

Spectroscopic notation:

R	Rotational angular momentum of the nuclear framework
I	Nuclear spin angular momentum
$L = \sum_i l_i$	Total electronic orbital angular momentum
$S = \sum_i s_i$	Total electronic spin
$F = R + L + S + I$	Total angular momentum
$J = F - I$	Total angular momentum excluding nuclear spin
$N = R + L = J - S$	Rotational angular momentum including electronic orbital angular momentum
Π	Parity defined as the result of inversion of all fixed space coordinates. This thesis adopts the standard phase convention that makes this operation equivalent to σ_v ⁴⁵ .
σ_v	The operator for reflection of the molecular wavefunction through a vertical mirror plane (i.e. coincident with the symmetry axis). By convention: $\sigma_v x,y,z\rangle = x,-y,z\rangle$.
v	Generic vibrational quantum number.
$V_1V_2V_3\dots V_n$	Compact notation for describing the vibrational state for the n non-degenerate modes of a molecule. An example follows.
$01^{lc/d}0$	This refers to the excitation $v_2 = 1$. c/d refers to lower or upper l -doublet component.
e/f	Lower or upper Λ -doublet component.
ϕ	Azimuthal angle for an unpaired electron with respect to the molecular symmetry axis. The phase convention: $\langle \Lambda = \pm 1 e^{\pm 2i\phi} \Lambda = \mp 1 \rangle = +1$, has been adopted.

Projections onto the symmetry axis:

$$S_z \equiv \Sigma$$

$$L_z \equiv \Lambda$$

$$J_z \equiv \Omega = \Lambda + \Sigma \quad \text{In states of non-zero orbital angular momentum}$$

$$N_z \equiv K \quad \text{For symmetric rotors without orbital angular momentum}$$

Vibronic coupling notation:

$$l \quad \text{Vibrational Angular Momentum}$$

$$K(\text{Kappa}) \equiv \Lambda + l$$

$$P \equiv K(\text{Kappa}) + \Sigma$$