# Spectroscopic notation of 2-atomic molecules

atoms: $^{2S+1}L_J$

Spin-multiplicity
orbital ang. mom.
total ang. momentum

$n$ ← principal / main q.n.

$L = 0 \quad 1 \quad 2 \quad 3 \quad \ldots$

$S \quad P \quad D \quad F$

---

molecules: $^{2S+1}\Lambda_{\Omega,g/u}^{\pm}$

$n$ ← principal quantum number

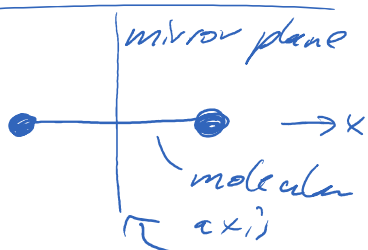
$\Lambda$ ← abs. value of projection of orbital angular momentum on molecular axis

$\Lambda = 0 \quad 1 \quad 2$

$\Sigma \quad \Pi \quad \Delta$

$\Omega$ (often discarded)
projection of $e^-$ total angular momentum onto molecular axis

Parity



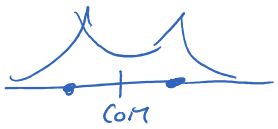

Sign change under mirroring at this plane

$\Psi^+(x,y,z) = +\Psi^+(-x,y,z)$

$\Psi^-(x,y,z) = -\Psi^-(-x,y,z)$

onto molecular axis

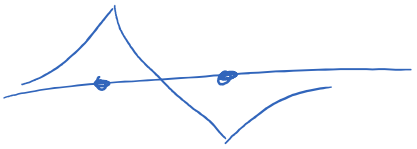
g/u for homonuclear molecules




symmetry of electrons w.r.t center of mass of the molecule

$\psi_g(\vec{r}) = +\psi_g(-\vec{r})$

$\psi_u(\vec{r} = -\psi_u(-\vec{r})$



e.g. $H_2$ (electronic states)

$2e^-$ → singlett, triplett states

ground state

$\Lambda = 0 \rightarrow {}^1\Sigma_g$

$\Omega = 0$ because $\Lambda = 0, \Sigma = 0$