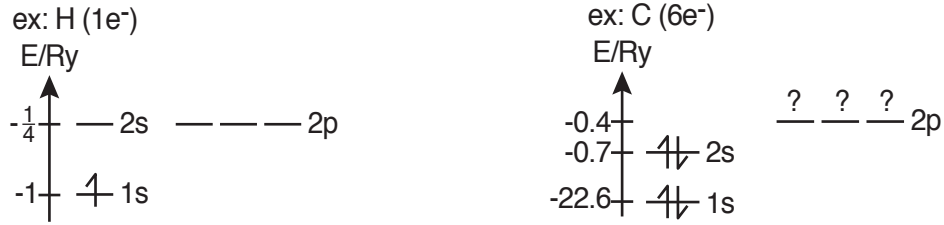
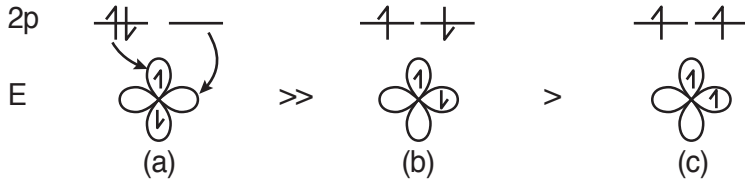


# Hund's rules: How spin lifts the degeneracy of spatial orbitals such as $p_x, p_y, p_z$ :

## A: Pauli exclusion at work again



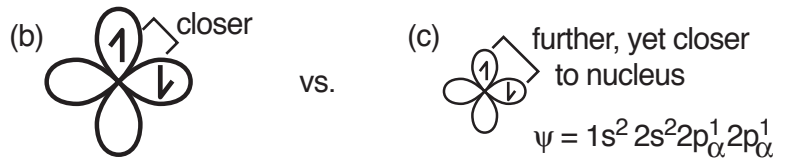
### Hund's rules:



- (b) has lower  $e^- - e^-$  repulsion (lower  $\langle \frac{1}{r_{12}} \rangle$ ) than (a) (different spatial orbital)
- (c) has slightly lower  $e^- - e^-$  repulsion than (b). Why?

Due to Pauli exclusion,  $\psi_{(c)} \rightarrow 0$  faster than  $\psi_{(b)}$  when  $r_{12} \rightarrow 0$  (or the two electrons would be in the same place with the same spin)

Thus the  $e^-$  shield each other less,  $Z_{\text{eff}}$  is larger, and the smaller orbitals are lower in  $e^-$



Purely a multi- $e^-$  (correlation) effect.

Note: magn. field effect is negligible

