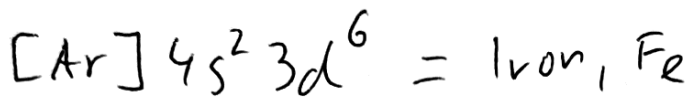
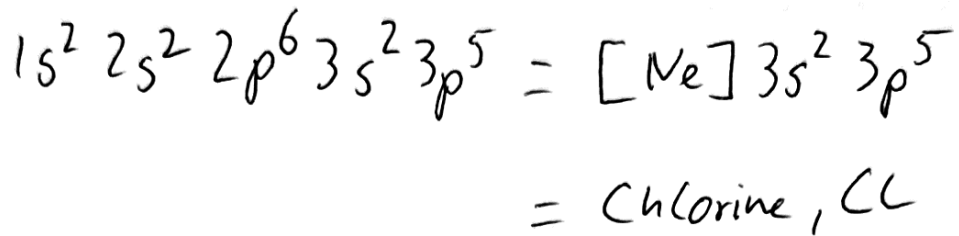


HW 3

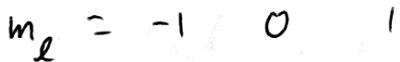
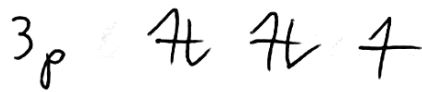
3.1

3.1.1



3.1.2 looking at valence e^- only

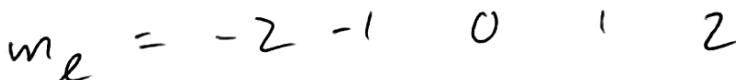
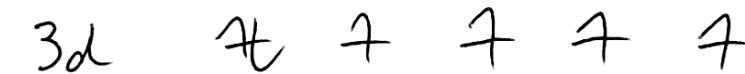
Cl.



$$\Rightarrow S=1 \quad L=1$$

\rightarrow paramagnetic (weak)

Fe

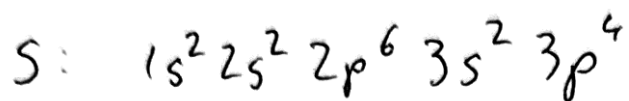


$$S=2$$

$$L=2$$

\rightarrow paramagnetic (strong)

3.2



shielding by $n < n_{\text{valence}}$: $n=1$ and $n=2$ shield

$$Z_{\text{eff}} = 16 - \underbrace{2}_{1s^2} - \underbrace{8}_{2s+2p} = 6$$

3.2.1

$$E_{\underset{\uparrow}{1s}} = - \frac{Z_{\text{eff}}^2}{n^2} R = - \frac{6^2}{3^2} R = -4R = \underline{\underline{-54 \text{ eV}}}$$

(removing a $3p \ e^-$)

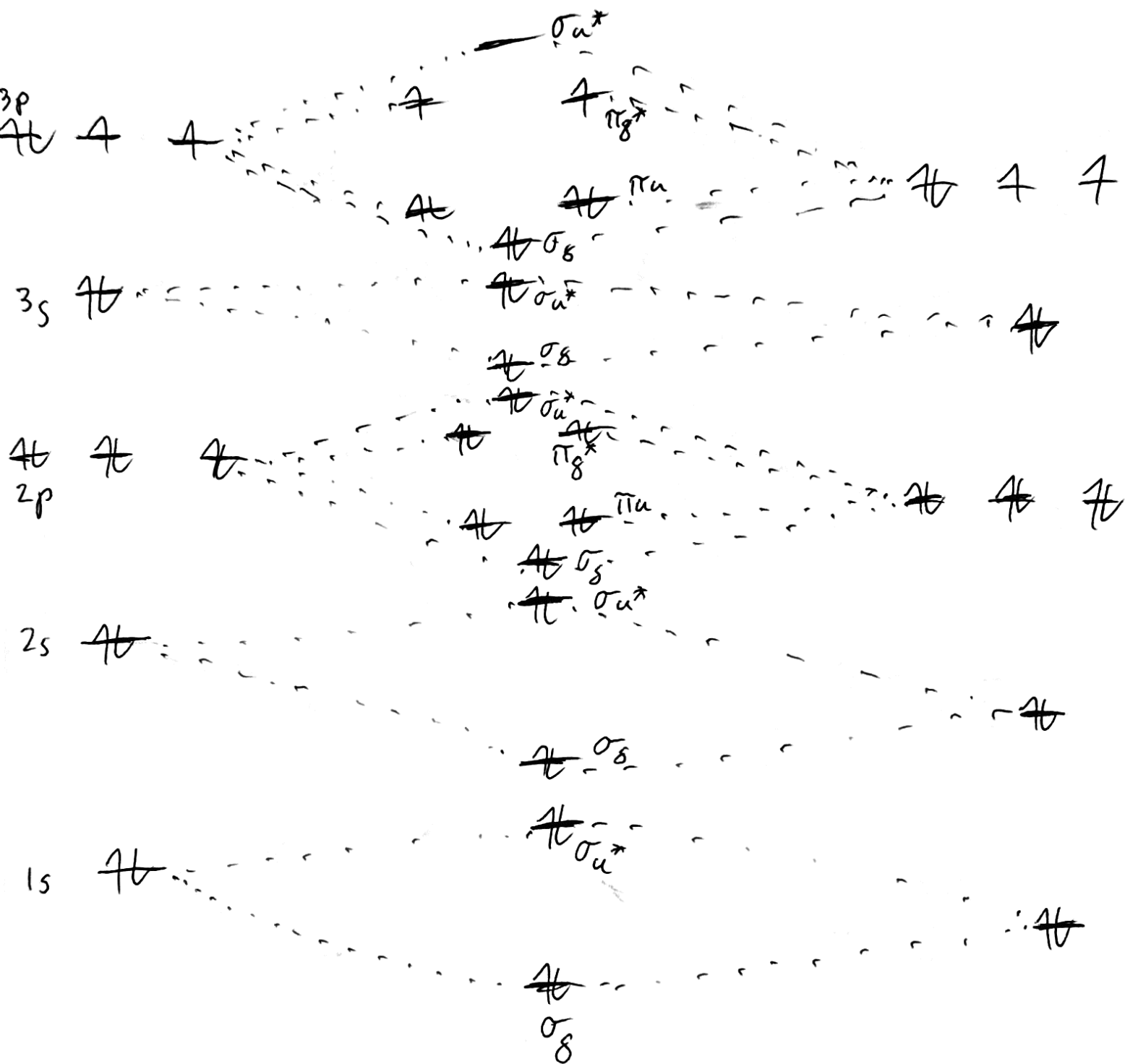
3.2.2

not realistic because:

- $3s^2$ and other $3p \ e^-$ have effect, too.
- $1s, 2s$ and $2p \ e^-$ will not shield completely as $3p$ wavefunctions extend towards nucleus.

3.3

3.3.1



3.3.2

$$B = \frac{18 - 14}{2} = 2 \rightarrow > 0 \rightarrow \text{stable}$$