Reflection Symmetry (+,−)

Orbital Degeneracy and Electron Indistinguishability:

\[ \hat{R}_z \]

\[ \lambda \rightarrow -\lambda. \]

with respect to exchange of spin labels:

\[ \Sigma^1_g \]

spin part: \{ \alpha(1)\alpha(2), \beta(1)\beta(2) \}

spatial part: symmetric

\[ \Sigma^3_g \]

spin part: \{ \alpha(1)\beta(2) + \beta(1)\alpha(2) \}

spatial part: anti-symmetric

These diagrams are still incomplete in that all electrons occupy each possible molecular orbital in the full set of Slater determinants that determine the state. However, the reflection symmetry can be determined by just focusing on the two unpaired electrons.

\[ (\sigma_{g,2p_z})^2(\pi_{u,2p})^3(\pi_{g,2p})^2 \]

\[ 3\Sigma^3_g \]

spin part: \{ \alpha(1)\alpha(2), \alpha(1)\beta(2), \beta(1)\alpha(2), \beta(1)\beta(2) \}

spatial part: anti-symmetric

\[ 1\Sigma^1_g \]

spin part: \{ \alpha(1)\beta(2) - \beta(1)\alpha(2) \}

spatial part: symmetric

\[ (\sigma_{g,2p_z})^2(\pi_{u,2p})^3(\pi_{g,2p})^3 \]

\[ 3\Sigma^3_u \]

spin part: symmetric

spatial part: anti-symmetric with respect to exchange of spin labels

\[ 3\Sigma^1_u \]

\[ 3\Sigma^3_u \]

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