(1) $1s^2$ ei yhtään paritonta e^-

$\Rightarrow S = 0 \Rightarrow 2S+1 = 1$ singletti

$\Rightarrow L = 0$

$\Rightarrow J = 0$

$^1S_0$ helium

$1s^2 2s^2 2p^1$ yksi pariton e^- p-orbitaalilla

$\Rightarrow S = 1/2 \Rightarrow 2S+1 = 2$ dubletti

$\Rightarrow L = 1$ koska p-orb

$\Rightarrow J = L+S,\ L+S-1,\ \dots,\ |L-S|$

$= 3/2$ tai $1/2$

$^2P_{3/2}$ ja $^2P_{1/2}$ Beryllium

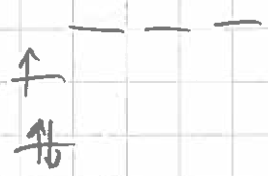
$1s^2 2s^1 2p^1$ yksi pariton e^- s-orb
+ yksi pariton e^- p-orb

$S = 1$ tai 0 $\Rightarrow 2S+1 = 3$ tai triplettl
$= 1$ singletti

$L = 0 + 1 = 1 \Rightarrow P$ (s ↓, L ↓)

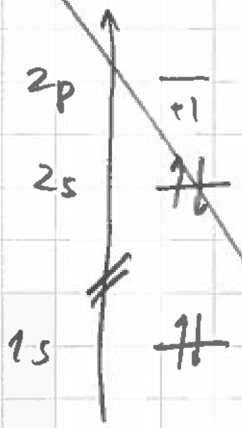
$S=1$: $J = 1+1,\ 1,\ 0$

$\Rightarrow$ $^3P_2$ $^3P_1$ $^3P_0$



$S=0$: $J = 1+0 = 1$ $^1P_1$

(2) Happo atomi $1s^2 2s^2 2p^4$



← nelpni elektrona

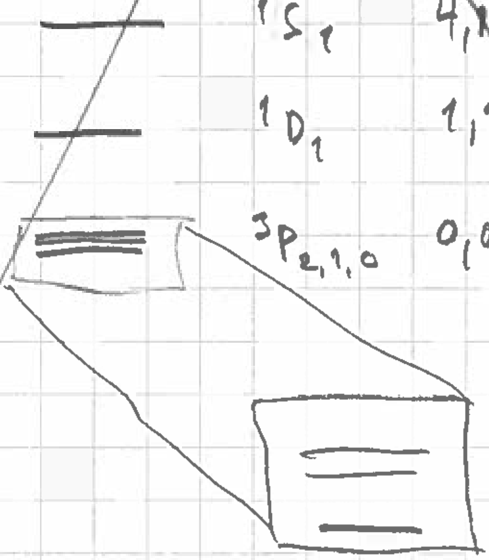
+1	0	-1	S	L (= max M_L)
↑↓	↑	↑	1	1+1+0-1 = 1
↑↓	↑	↓	0	1+1+0-1 = 1
↑↓	↑↓		0	1+1+0 0 = 2

$S=1 \quad L=1 \Rightarrow {}^3P_2, \; {}^3P_1, \; {}^3P_0$

$S=0 \quad L=1 \Rightarrow {}^1P_1$

$S=0 \quad L=2 \Rightarrow {}^1D_2$

NIST atomic spectra database



${}^1S_1$ 4,19 eV

${}^1D_1$ 1,97 eV

${}^3P_{2,1,0}$ 0,00 eV

${}^2P_0$ 0,03 eV

${}^2P_1$ 0,02 eV

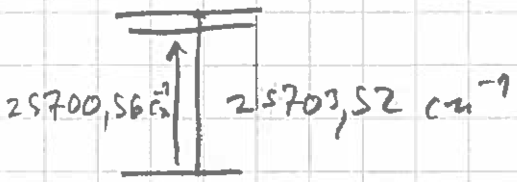
${}^3P_2$ 0,00 eV

(3) $4p^6 5d^1$ ← yksi pariton e^- d-orb

↑ täysi kuori

$J = 2 + 1/2,\ 2 - 1/2 = 5/2,\ 3/2$

$^1D_{5/2}$ ja $^1D_{3/2}$



$$\Delta\nu = 2{,}96\ \text{cm}^{-1}$$

$$E_{l,s,j} = \frac{1}{2} hcA\left[j(j+1) - l(l+1) - s(s+1)\right]$$

$$E_{2,1/2,5/2} = \frac{1}{2} hcA\left[\frac{5}{2}\left(\frac{5}{2}+1\right) - \frac{4}{2}\left(\frac{4}{2}+1\right) - \frac{1}{2}\left(\frac{1}{2}+1\right)\right]$$

$$= \frac{1}{8} hcA\left[5\cdot(5+2) - 4(4+2) - 1(1+2)\right]$$

$$= \frac{1}{8} hcA \cdot 8 = hcA$$

$$E_{2,1/2,3/2} = \frac{1}{8} hcA\left[3(3+2) - 4(4+2) - 1(1+2)\right]$$

$$= \frac{1}{8} hcA \cdot (-12) = -\frac{3}{2} hcA$$

$$\Delta E = hcA - -\frac{3}{2} hcA = \frac{5}{2} hcA$$

$$A = \frac{2}{5}\frac{\Delta E}{hc} = \frac{2}{5}\frac{hc\Delta\tilde{\nu}}{hc} = \frac{2}{5}\Delta\tilde{\nu}$$

$$= \frac{2}{5}\cdot 2{,}96\ \text{cm}^{-1} = \underline{1{,}184\ \text{cm}^{-1}}$$

(4)

$$\phi_1 = \left(\frac{1}{3}\right)^{1/2} 2s - \left(\frac{1}{3}\right)^{1/2} 2p_x + \left(\frac{1}{3}\right)^{1/2} p_z$$

$$\langle \phi_1 | \phi_1 \rangle = \left[\left(\frac{1}{3}\right)^{1/2}\right]^2 \Big(\langle 2s | 2s \rangle - \cancel{\langle 2s | 2p_x \rangle} + \cancel{\langle 2s | 2p_z \rangle} - \cancel{\langle 2p_x | 2s \rangle} + \langle 2p_x | 2p_x \rangle - \cancel{\langle 2p_x | 2p_z \rangle} + \cancel{\langle 2p_z | 2s \rangle} - \underbrace{\cancel{\langle 2p_z | 2p_x \rangle}}_{0} + \underbrace{\langle 2p_z | 2p_z \rangle}_{1} \Big)$$

$$= \frac{1}{3} \cdot 3 = \underline{\underline{1}}$$

$$\phi_2 = \frac{1}{\sqrt{3}} 2s + \frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right) 2p_x + \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right) 2p_z$$

$$\langle \phi_2 | \phi_2 \rangle = \left[\frac{1}{\sqrt{3}}\right]^2 \langle 2s | 2s \rangle + \frac{1}{\sqrt{3}} \frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right) \underbrace{\langle 2s | 2p_x \rangle}_{0}$$

$$+ \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right) \underbrace{\langle 2s | 2p_z \rangle}_{0}$$

$$+ \ 0 \quad + \left[\frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right)\right]^2 \langle 2p_x | 2p_x \rangle + 0$$

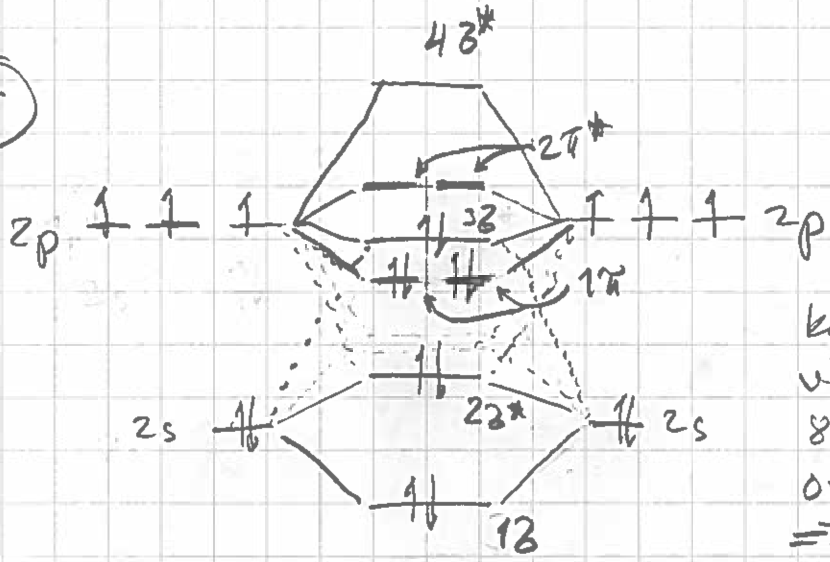
$$+ \ 0 \quad + 0 \quad + \left[\frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right)\right]^2 \langle 2p_z | 2p_z \rangle$$

$$= \frac{1}{3} + \frac{1}{4}\left(1 + \frac{1}{\sqrt{3}}\right)^2 + \frac{1}{4}\left(1 - \frac{1}{\sqrt{3}}\right)^2 = \underline{1}$$

$$\phi_3 = \left(\frac{1}{\sqrt{3}}\right)^2 + \left(\frac{1}{2}\right)^2 \left(-1 + \frac{1}{\sqrt{3}}\right)^2 + \left(\frac{1}{2}\right)^2 \left(1 + \frac{1}{\sqrt{3}}\right)^2$$

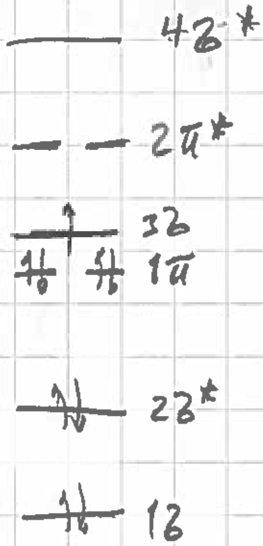
$$= \underline{\underline{1}}$$

(5)



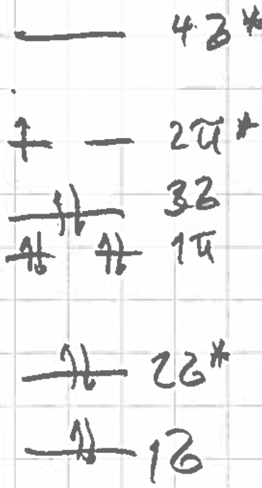
N_2

kymmenestä valenssielektronista 8 on sitovilla orbitaaleilla
=> erittäin vahva sidos



N_2^+

yksi elektroni vähemmän sitovalla 3σ orbitaalilla
=> sidos heikkenee



N_2^-

yksi elektroni lisää hajottavalla 2π* orbitaalilla
=> sidos heikkenee