$\mathbf{H_{mhf}}$:

Σ's refer to magnitudes (Ω-Λ) and π is only referred to in the 'd' term.

$$
\begin{aligned}
&\langle \pi' \Lambda S \Sigma' J' \Omega' I F | H_{mhf} | \pi \Lambda S \Sigma J \Omega I F \rangle \\
&= \left[
\begin{array}{l}
a\delta_{\Omega\Omega'}\Lambda(-1)^{J'+J-\Omega'+I+F}\sqrt{(2J'+1)(2J+1)I(I+1)(2I+1)}\begin{pmatrix} J' & 1 & J \\ -\Omega & 0 & \Omega \end{pmatrix} \\
\\
+b(1-\delta_{\Omega\Omega'})(-1)^{S-\Sigma'+J'+J-\Omega'+I+F}\sqrt{S(S+1)(2S+1)(2J'+1)(2J+1)I(I+1)(2I+1)} \\
\times\begin{pmatrix} J' & 1 & J \\ -\Omega' & \Omega'-\Omega & \Omega \end{pmatrix}\begin{pmatrix} S & 1 & S \\ -\Sigma' & \Sigma'-\Sigma & \Sigma \end{pmatrix} \\
\\
+(b+c)\delta_{\Omega\Omega'}\Sigma(-1)^{J'+J-\Omega'+I+F}\sqrt{(2J'+1)(2J+1)I(I+1)(2I+1)}\begin{pmatrix} J' & 1 & J \\ -\Omega & 0 & \Omega \end{pmatrix} \\
\\
+d\pi\delta_{\Omega+\Omega',1}(-1)^{J'+2J-\Omega'+I+F-\Sigma'}\sqrt{S(S+1)(2S+1)(2J'+1)(2J+1)I(I+1)(2I+1)} \\
\times\begin{pmatrix} J' & 1 & J \\ -\Omega' & 1 & \Omega \end{pmatrix}\begin{pmatrix} S & 1 & S \\ -\Sigma' & -1 & \Sigma \end{pmatrix} \\
\\
+C_I\delta_{\Omega\Omega'}\delta_{JJ'}(-1)^{J+I+F}\sqrt{I(I+1)(2I+1)J(J+1)(2J+1)}
\end{array}
\right]
\begin{Bmatrix} I & J' & F \\ J & I & 1 \end{Bmatrix}
\end{aligned}
$$

In the centrifugal distortion term, it is assumed that the 'b' term is used exclusively in H_{mhf}:

$$
\begin{aligned}
&\langle \Lambda S \Sigma' J' \Omega' I F | H_{mhfcd} | \Lambda S \Sigma J \Omega I F \rangle = \frac{b_D}{2Bb}\{H_{rot}, H_{mhf}\} \\
&= \frac{b_D}{2Bb}\left[
\begin{array}{l}
\langle \Lambda S \Sigma' J' \Omega' F | H_{rot}\left(\sum_{\Sigma''\Omega''J''}|\Lambda S \Sigma'' J'' \Omega'' F\rangle\langle \Lambda S \Sigma'' J'' \Omega'' F|\right) H_{mhf} | \Lambda S \Sigma J \Omega F \rangle \\
+\langle \Lambda S \Sigma' J' \Omega' F | H_{mhf}\left(\sum_{\Sigma''\Omega''J''}|\Lambda S \Sigma'' J'' \Omega'' F\rangle\langle \Lambda S \Sigma'' J'' \Omega'' F|\right) H_{rot} | \Lambda S \Sigma J \Omega F \rangle
\end{array}
\right]
\end{aligned}
$$

For S > 1*:

$$\left\langle \Lambda S\Sigma' J'\Omega' IF \left| H^{(3)}_{mhf} \right| \Lambda S\Sigma J\Omega IF \right\rangle = -b_s \frac{\sqrt{35}}{4\sqrt{3}} \prod_{k=0}^{6} \sqrt{2S-2+k}\,(-1)^{J'+J+I+F+S-\Sigma-\Omega}$$
$$\times \sqrt{I(I+1)(2I+1)(2J+1)(2J'+1)} \begin{Bmatrix} F & J' & I \\ 1 & I & J \end{Bmatrix}$$
$$\times \sum_q (-1)^q \begin{pmatrix} J' & 1 & J \\ -\Omega' & q & \Omega \end{pmatrix} \begin{pmatrix} S & 3 & S \\ -\Sigma' & q & \Sigma \end{pmatrix} \begin{pmatrix} 3 & 1 & 2 \\ q & -q & 0 \end{pmatrix}$$

***** A.S-C. Cheung and A.J. Merer, *Molecular Physics*, **46** (1), 111-128 (1982).