C'(Tl) -term in uncoupled basis

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This document goes through the derivation of the matrix elements of the C'(Tl)-term as defined by Brown et al. in "A determination of fundamental Zeeman parameters for the OH radical" (1978):

$$H'_{nsr} = C'_I \sum_{q=\pm 1} \exp(-2iq\phi) \frac{1}{2} \left[T^2_{2q}(I, J-S) + T^2_{2q}(J-S, I) \right] \tag{0.1}$$

We'll be using a basis set where the nuclear spin I is decoupled from J: $|\eta; J, \Omega, m_J, I_1, m_1, I_2, m_2\rangle$. Since we're only interested in matrix elements for the Tl-spin, the quantum numbers for the fluorine will be suppressed; the selection rules for them will be $\delta_{I_2,I'_2}\delta_{m_2,m'_2}$. We will also drop the electron spin operator S since it only couples to different electronic states, and thus does not contribute significantly. We can thus write the operators as $T^2_{\pm 2}(I, J) = T^1_{\pm 1}(I)T^1_{\pm 1}(J)$. To evaluate the matrix elements we'll use the following relations:

- B&C 5.162:

$$\langle J', \Omega', m'_J, I'_1, m'_1 | \, T^1_q(J) \, |J, \Omega, m_J, I_1, m_1\rangle \tag{0.2}$$

$$= (-1)^{J'-\Omega'} \begin{pmatrix} J' & 1 & J' \\ -\Omega' & -q & \Omega \end{pmatrix} \left[J'\left(J'+1\right)\left(2J'+1\right) \right]^{1/2} \delta_{J,J'}\delta_{m_J,m'_J}\delta_{I_1,I'_1}\delta_{m_1,m'_1} \tag{0.3}$$

- B&C5.144 (transforming operator to lab frame), B&C5.172 (W-E theorem), 5.179 (reduced ME for 1st rank tensor)

$$\langle J', \Omega', m'_J, I'_1, m'_1| \, T^1_q(I) \, |J, \Omega, m_J, I_1, m_1\rangle \tag{0.4}$$

$$= \sum_p (-1)^{p-q} \, \langle J', \Omega', m'_J, I'_1, m'_1| \, D^{(1)*}_{-p,-q} T^1_p(I) \, |J, \Omega, m_J, I_1, m_1\rangle \tag{0.5}$$

$$= \sum_p (-1)^{p-q} (-1)^{J'-\Omega'} \left[(2J'+1)\,(2J+1)\right]^{1/2} \begin{pmatrix} J' & 1 & J \\ -m'_J & -p & m_J \end{pmatrix} \begin{pmatrix} J' & 1 & J \\ -\Omega' & -q & \Omega \end{pmatrix} \tag{0.6}$$

$$(-1)^{I'_1-m'_1} \begin{pmatrix} I' & 1 & I \\ -m'_1 & p & m_1 \end{pmatrix} \left[I_1\,(I_1+1)\,(2I_1+1)\right] \delta_{I_1, I'_1} \tag{0.7}$$

$$=(-1)^{p-q+J'-\Omega'+I'_1-m'_1} \left[(2J'+1)\,(2J+1)\,I_1\,(I_1+1)\,(2I_1+1)\right]^{1/2} \tag{0.8}$$

$$\begin{pmatrix} J' & 1 & J \\ -m'_J & -p & m_J \end{pmatrix} \begin{pmatrix} J' & 1 & J \\ -\Omega' & -q & \Omega \end{pmatrix} \begin{pmatrix} I' & 1 & I \\ -m'_1 & p & m_1 \end{pmatrix} \tag{0.9}$$