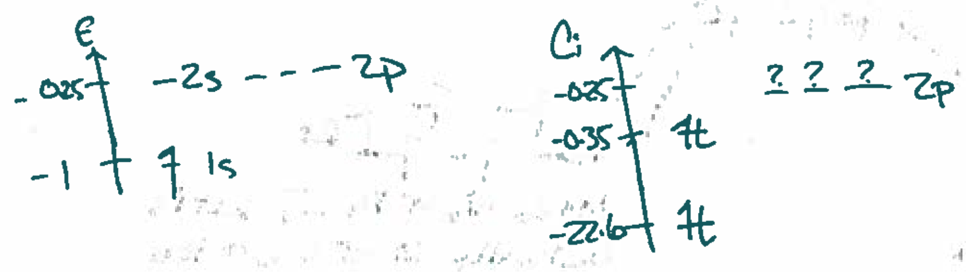
Hunds Rules



Hund's rules

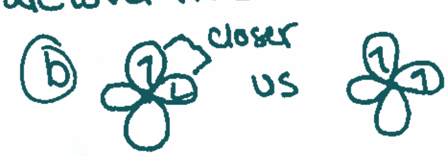
(b) has lower e⁻-e⁻ repulsion → lower $\langle \frac{1}{r_{12}} \rangle$ than (a)

(c) lower e⁻-e⁻ repulsion than (b) ... why?

→ Pauli exclusion

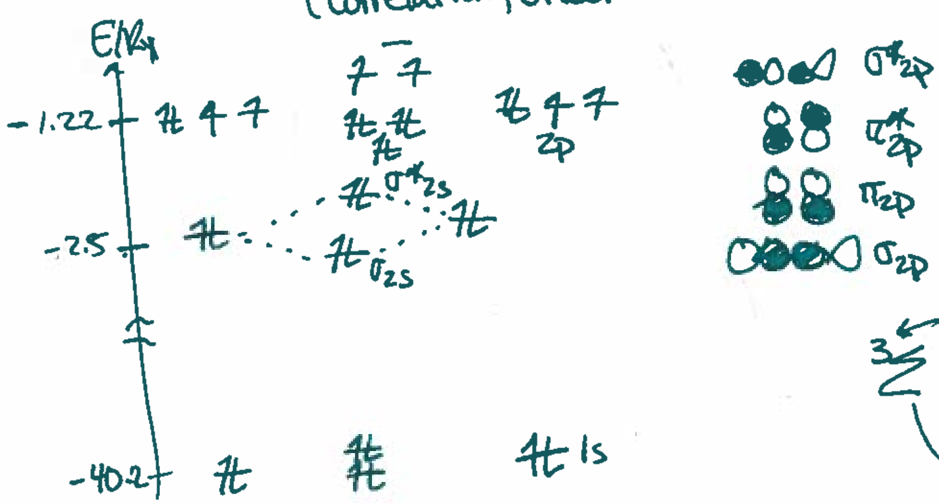
$\psi_{(c)} \rightarrow 0$ faster than $\psi_{(b)}$ when $r_{12} \rightarrow 0$

Thus the e⁻ shield each other less → Zeff is larger and the smaller orbitals are lower in e⁻



$\psi = 1s^2 2s^2 2p\alpha' \; 2p\alpha$

purely a multi e⁻ (correlation) effect



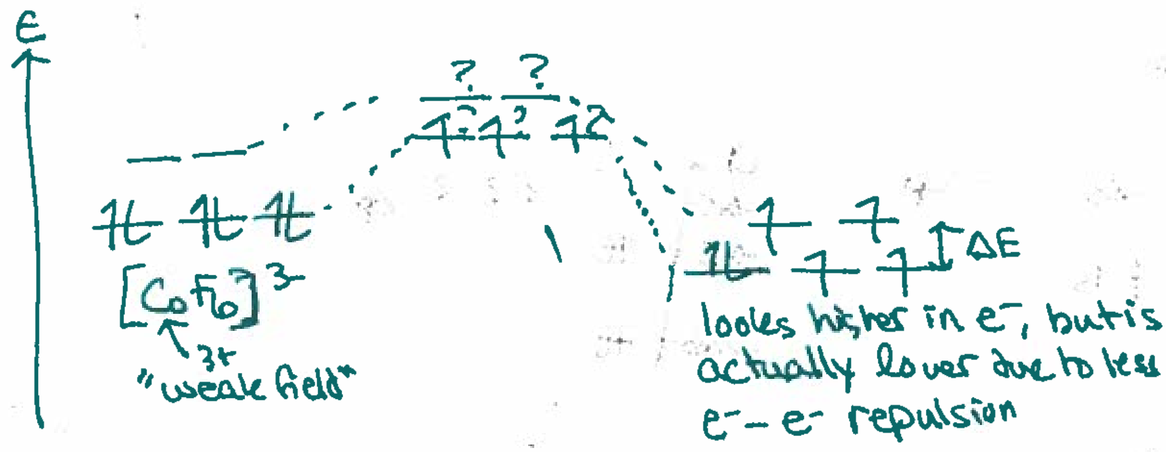
$^3\Sigma$ ← S=1, Ms = 0, ±1

ground state

→ $M_L = M_{L1} + M_{L2}$

$= \pm1 \pm1$

$= 0$ (lowest E)



E
$[CoF_6]^{3-}$
3+
"weak field"
?
?
ΔE
looks higher in e⁻, but is actually lower due to less e⁻ – e⁻ repulsion