

HW #5 Chem 1410

1. Li atom ( $1s^2 2s$ )

$$\psi = \frac{1}{\sqrt{3!}} \begin{vmatrix} 1s & \bar{1s} & 2s \\ 1s & \bar{1s} & 2s \\ 1s & 1s & 2s \end{vmatrix} = \frac{1}{\sqrt{6}} \left\{ 1s \begin{vmatrix} \bar{1s} & 2s \\ 1s & 2s \end{vmatrix} - \bar{1s} \begin{vmatrix} 1s & 2s \\ 1s & 2s \end{vmatrix} + 2s \begin{vmatrix} 1s & \bar{1s} \\ 1s & \bar{1s} \end{vmatrix} \right\}$$
$$= \frac{1}{\sqrt{6}} \left\{ 1s \bar{1s} 2s - 1s 2s \bar{1s} - \bar{1s} 1s 2s + 1s 2s 1s + 2s 1s \bar{1s} - 2s \bar{1s} 1s \right\}$$

2. Energy of Li ( $1s^2 2s$ )

$$\bar{E} = 2h_{1s} + h_{2s} + J_{1s,1s} + 2J_{1s,2s} - K_{1s,2s}$$

$$= 2E_{1s} + E_{2s} - J_{1s,1s} - 2J_{1s,2s} + K_{1s,2s}, \text{ using HF orbitals}$$

3. Energy of Be ( $1s^2 2s^2$ )

$$E = 2h_{1s} + 2h_{2s} + J_{1s,1s} + J_{2s,2s} + 2J_{1s,2s} - 2K_{1s,2s}$$

$$= 2E_{1s} + 2E_{2s} - J_{1s,1s} - J_{2s,2s} - 2J_{1s,2s} + 2K_{1s,2s} \leftarrow$$

using HF orbitals