Supplementary Material:
Second-order average Hamiltonian theory of symmetry-based pulse schemes in the Nuclear Magnetic Resonance of rotating solids: Application to triple-quantum dipolar recoupling

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I. Analytical Expressions for 3Q terms

A. Symmetries of Scaling Factors

Here we examine the relationship between $\kappa_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$ and $\kappa_{\substack{l_1m_1\lambda_1\mu_1\\ l_2m_2\lambda_2\mu_2}}$, i.e., the dependence of the second-order scaling factors upon permutation of the two sets of quantum numbers comprised in the cross-term: $\{(l_2m_2\lambda_2\mu_2),(l_1m_1\lambda_1\mu_1)\} \longleftrightarrow \{(l_1m_1\lambda_1\mu_1),(l_2m_2\lambda_2\mu_2)\}$. This has consequences for the expressions of the symmetrized second-order scaling factors, depending on the R/C category 2-4 that the symmetry-allowed term belongs. According to Eqs. (30)-(35), the scaling factor depends on products of the sums $S^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$ and $S^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$ with the corresponding integrals $A^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$ and $A^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$. From Eqs. (31) and (34) follow directly that $A^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$ is invariant to exchange of the order of the terms, i.e.,

$$A^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}} = A^{\square}_{\substack{l_1m_1\lambda_1\mu_1\\ l_2m_2\lambda_2\mu_2}} \tag{S-1}$$

whereas no such symmetry exists for $A^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$; in the general case, $A^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}} \neq A^{\triangle}_{\substack{l_1m_1\lambda_1\mu_1\\ l_2m_2\lambda_2\mu_2}}$. Further, the expressions for the sum terms, $S^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$ and $S^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$, depend on which R/C category (2, 3a, 3b or 4) the recoupled term belongs (Table I and S-I):

$$S^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}} = S^{\triangle}_{\substack{l_1m_1\lambda_1\mu_1\\ l_2m_2\lambda_2\mu_2}} = \begin{cases} 0 & \text{for class 1, 3a and 3b} \\ 1/N & \text{for class 2 and 4} \end{cases} \tag{S-2}$$

$$S^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}[2] = \left(S^{\square}_{\substack{l_1m_1\lambda_1\mu_1\\ l_2m_2\lambda_2\mu_2}}[2] \right)^* \tag{S-3}$$

$$S^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}[3a] = -S^{\square}_{\substack{l_1m_1\lambda_1\mu_1\\ l_2m_2\lambda_2\mu_2}}[3b] \tag{S-4}$$

$$S^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}[4] = S^{\square}_{\substack{l_1m_1\lambda_1\mu_1\\ l_2m_2\lambda_2\mu_2}}[4] \tag{S-5}$$

The number within brackets denotes the category of the term. Note that most of them are invariant to exchange of the order of the two rows of subscripts (i.e., the order of $(l_2m_2\lambda_2\mu_2)$ and $(l_1m_1\lambda_1\mu_1)$) in the cross-term, except $S^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$ if the term falls into R/C categories 2, 3a, or 3b. Eq. S-4 means that if the term $\{(l_2m_2\lambda_2\mu_2),(l_1m_1\lambda_1\mu_1)\}$ belongs to class 3a, then $\{(l_1m_1\lambda_1\mu_1),(l_2m_2\lambda_2\mu_2)\}$ belongs to class 3b, and that the two sums are related by sign reversal. The equations above imply that only $\kappa^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$ contributes to the scaling factor for terms of R/C categories 3a and 3b, whereas only $\kappa^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$ is contributing in the case of a category 4 term. From these expressions, combined with Eqs. (31), (34), (30) follow that the general form of the symmetrized scaling factor,

$$\kappa_{\binom{l_2m_2\lambda_2\mu_2}{l_1m_1\lambda_1\mu_1}} = \frac{-ni}{2}\left\{\left(S^{\Box}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}} - S^{\Box}_{\substack{l_1m_1\lambda_1\mu_1\\ l_2m_2\lambda_2\mu_2}}\right)A^{\Box}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}} + S^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}\left(A^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}} - A^{\triangle}_{\substack{l_1m_1\lambda_1\mu_1\\ l_2m_2\lambda_2\mu_2}}\right)\right\} \tag{S-6}$$

reduces to one of the following expressions, depending on the relevant R/C category 2-4:

$$\kappa_{\binom{l_2m_2\lambda_2\mu_2}{l_1m_1\lambda_1\mu_1}}[2] = \frac{-in\tau_r}{2}\left\{2i\,\mathrm{Im}\left(S^{\Box}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}\right)A^{\Box}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}} + \frac{1}{N}\left(A^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}} - A^{\triangle}_{\substack{l_1m_1\lambda_1\mu_1\\ l_2m_2\lambda_2\mu_2}}\right)\right\} \tag{S-7}$$

$$\kappa_{\binom{l_2m_2\lambda_2\mu_2}{l_1m_1\lambda_1\mu_1}}[3a,3b] = -in\tau_r S^{\Box}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}A^{\Box}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}} \tag{S-8}$$

$$\kappa_{\binom{l_2m_2\lambda_2\mu_2}{l_1m_1\lambda_1\mu_1}}[4] = \frac{-in\tau_r}{2N}\left(A^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}} - A^{\triangle}_{\substack{l_1m_1\lambda_1\mu_1\\ l_2m_2\lambda_2\mu_2}}\right) \tag{S-9}$$

B. 3Q Average Hamiltonian Frequencies

The explicit forms of the frequencies in Eq. (70) depends on the category 2-4 to which the cross-term belongs. It follows from the general expressions of the symmetrized terms that the frequency $\bar{\omega}^{(ij\times ik)}_{\mathcal{T}_r}$ may be written

$$\bar{\omega}^{(ij\times ik)}_{\mathcal{T}_r} = \frac{-ni\tau_r}{2}\left\{\begin{array}{c}\left(S^{\Box}_{\substack{2m_222\\ 2m_121}} - S^{\Box}_{\substack{2m_121\\ 2m_222}}\right)A^{\Box}_{\substack{2m_222\\ 2m_121}}\\ +S^{\triangle}_{\substack{2m_222\\ 2m_121}}\left(A^{\triangle}_{\substack{2m_222\\ 2m_121}} - A^{\triangle}_{\substack{2m_121\\ 2m_222}}\right)\end{array}\right\}\mathcal{A}^{(ij\times ik)}_{m_2m_1} \tag{S-10}$$

$$= \kappa_{\binom{2m_222}{2m_121}}\mathcal{A}^{(ij\times ik)}_{m_2m_1} \tag{S-11}$$

where $\mathcal{A}^{(ij\times ik)}_{m_2m_1}$ is given by a product of rotor-frame dipolar coupling components according to

$$\mathcal{A}^{(ij\times ik)}_{m_2m_1} = \left[A^{ij}_{m_2}\right]^R\left[A^{ik}_{m_1}\right]^R + \left[A^{ij}_{m_1}\right]^R\left[A^{ik}_{m_2}\right]^R \tag{S-12}$$

Terms belonging to different categories (2, 3a, 3b or 4) provide different expressions; they are obtained by substitution of the symmetrized scaling factors (Eqs. (S-7), (S-8) and (S-9) into Eq. (S-11).

II. Heteronuclear Decoupling during 3Q Recoupling

Heteronuclear ^{1}H-^{13}C decoupling is well-known to be problematic when simultaneously applying ^{13}C recoupling pulses.[S1–5] It has been shown that a ratio between the nutation frequencies $\omega^{H}_{\mathrm{nut}}/\omega^{C}_{\mathrm{nut}} > 3$ is required to reduce signal losses.[S1,2] The complications are particularly acute when employing windowed pulse elements,[S6] as they require strong rf recoupling pulses to minimize the pulse fraction. For 3Q recoupling, signal losses occur otherwise due to increased interferences from ZQ dipolar and chemical shift interactions. Therefore, the unfortunate condition $\omega_{\mathrm{nut}}^{H}/\omega_{\mathrm{nut}}^{C} \approx 1$ had to be employed in our experiments at $B_0 = 4.7$ T.

We observed that the heteronuclear decoupling performance was strongly dependent on the spinning frequency. The experiments on dAla using low spinning speeds employed "CW" decoupling with slightly different amplitudes (optimized individually) during ^{13}C pulses and windows of the $\mathrm{R}18_3^7$-based schemes at both magnetic fields. However, this approach gave severe losses both for dAla and tyrosine at spinning frequencies $\omega_r/2\pi > 7$ kHz. For example, using $\omega_{\mathrm{nut}}^{H} \approx 115$ kHz CW decoupling on tyrosine resulted only in $\approx 2\%$ 3QF efficiency.

We found empirically that the heteronuclear decoupling performance could sometimes be dramatically improved by changing the ^{1}H rf phases synchronously with the various fragments (i.e., pulses and windows) of the ^{13}C rf pulse sequence. Consequently, we optimized the sequence of ^{1}H rf phases and amplitudes individually for each sample. In the experiments of Fig. 6 for dAla, we employed the following sequence of phases: $\left(\phi_{p_1}^H, \phi_{w_1}^H, \phi_{p_2}^H, \phi_{w_2}^H, \phi_{p_3}^H\right) = (0, \pi, 0, \pi, \pi)$, where $\phi_{p_j}^H$ and $\phi_{w_j}^H$ denote the ^{1}H rf phase during the jth ^{13}C pulse and window of $\mathcal{R}_w(\beta)$, respectively (see Eq. (75)). The following phases gave best result for tyrosine: $(0, \pi, \pi, 0, \pi)$. Many combinations provided similar decoupling performance but were consistently reproducible and identical for $(\mathrm{R}18_3^7)3^1$ and $(\mathrm{R}18_3^7\mathrm{R}18_3^{-7})3^1$ on each sample. The reasons for the improved decoupling results are at the moment not fully understood and further investigations along these lines are underway. No improvements over CW decoupling were observed at lower spinning frequencies ($\omega_r/2\pi \lesssim 7$ kHz) at either magnetic field.

III. 3Q-1Q Correlation Experiments

To allow an unrestricted spectral width in ω_1, i.e., an arbitrary incrementation of t_1, the 3Q recoupling sequence must fulfil the condition that *all* its recoupled second-order 3Q terms $\{(l_2, m_2, \lambda_2, \mu_2), (l_1, m_1, \lambda_1, \mu_1)\}$ have *equal* ratios $(m_2 + m_1)/(\mu_2 + \mu_1)$. The requirement for second-order symmetry-based correlation spectroscopy is analogous to that discussed in Refs.[S5,7,8] for first order recoupling scenarios. For instance, from Table III follows that $\mathrm{R}8_1^{-1}$ and $\mathrm{C}7_2^{-1}$ do not meet this condition (and neither do $(\mathcal{S}\mathcal{S}')3^1$ schemes in general) whereas $\mathrm{R}18_3^7$ and $\mathrm{R}14_3^2$ do. t_1 may then be incremented arbitrarily, provided that the following t_1-dependent phase-shift is applied to the reconversion pulse block

$$\Phi_{\mathrm{rec}}(t_1) = \frac{\pi}{3}k + \frac{m_2 + m_1}{\mu_2 + \mu_1}\omega_r t_1 \tag{S-13}$$

where the spin and spatial components depend on the recoupled second-order terms and k is any integer.

In the 3Q-1Q correlation experiment of Fig. 10, the TPPI scheme[S9] was used to obtain a purely absorptive 2D spectrum with sign discrimination along both spectral The spectral widths (after TPPI processing) were 25 kHz and 20 kHz in the first and second spectral dimensions, and (128×350) time-points were recorded.

IV. Second-Order Terms: Generic Analytical Expressions

Here we present the generic closed analytical sums derived from $S^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\l_1m_1\lambda_1\mu_1}}$ (Eq. (32)) and $S^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\l_1m_1\lambda_1\mu_1}}$ (Eq. (35) in the case of $\mathrm{C}N_n^\nu$ and $\mathrm{R}N_n^\nu$ sequences (Table S-I) and for $\mathbb{S}^{\square}_{\mu_2\mu_1}$ (Eq. (58)) and $\mathbb{S}^{\triangle}_{\mu_2\mu_1}$ (Eq. (60)) for MQ phase cycles $\mathcal{S}M^{\chi}$ (Table S-II). These results may be evaluated to the expressions given in Tables I and II.

Table S-I: The generic closed analytical form of $S^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\l_1m_1\lambda_1\mu_1}}$ (Eq. (32)) and $S^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\l_1m_1\lambda_1\mu_1}}$ (Eq. (35)) depending on each category of the second order average Hamiltonian term. These expressions apply both for $\mathrm{C}N_n^\nu$ and $\mathrm{R}N_n^\nu$ sequences. The symbol "$\wedge$" represents the mathematical AND operator. $\mathcal{Q}_1$ and $\mathcal{Q}_2$ are defined as in Eq. (15), e. g., $\mathcal{Q}_1 = \exp\{i2\pi(m_1n-\mu_1\nu)/N\}$ for $\mathrm{C}N_n^\nu$ sequences and $\mathcal{Q}_1 = \exp\{i2\pi(m_1n-\mu_1\nu-\lambda_1N/2)/N\}$ for $\mathrm{R}N_n^\nu$ sequences.

$S^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\l_1m_1\lambda_1\mu_1}}$	$S^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\l_1m_1\lambda_1\mu_1}}$	$\mathrm{C}N_n^\nu/\mathrm{R}N_n^\nu$ Selection Rules	C/R Category
0	0	$\mathcal{Q}_1\neq1 \ \wedge\ \mathcal{Q}_2\neq1\ \wedge\ \mathcal{Q}_1\mathcal{Q}_2\neq1$	1
$\frac{1}{N(\mathcal{Q}_1-1)}=-\frac{\mathcal{Q}_2}{N(\mathcal{Q}_2-1)}$	$\frac{1}{N}$	$\mathcal{Q}_1\neq1 \ \wedge\ \mathcal{Q}_2\neq1\ \wedge\ \mathcal{Q}_1\mathcal{Q}_2=1$	2
$\frac{1}{N(\mathcal{Q}_2-1)}$	0	$\mathcal{Q}_1=1 \ \wedge\ \mathcal{Q}_2\neq1\ \wedge\ \mathcal{Q}_1\mathcal{Q}_2\neq1$	3a
$-\frac{1}{N(\mathcal{Q}_1-1)}$	0	$\mathcal{Q}_1\neq1 \ \wedge\ \mathcal{Q}_2=1\ \wedge\ \mathcal{Q}_1\mathcal{Q}_2\neq1$	3b
$\frac{N-1}{2N}$	$\frac{1}{N}$	$\mathcal{Q}_1=1 \ \wedge\ \mathcal{Q}_2=1\ \wedge\ \mathcal{Q}_1\mathcal{Q}_2=1$	4

Table S-II: The generic expressions for $\mathbb{S}^{\square}_{\mu_2\mu_1}$ (Eq. (58)) and $\mathbb{S}^{\triangle}_{\mu_2\mu_1}$ (Eq. (60)) depending on the category of the second order average Hamiltonian term for MQ phase cycles $\mathcal{S}M^{\chi}$. The symbol "$\wedge$" represents the mathematical AND operator. $\mathcal{P}_1$ and $\mathcal{P}_2$ are defined as in Eq. (47), e. g., $\mathcal{P}_1 = \exp\{-i2\pi\mu_1\nu/N\}$.

$\mathbb{S}^{\square}_{\mu_2\mu_1}$	$\mathbb{S}^{\triangle}_{\mu_2\mu_1}$	MQ Selection Rules	MQ Category
0	0	$\mathcal{P}_1 \neq 1 \ \wedge \ \mathcal{P}_2 \neq 1 \ \wedge \ \mathcal{P}_1\mathcal{P}_2 \neq 1$	1
$\frac{1}{M(\mathcal{P}_1-1)} = -\frac{\mathcal{P}_2}{M(\mathcal{P}_2-1)}$	$\frac{1}{M}$	$\mathcal{P}_1 \neq 1 \ \wedge \ \mathcal{P}_2 \neq 1 \ \wedge \ \mathcal{P}_1\mathcal{P}_2 = 1$	2
$\frac{1}{M(\mathcal{P}_2-1)}$	0	$\mathcal{P}_1 = 1 \ \wedge \ \mathcal{P}_2 \neq 1 \ \wedge \ \mathcal{P}_1\mathcal{P}_2 \neq 1$	3a
$-\frac{1}{M(\mathcal{P}_1-1)}$	0	$\mathcal{P}_1 \neq 1 \ \wedge \ \mathcal{P}_2 = 1 \ \wedge \ \mathcal{P}_1\mathcal{P}_2 \neq 1$	3b
$\frac{M-1}{2M}$	$\frac{1}{M}$	$\mathcal{P}_1 = 1 \ \wedge \ \mathcal{P}_2 = 1 \ \wedge \ \mathcal{P}_1\mathcal{P}_2 = 1$	4

Table S-III: Summary of the second order selection rules and average Hamiltonian properties for the MQ-phase cycled $\mathcal{S}M^{\chi}$ sequences. The symbol "$\wedge$" represents the mathematical AND operator. For each case, the selection rules and the corresponding MQ-category and R/C-category are indicated and *which* sums $\mathbb{S}^{\square}_{\mu_2\mu_1}$ and/or $\mathbb{S}^{\triangle}_{\mu_2\mu_1}$ that vanish. It is important to note that indication of $\bar{H}^{\Lambda_2\times\Lambda_1}_{\substack{l_2m_2\lambda_2\mu_2\\l_1m_1\lambda_1\mu_1}} \neq 0$ only implies that the term is *symmetry-allowed*: its scaling factor Eq. (56) may still vanish due to additional symmetries of the basic element $\mathcal{E}^0$.

$\bar{H}^{\Lambda_2\times\Lambda_1}_{\substack{l_2m_2\lambda_2\mu_2\\l_1m_1\lambda_1\mu_1}}$	$\mathbb{S}^{\square}_{\mu_2\mu_1}$	$\mathbb{S}^{\triangle}_{\mu_2\mu_1}$	$S^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\l_1m_1\lambda_1\mu_1}}$	$S^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\l_1m_1\lambda_1\mu_1}}$	$S_{l_1m_1\lambda_1\mu_1}$	$S_{l_2m_1\lambda_2\mu_2}$	Selection Rules	MQ Category	R/C Category
$=0$	$=0$	$=0$	$=0$	$=0$	$=0$	$=0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1\neq1 \wedge \mathcal{Q}_2\neq1 \wedge \mathcal{Q}_1\mathcal{Q}_2\neq1)$	1	1
$=0$	$=0$	$=0$	$\neq0$	$\neq0$	$=0$	$=0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1\neq1 \wedge \mathcal{Q}_2\neq1 \wedge \mathcal{Q}_1\mathcal{Q}_2=1)$	1	2
$=0$	$=0$	$=0$	$\neq0$	$=0$	$\neq0$	$=0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1=1 \wedge \mathcal{Q}_2\neq1 \wedge \mathcal{Q}_1\mathcal{Q}_2\neq1)$	1	3a
$=0$	$=0$	$=0$	$\neq0$	$=0$	$=0$	$\neq0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1\neq1 \wedge \mathcal{Q}_2=1 \wedge \mathcal{Q}_1\mathcal{Q}_2\neq1)$	1	3b
$=0$	$=0$	$=0$	$\neq0$	$\neq0$	$\neq0$	$\neq0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1=1 \wedge \mathcal{Q}_2=1 \wedge \mathcal{Q}_1\mathcal{Q}_2=1)$	1	4
$=0$	$\neq0$	$\neq0$	$=0$	$=0$	$=0$	$=0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2=1) \wedge (\mathcal{Q}_1\neq1 \wedge \mathcal{Q}_2\neq1 \wedge \mathcal{Q}_1\mathcal{Q}_2\neq1)$	2	1
$\neq0$	$\neq0$	$\neq0$	$\neq0$	$\neq0$	$=0$	$=0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2=1) \wedge (\mathcal{Q}_1\neq1 \wedge \mathcal{Q}_2\neq1 \wedge \mathcal{Q}_1\mathcal{Q}_2=1)$	2	2
$\neq0$	$\neq0$	$\neq0$	$\neq0$	$=0$	$\neq0$	$=0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2=1) \wedge (\mathcal{Q}_1=1 \wedge \mathcal{Q}_2\neq1 \wedge \mathcal{Q}_1\mathcal{Q}_2\neq1)$	2	3a
$\neq0$	$\neq0$	$\neq0$	$\neq0$	$=0$	$=0$	$\neq0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2=1) \wedge (\mathcal{Q}_1\neq1 \wedge \mathcal{Q}_2=1 \wedge \mathcal{Q}_1\mathcal{Q}_2\neq1)$	2	3b
$\neq0$	$\neq0$	$\neq0$	$\neq0$	$\neq0$	$\neq0$	$\neq0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2=1) \wedge (\mathcal{Q}_1=1 \wedge \mathcal{Q}_2=1 \wedge \mathcal{Q}_1\mathcal{Q}_2=1)$	2	4
$=0$	$\neq0$	$=0$	$=0$	$=0$	$=0$	$=0$	$(\mathcal{P}_1=1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1\neq1 \wedge \mathcal{Q}_2\neq1 \wedge \mathcal{Q}_1\mathcal{Q}_2\neq1)$	3a	1
$=0$	$\neq0$	$=0$	$\neq0$	$\neq0$	$=0$	$=0$	$(\mathcal{P}_1=1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1\neq1 \wedge \mathcal{Q}_2\neq1 \wedge \mathcal{Q}_1\mathcal{Q}_2=1)$	3a	2
$=0$	$\neq0$	$=0$	$\neq0$	$=0$	$\neq0$	$=0$	$(\mathcal{P}_1=1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1=1 \wedge \mathcal{Q}_2\neq1 \wedge \mathcal{Q}_1\mathcal{Q}_2\neq1)$	3a	3a
$=0$	$\neq0$	$=0$	$\neq0$	$=0$	$=0$	$\neq0$	$(\mathcal{P}_1=1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1\neq1 \wedge \mathcal{Q}_2=1 \wedge \mathcal{Q}_1\mathcal{Q}_2\neq1)$	3a	3b
$\neq0$	$\neq0$	$=0$	$\neq0$	$\neq0$	$\neq0$	$\neq0$	$(\mathcal{P}_1=1 \wedge \mathcal{P}_2\neq1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1=1 \wedge \mathcal{Q}_2=1 \wedge \mathcal{Q}_1\mathcal{Q}_2=1)$	3a	4
$=0$	$\neq0$	$=0$	$=0$	$=0$	$=0$	$=0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2=1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1\neq1 \wedge \mathcal{Q}_2\neq1 \wedge \mathcal{Q}_1\mathcal{Q}_2\neq1)$	3b	1
$=0$	$\neq0$	$=0$	$\neq0$	$\neq0$	$=0$	$=0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2=1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1\neq1 \wedge \mathcal{Q}_2\neq1 \wedge \mathcal{Q}_1\mathcal{Q}_2=1)$	3b	2
$=0$	$\neq0$	$=0$	$\neq0$	$=0$	$\neq0$	$=0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2=1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1=1 \wedge \mathcal{Q}_2\neq1 \wedge \mathcal{Q}_1\mathcal{Q}_2\neq1)$	3b	3a
$=0$	$\neq0$	$=0$	$\neq0$	$=0$	$=0$	$\neq0$	$(\mathcal{P}_1\neq1 \wedge \mathcal{P}_2=1 \wedge \mathcal{P}_1\mathcal{P}_2\neq1) \wedge (\mathcal{Q}_1\neq1 \wedge \mathcal{Q}_2=1 \wedge \mathcal{Q}_1\mathcal{Q}_2\neq1)$	3b	3b

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$\bar{H}^{\Lambda_2\times\Lambda_1}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$	$\mathbb{S}^{\square}_{\mu_2\mu_1}$	$\mathbb{S}^{\triangle}_{\mu_2\mu_1}$	$S^{\square}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$	$S^{\triangle}_{\substack{l_2m_2\lambda_2\mu_2\\ l_1m_1\lambda_1\mu_1}}$	$S_{l_1m_1\lambda_1\mu_1}$	$S_{l_2m_1\lambda_2\mu_2}$	Selection Rules	MQ Category	R/C Category
$\neq 0$	$\neq 0$	$= 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$(\mathcal{P}_1 \neq 1 \ \wedge \ \mathcal{P}_2 = 1 \ \wedge \ \mathcal{P}_1\mathcal{P}_2 \neq 1) \ \wedge \ (\mathcal{Q}_1 = 1 \ \wedge \ \mathcal{Q}_2 = 1 \ \wedge \ \mathcal{Q}_1\mathcal{Q}_2 = 1)$	3b	4
$= 0$	$\neq 0$	$\neq 0$	$= 0$	$= 0$	$= 0$	$= 0$	$(\mathcal{P}_1 = 1 \ \wedge \ \mathcal{P}_2 = 1 \ \wedge \ \mathcal{P}_1\mathcal{P}_2 = 1) \ \wedge \ (\mathcal{Q}_1 \neq 1 \ \wedge \ \mathcal{Q}_2 \neq 1 \ \wedge \ \mathcal{Q}_1\mathcal{Q}_2 \neq 1)$	4	1
$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$= 0$	$= 0$	$(\mathcal{P}_1 = 1 \ \wedge \ \mathcal{P}_2 = 1 \ \wedge \ \mathcal{P}_1\mathcal{P}_2 = 1) \ \wedge \ (\mathcal{Q}_1 \neq 1 \ \wedge \ \mathcal{Q}_2 \neq 1 \ \wedge \ \mathcal{Q}_1\mathcal{Q}_2 = 1)$	4	2
$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$= 0$	$\neq 0$	$= 0$	$(\mathcal{P}_1 = 1 \ \wedge \ \mathcal{P}_2 = 1 \ \wedge \ \mathcal{P}_1\mathcal{P}_2 = 1) \ \wedge \ (\mathcal{Q}_1 = 1 \ \wedge \ \mathcal{Q}_2 \neq 1 \ \wedge \ \mathcal{Q}_1\mathcal{Q}_2 \neq 1)$	4	3a
$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$= 0$	$= 0$	$\neq 0$	$(\mathcal{P}_1 = 1 \ \wedge \ \mathcal{P}_2 = 1 \ \wedge \ \mathcal{P}_1\mathcal{P}_2 = 1) \ \wedge \ (\mathcal{Q}_1 \neq 1 \ \wedge \ \mathcal{Q}_2 = 1 \ \wedge \ \mathcal{Q}_1\mathcal{Q}_2 \neq 1)$	4	3b
$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	$(\mathcal{P}_1 = 1 \ \wedge \ \mathcal{P}_2 = 1 \ \wedge \ \mathcal{P}_1\mathcal{P}_2 = 1) \ \wedge \ (\mathcal{Q}_1 = 1 \ \wedge \ \mathcal{Q}_2 = 1 \ \wedge \ \mathcal{Q}_1\mathcal{Q}_2 = 1)$	4	4

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