

ATOMS, MOLECULES 2 RESEARCH

QUANTUM MECHANICS - SPRING - WEEK 3

$$\textcircled{1} \quad \psi = \frac{1}{\sqrt{2} 2(1+S)} \left[1S_A(1) 1S_A(2) + 1S_A(1) 1S_B(2) + 1S_B(1) 1S_A(2) + 1S_B(1) 1S_B(2) \right] [\alpha(1)\beta(2) - \beta(1)\alpha(2)]$$

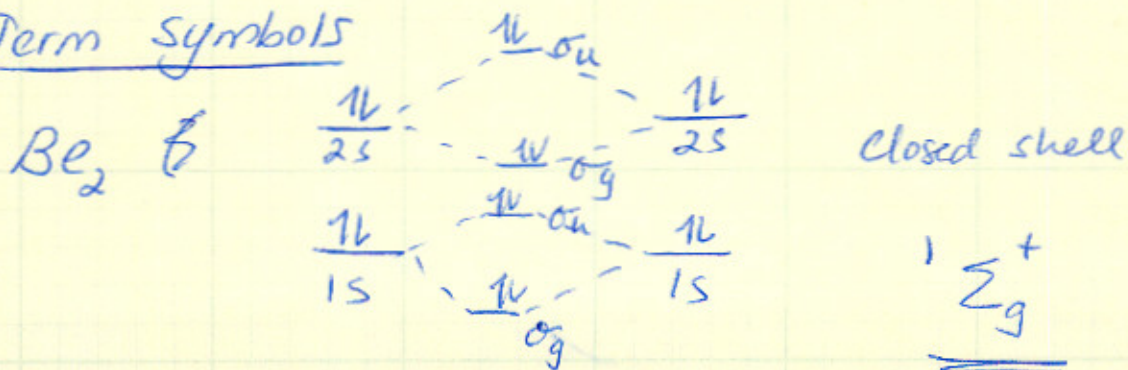
$$\hat{P}_{12} \psi = \frac{1}{\sqrt{2} 2(1+S)} \left[1S_A(2) 1S_A(1) + 1S_A(2) 1S_B(1) + 1S_B(2) 1S_A(1) + 1S_B(2) 1S_B(1) \right] [\alpha(2)\beta(1) - \beta(2)\alpha(1)]$$

$$= \frac{-1}{\sqrt{2} 2(1+S)} \left[1S_A(2) 1S_A(1) + 1S_A(2) 1S_B(1) + 1S_B(2) 1S_A(1) + 1S_B(2) 1S_B(1) \right] [\alpha(1)\beta(2) - \beta(1)\alpha(2)]$$

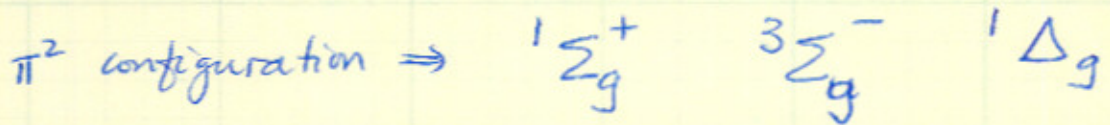
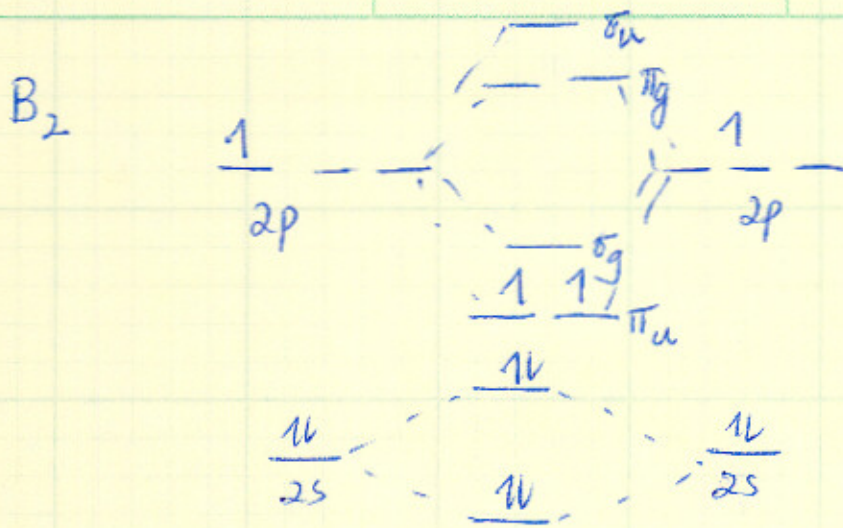
$$= -\psi$$

Since $\hat{P}_{12} \psi = -\psi$, the wavefunction ψ is antisymmetric with respect to permutation.

Term symbols



2/



Ground state is $3\Sigma_g^-$

