

**H<sub>sr</sub>:**

$$\langle N\Lambda SJ | H_{sr} | N\Lambda SJ \rangle = \frac{1}{2} \left[ \gamma(J(J+1) - N(N+1) - S(S+1)) + \gamma_D N(N+1)(J(J+1) - N(N+1) - S(S+1)) \right]$$

Higher order spin-rotation (S>1)<sup>1,2</sup> (Λ=0):

$$\begin{aligned} \langle N'\Lambda SJ | H_{sr}^{(3)} | N\Lambda SJ \rangle &= \frac{\gamma_s \sqrt{70}}{4\sqrt{6}} (-1)^{2N+2N'+S+J-\Lambda+1} (2N+1) \sqrt{N(N+1)(2N'+1)} \\ &\times \begin{pmatrix} N' & 2 & N \\ -\Lambda & 0 & \Lambda \end{pmatrix} \begin{Bmatrix} S & N' & J \\ N & S & 3 \end{Bmatrix} \begin{Bmatrix} 2 & 1 & 3 \\ N & N' & N \end{Bmatrix} \prod_{k=0}^6 \sqrt{2S+k-2} \end{aligned}$$

Note that, as discussed in Ref. 1, if one transforms this representation of the matrix elements to case (a), in addition to regenerating all of the off diagonal matrix elements derived in Ref. 2, one introduces diagonal case (a) matrix elements which were ignored by Brown and Milton. Be careful when comparing results that use this term in different bases.

1. T. Nelis, T., J. M. Brown, K. M. Evenson, *J. Chem. Phys.*, **92** (7), 4067-4076 (1990).
2. J.M. Brown and D.J. Milton, *Molec. Phys.*, **31** (2), 409-422 (1976).