

$\mathbf{H}_{\Lambda\text{-doubling}}$:

$\Sigma = \Omega - 1$. The raising and lowering operators are implicitly Λ dependent*. The convention is that, for example, $\langle \Lambda = 1 | S_-^2 | \Lambda = -1 \rangle$ and $\langle \Lambda = -1 | S_+^2 | \Lambda = 1 \rangle$ (i.e. the matrix elements are assumed to connect states of opposite Λ exclusively).

$$\begin{aligned} \langle \Lambda = \pm 1, S\Sigma'J\Omega'\pi' | H_{\Lambda\text{-doubling}} | \Lambda = \mp 1, S\Sigma J\Omega\pi \rangle &= \delta_{\Omega+\Omega',0} (o+p+q) \frac{\pi}{2} (-1)^{J-S} \\ &\times \sqrt{\frac{[S(S+1) - \Sigma(\Sigma+1)]}{[S(S+1) - (\Sigma+1)(\Sigma+2)]}} \\ &+ \delta_{\Omega+\Omega',1} (p+2q) \frac{\pi}{2} (-1)^{J-S+1} \sqrt{[S(S+1) - \Sigma(\Sigma+1)][J(J+1) - \Omega(\Omega-1)]} \\ &+ \delta_{\Omega+\Omega',2} q \frac{\pi}{2} (-1)^{J-S} \sqrt{[J(J+1) - \Omega(\Omega-1)][J(J+1) - (\Omega-1)(\Omega-2)]} \end{aligned}$$

$$\begin{aligned} \langle \Lambda = \pm 1, S\Sigma'J\Omega'\pi' | H_{\Lambda\text{-doubling},cd} | \Lambda = \mp 1, S\Sigma J\Omega\pi \rangle &= (o_D + p_D + q_D) \frac{1}{4} (-1)^{J-S} \\ &\times \left[\begin{aligned} &\pi' \delta_{\Omega+\Omega',0} \sqrt{\frac{[S(S+1) - \Sigma'(\Sigma'+1)]}{[S(S+1) - (\Sigma'+1)(\Sigma'+2)]}} \frac{\langle \Lambda, S\Sigma''J\Omega''\pi'' | H_{rot} | \Lambda = \mp 1, S\Sigma J\Omega\pi \rangle}{B} \\ &+ \pi \delta_{\Omega'+\Omega'',0} \sqrt{\frac{[S(S+1) - \Sigma(\Sigma+1)]}{[S(S+1) - (\Sigma+1)(\Sigma+2)]}} \frac{\langle \Lambda = \pm 1, S\Sigma'J\Omega'\pi' | H_{rot} | \Lambda, S\Sigma''J\Omega''\pi'' \rangle}{B} \end{aligned} \right] \\ &+ (p_D + 2q_D) \frac{1}{4} (-1)^{J-S+1} \\ &\times \left[\begin{aligned} &\pi' \delta_{\Omega+\Omega',1} \sqrt{[S(S+1) - \Sigma'(\Sigma'+1)][J(J+1) - \Omega'(\Omega'-1)]} \frac{\langle \Lambda, S\Sigma''J\Omega''\pi'' | H_{rot} | \Lambda = \mp 1, S\Sigma J\Omega\pi \rangle}{B} \\ &+ \pi \delta_{\Omega'+\Omega'',1} \sqrt{[S(S+1) - \Sigma(\Sigma+1)][J(J+1) - \Omega(\Omega-1)]} \frac{\langle \Lambda = \pm 1, S\Sigma'J\Omega'\pi' | H_{rot} | \Lambda S\Sigma''J\Omega''\pi'' \rangle}{B} \end{aligned} \right] \\ &+ q_D \frac{1}{4} (-1)^{J-S} \\ &\times \left[\begin{aligned} &\pi' \delta_{\Omega+\Omega',2} \sqrt{[J(J+1) - \Omega'(\Omega'-1)][J(J+1) - (\Omega'-1)(\Omega'-2)]} \frac{\langle \Lambda S\Sigma''J\Omega''\pi'' | H_{rot} | \Lambda = \mp 1, S\Sigma J\Omega\pi \rangle}{B} \\ &+ \pi \delta_{\Omega'+\Omega'',2} \sqrt{[J(J+1) - \Omega(\Omega-1)][J(J+1) - (\Omega-1)(\Omega-2)]} \frac{\langle \Lambda = \pm 1, S\Sigma'J\Omega'\pi' | H_{rot} | \Lambda S\Sigma''J\Omega''\pi'' \rangle}{B} \end{aligned} \right] \end{aligned}$$

* J.M. Brown and A.J. Merer, *J. Mol. Spec.*, **74**, 488-494 (1979).