

H_{sr}:

$$\langle \Lambda S \Sigma' J M_J \Omega' | H_{sr} | \Lambda S \Sigma J M_J \Omega \rangle = \gamma \left[\begin{array}{l} -\delta_{\Omega\Omega'} S(S+1) + (-1)^{J-\Omega'+S-\Sigma'} \begin{pmatrix} J & 1 & J \\ -\Omega' & (\Omega' - \Omega) & \Omega \end{pmatrix} \begin{pmatrix} S & 1 & S \\ -\Sigma' & (\Sigma' - \Sigma) & \Sigma \end{pmatrix} \\ \times \sqrt{J(J+1)(2J+1)S(S+1)(2S+1)} \end{array} \right]$$

$$\begin{aligned} \langle \Lambda S \Sigma' J M_J \Omega' | H_{sr} | \Lambda S \Sigma J M_J \Omega \rangle &= \frac{\gamma_D}{2B\gamma} \{ H_{rot}, H_{sr} \} \\ &= \frac{\gamma_D}{2B\gamma} \left[\begin{array}{l} \langle \Lambda S \Sigma' J M_J \Omega' | H_{rot} \left(\sum_{\Sigma'' \Omega''} | \Lambda S \Sigma'' J M_J \Omega'' \rangle \langle \Lambda S \Sigma'' J M_J \Omega'' | \right) H_{sr} | \Lambda S \Sigma J M_J \Omega \rangle \\ + \langle \Lambda S \Sigma' J M_J \Omega' | H_{sr} \left(\sum_{\Sigma'' \Omega''} | \Lambda S \Sigma'' J M_J \Omega'' \rangle \langle \Lambda S \Sigma'' J M_J \Omega'' | \right) H_{rot} | \Lambda S \Sigma J M_J \Omega \rangle \end{array} \right] \end{aligned}$$

For $S > 1^*$ ($\Lambda = 0$):

$$\begin{aligned} \langle S, \Sigma; J, \Omega, M | H_{sr}^{(3)} | S, \Sigma \pm 1; J, \Omega \pm 1, M \rangle &= \frac{-\gamma_s}{2} (S(S+1) - 5\Sigma(\Sigma \pm 1) - 2) \\ &\times \sqrt{J(J+1) - \Omega(\Omega \pm 1)} \sqrt{S(S+1) - \Sigma(\Sigma \pm 1)} \end{aligned}$$

* J.M. Brown, D.J. Milton, J.K.G. Watson, R.N. Zare, D.L. Albritton, M. Horani, and J. Rostas, *J. Mol. Spec.*, **90**, 139-151 (1981).