

H_{ss}:

$$\begin{aligned} \langle N'\Lambda SJ | H_{ss} | N\Lambda SJ \rangle &= \lambda \frac{(-1)^{N+N'+S+J-\Lambda}}{3} \sqrt{(2N+1)(2N'+1)} \begin{pmatrix} N' & 2 & N \\ -\Lambda & 0 & \Lambda \end{pmatrix} \begin{Bmatrix} S & N' & J \\ N & S & 2 \end{Bmatrix} \\ &\times \prod_{k=0}^4 \sqrt{2S+k-1} + \lambda_D \frac{(-1)^{N+N'+S+J-\Lambda}}{6} (N(N+1) + N'(N'+1)) \\ &\times \sqrt{(2N+1)(2N'+1)} \begin{pmatrix} N' & 2 & N \\ -\Lambda & 0 & \Lambda \end{pmatrix} \begin{Bmatrix} S & N' & J \\ N & S & 2 \end{Bmatrix} \prod_{k=0}^4 \sqrt{2S+k-1} \end{aligned}$$

Fourth-order spin-spin (S>1.5)* ($\Lambda = 0$):

$$\begin{aligned} \langle \Lambda'N'SJM_J | H_{ss}^{(4)} | \Lambda NSJM_J \rangle &= \frac{\theta}{24} (-1)^{N+S+J+N'-\Lambda'} \begin{Bmatrix} J & S & N' \\ 4 & N & S \end{Bmatrix} \begin{pmatrix} N' & 4 & N \\ -\Lambda' & 0 & \Lambda \end{pmatrix} \\ &\times \sqrt{(2N+1)(2N'+1)} \prod_{k=0}^8 \sqrt{2S+k-3} \\ &+ \frac{\theta_D}{48} (-1)^{N+S+J+N'-\Lambda'} (N(N+1) + N'(N'+1)) \\ &\times \begin{Bmatrix} J & S & N' \\ 4 & N & S \end{Bmatrix} \begin{pmatrix} N' & 4 & N \\ -\Lambda' & 0 & \Lambda \end{pmatrix} \sqrt{(2N+1)(2N'+1)} \prod_{k=0}^8 \sqrt{2S+k-3} \end{aligned}$$

* Corkery, S.M. and Brown, J.M., *J. Mol. Spec.*, **149**, 257-273 (1991).