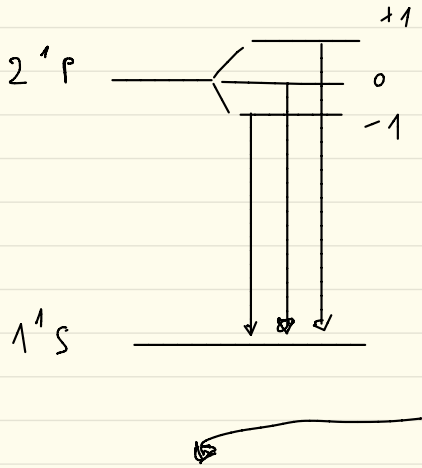
REGOLE DI SELEZIONE

$\Delta S = 0 \qquad \Delta L = \pm 1 \qquad \Delta M_L = 0, \pm 1$

È POSSIBILE SOLO LA TRANS.

$2^1P \rightarrow 1^1S$

CON $S = 0$ NON CI SONO EFFETTI S.O.



$\Delta E = \mu_B B (M_L + 2 M_S)$

$(M_S = 0)$

$\mu_B B = 0.047 \ cm^{-1}$

→ TRASCURABILE

1 LINEA DEGENERE A

$\nu = 171129 \ cm^{-1} \rightarrow 21.2 \ eV$

$$\psi_{1s}(\vec{r}) = R_{10}(r)\, Y_{00} = \frac{1}{\sqrt{4\pi}} R_{10}(r)$$

$$\psi(2^1P) = \frac{1}{\sqrt{2}} \left[\psi_{1s}(r_1)\, \psi_{21m}(r_2) + \psi_{21m}(r_1)\, \psi_{1s}(r_2) \right] \cdot \chi_{00}$$

$$\psi(2^3P) = \frac{1}{\sqrt{2}} \left[\psi_{1s}(r_1)\, \psi_{21m}(r_2) - \psi_{21m}(r_1)\, \psi_{1s}(r_2) \right] \chi_{1m_s}$$

$$\chi_{00} = \frac{1}{\sqrt{2}} \left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right]$$

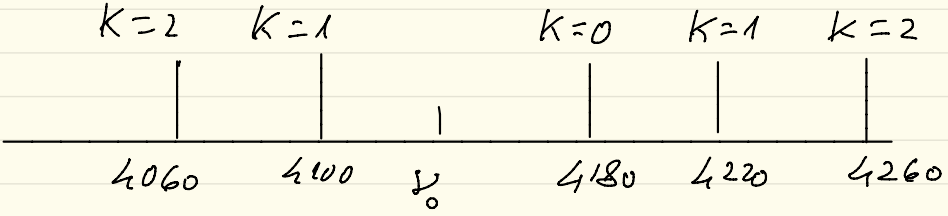
$$\chi_{1m_s} = \begin{cases} |\uparrow\uparrow\rangle & m_s = 1 \\ \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \right) & m_s = 0 \\ |\downarrow\downarrow\rangle & m_s = -1 \end{cases}$$

PROBLEMA 2

4060 4100 4180 4220 4260 cm^{-1}

| 2B | 4B | 2B | 2B |

$2B = 40\ cm^{-1}$ $B = 20\ cm^{-1}$



$(v=0, K) \Rightarrow (v=1, K-1)$ $(v=0, K) \Leftrightarrow (v=1, K+1)$

A $T = 0\ K$ SOLO $v=0, K=0$ OCUPADO

QUIMPI SE VEDE SOLO RIGA A $4180\ cm^{-1}$

$\nu_0 = 4140 \ cm^{-1}$

$$B = \frac{\hbar^2}{4\pi \mu C R_0^2} \qquad \text{con } B \text{ in } cm^{-1}$$

$\mu = 0.95$ amu

$$R_0^2 = \frac{1.055\ 10^{-34}}{4\pi \cdot (0.95 \cdot 1.66\ 10^{-27}) \cdot 3 \cdot 10^{10} \cdot B}$$

$$R_0^2 = \frac{1.055}{4\pi \cdot 0.95 \cdot 1.66 \cdot 3 \cdot 20}\ 10^{-34}\ 10^{27}\ 10^{-10}$$

$R_0^2 = 8.41\ 10^{-4}\ 10^{-17} = 8.41\ 10^{-21}\ m^2$

$R_0^2 = 0.841\ 10^{-20}\ m^2$

$R_0 = 0.92$ Å

$$E(R) = \frac{A}{R^{12}} - \frac{B}{R^6}$$

$$\left.\frac{dE}{dR}\right|_{R_0} = \left(-\frac{12A}{R^{13}} + \frac{6B}{R^7} \right)_{R_0} = 0$$

$$-\frac{6}{R_0^7}\left(\frac{2A}{R_0^6} - B \right) = 0$$

$$B = \frac{2A}{R_0^6}$$

$$\left.\frac{d^2E}{dR^2}\right|_{R_0} = +\frac{12 \cdot 13\ A}{R_0^{14}} - \frac{7 \cdot 6\ B}{R_0^8}$$

$$k = \frac{12 \cdot 13\ A}{R_0^{14}} - \frac{7 \cdot 6}{R_0^8}\ \frac{2A}{R_0^6}$$

$$k = \frac{12 \cdot 13\, A}{R_0^{14}} - \frac{12 \cdot 7\, A}{R_0^{14}}$$

$$= \frac{12 \cdot A}{R_0^{14}} (13 - 7) = \frac{72\, A}{R_0^{14}}$$

$$A = \frac{1}{72} K R_0^{14}$$

$$\nu_0 = \frac{1}{2\pi c} \sqrt{\frac{K}{\mu}} \qquad K = (2\pi c)^2 \nu_0^2 \cdot \mu$$

$$K = (2\pi 3)^2 10^{20} (4140)^2 \cdot 0{,}95 \cdot 1{,}66\, 10^{-27}\ J/m^2$$

$$K = 960\ J/m^2 .$$

$$E(R_0) = \frac{A}{R_0^{12}} - \frac{B}{R_0^{6}} =$$

$$= \frac{A}{R_0^{12}} - \frac{2A}{R_0^{12}} = -\frac{A}{R_0^{12}}$$

$$E(R_0) = -\frac{1}{72} K \frac{R_0^{14}}{R_0^{12}} = -\frac{1}{72} K R_0^2$$

$$E(R_0) = -\frac{1}{72} 960 \cdot 0.841\, 10^{-20}\ \text{J}$$

$$= -11.21\ 10^{-20}\ \text{J}$$

$$E(R_0) = -11.21\ 10^{-20}\ \text{J} \,/\, 1.602\ 10^{-19}\ \text{eV}$$

$$7.10^{-1}\ \text{eV} = 0.70\ \text{eV}$$

$$h\nu_0 = 4120 / 8065\ \text{eV} = 0.51\ \text{eV}$$

$$D_0 = \left(0.7 - \frac{1}{2} 0.51\right) \text{eV} = 0.445\ \text{eV}$$