



Supplement of

Efficient polynomial analysis of magic-angle spinning sidebands and application to order parameter determination in anisotropic samples

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S1. AVERAGES OVER POWER PRODUCTS OF TRIGONOMETRIC FUNCTIONS

A. Azimuthal average

1. Proposition

$$\langle \sin^m \gamma \cos^n \gamma \rangle_\gamma = \begin{cases} \frac{(m-1)!!(n-1)!!}{(m+n)!!} & \text{if } m \text{ and } n \text{ even} \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

Meaning of the averaging symbol:

$$\langle A(\gamma) \rangle_\gamma = \frac{1}{2\pi} \int_a^{a+2\pi} A(\gamma) d\gamma \quad ; \quad a \in \mathbb{R} \quad (2)$$

For sake of shortness of the expressions, the index γ is omitted in the following.

2. Proof for odd exponents:

If the sine power m is odd:

We set $a = -\pi$, split the integration range in $[-\pi, 0]$ and $[0, \pi]$ and substitute in the first part $\gamma \rightarrow -\gamma$:

$$\int_{-\pi}^0 \sin^m \gamma \cos^n \gamma d\gamma + \int_0^\pi \sin^m \gamma \cos^n \gamma d\gamma = \int_0^\pi \sin^m(-\gamma) \cos^n(-\gamma) d(-\gamma) + \int_0^\pi \sin^m \gamma \cos^n \gamma d\gamma = 0 \quad (3)$$

If the cosine power n is odd: We substitute $\gamma \rightarrow \pi/2 - \gamma$ and get again an integral with odd sine power which therefore will be zero likewise.

3. Proof for even exponents

This will be done by mathematical induction from n to $n+2$ with base case $n=0$. The latter has to be proven with an induction from m to $m+2$.

Base case $n=0$: The proposition eqn. (1) has here the form:

$$\langle \sin^m \gamma \rangle = \frac{(m-1)!!}{m!!} \quad (4)$$

To prove this by a further induction we check first that the base case is obviously valid for $m=0$. The inductive step $m \rightarrow m+2$ is done by

$$\begin{aligned} \int \sin^{m+2} \gamma d\gamma &= -\cos \gamma \sin^{m+1} \gamma + (m+1) \int \cos^2 \gamma \sin^m \gamma d\gamma \\ &= -\cos \gamma \sin^{m+1} \gamma + (m+1) \int \sin^m \gamma d\gamma - (m+1) \int \sin^{m+2} \gamma d\gamma \end{aligned} \quad (5)$$

Inserting the integration limits: first term at the right-hand side is cancelled, and we get

$$\langle \sin^{m+2} \gamma \rangle = \frac{m+1}{m+2} \langle \sin^m \gamma \rangle = \frac{m+1}{m+2} \cdot \frac{(m-1)!!}{m!!} = \frac{(m+1)!!}{(m+2)!!} \quad (6)$$

That means, the validity of the sub-proposition (4) for m implies the validity of that also for $m+2$. This proves sub-proposition (4) for all even m . Therefore the base case for the following induction is valid.

Inductive step $n \rightarrow n+2$: Suppose proposition (1) is valid for a particular n . We investigate this expression for $n \rightarrow n+2$ by replacing $\cos^{n+2} \gamma = \cos^n \gamma (1 - \sin^2 \gamma)$:

$$\begin{aligned}
\langle \sin^m \gamma \cos^{n+2} \gamma \rangle &= \langle \sin^m \gamma \cos^n \gamma \rangle - \langle \sin^{m+2} \gamma \cos^n \gamma \rangle = \frac{(m-1)!!(n-1)!!}{(m+n)!!} - \frac{(m+1)!!(n-1)!!}{(m+2+n)!!} \\
&= \frac{(m-1)!!(n-1)!!}{(m+2+n)!!} [(m+n+2) - (m+1)] = \frac{(m-1)!!(n+1)!!}{(m+2+n)!!}
\end{aligned} \tag{7}$$

which is exactly the proposition for $n+2$.

The validity of proposition (1) for n implies the validity of the proposition also for $n+2$. This proves that proposition for all even m and n .

□

B. Polar average

1. Proposition

$$\langle \cos^n \alpha \sin^m \alpha \rangle_{\cos \alpha} = \begin{cases} \frac{m!!(n-1)!!}{(m+n+1)!!} & \text{if } m \text{ and } n \text{ even} \\ \frac{m!!(n-1)!!}{(m+n+1)!!} \cdot \frac{\pi}{2} & \text{if } m \text{ odd and } n \text{ even} \\ 0 & \text{if } n \text{ odd} \end{cases} \tag{8}$$

Meaning of the averaging symbol:

$$\langle A(\alpha) \rangle_{\cos \alpha} = \frac{1}{\pi} \int_0^\pi A(\alpha) \sin \alpha \, d\alpha = \frac{1}{2} \int_{-1}^1 A(\alpha) \, d(\cos \alpha) \tag{9}$$

For sake of shortness of the expressions, the index $\cos \alpha$ is omitted in the following.

For odd n : Split of the integration interval into the parts $[0, \pi/2]$ and $[\pi/2, \pi]$; in the second part: substitution $\alpha \rightarrow \pi - \alpha$, then $d\alpha$ and $\cos \alpha$ alternate the sign:

$$\begin{aligned}
\langle \cos^n \alpha \sin^m \alpha \rangle &= \frac{1}{\pi} \int_0^\pi \cos^n \alpha \sin^{m+1} \alpha \, d\alpha = \frac{1}{\pi} \int_0^{\pi/2} \cos^n \alpha \sin^{m+1} \alpha \, d\alpha + \frac{1}{\pi} \int_{\pi/2}^\pi \cos^n \alpha \sin^{m+1} \alpha \, d\alpha \\
&= \frac{1}{\pi} \int_0^{\pi/2} \cos^n \alpha \sin^{m+1} \alpha \, d\alpha + \frac{1}{\pi} \int_{\pi/2}^0 \cos^n \alpha \sin^{m+1} \alpha \, d\alpha = 0
\end{aligned} \tag{10}$$

This proves proposition (8) for odd n .

For even n : Prove by mathematical induction $m \rightarrow m+2$; therefore two base cases (here $m=0$ and $m=1$) are needed.

Base case 1 ($m=0$): Substitution $\cos \alpha \rightarrow c$:

$$\langle \cos^n \alpha \rangle = \frac{1}{2} \int_{-1}^1 c^n \, dc = \frac{1}{2} \left[\frac{1}{n+1} c^{n+1} \right]_{-1}^1 = \frac{1}{n+1} \tag{11}$$

which proves proposition (8) for $m=0$ and $n \in \mathbb{N}$.

Base case 2 ($m=1$): To be shown here:

$$\langle \cos^n \alpha \sin \alpha \rangle = \frac{(n-1)!!}{(n+2)!!} \cdot \frac{\pi}{2} \tag{12}$$

This is done by the following steps:

$$\langle \cos^{n+2} \alpha \sin \alpha \rangle = \frac{1}{2} \int_0^\pi \cos^{n+2} \alpha \sin^2 \alpha \, d\alpha = \frac{1}{2} \int_0^\pi (\cos^{n+2} \alpha - \cos^{n+4} \alpha) \, d\alpha \quad (13)$$

Partial integration of a cosine power:

$$\int_0^\pi \cos^p \alpha \, d\alpha = [\sin \alpha \cos^{p-1} \alpha]_0^\pi - (p-1) \int_0^\pi (-\sin^2 \alpha) \cos^{p-2} \alpha \, d\alpha = (p-1) \cdot 2 \langle \cos^{p-2} \alpha \sin \alpha \rangle \quad (14)$$

Inserting this rule into eqn. (13):

$$\langle \cos^{p+2} \alpha \sin \alpha \rangle = (p+1) \langle \cos^p \alpha \sin \alpha \rangle - (p+3) \langle \cos^{p+2} \alpha \sin \alpha \rangle \quad (15)$$

or

$$\langle \cos^{n+2} \alpha \sin \alpha \rangle = \frac{n+1}{n+4} \langle \cos^n \alpha \sin \alpha \rangle = \frac{n+1}{n+4} \cdot \frac{(n-1)!!}{(n+2)!!} \cdot \frac{\pi}{2} = \frac{(n+1)!!}{(n+4)!!} \cdot \frac{\pi}{2} \quad (16)$$

It can be shown easily that eqn. (12) is fulfilled for $n = 0$. This together with eqn. (16) as induction step proves base case 2.

Inductive step $m \rightarrow m+2$: Suppose proposition (8) would be valid for a particular m and all even n . We calculate the average for $m+2$ by replacing $\sin^{m+2} \gamma = \sin^m \gamma (1 - \cos^2 \gamma)$:

$$\begin{aligned} \langle \cos^n \alpha \sin^{m+2} \alpha \rangle &= \langle \cos^n \alpha \sin^m \alpha \rangle - \langle \cos^{n+2} \alpha \sin^m \alpha \rangle \\ &= \frac{m!! (n-1)!!}{(m+n+1)!!} f_n - \frac{m!! (n+1)!!}{(m+n+3)!!} f_n \\ &= \frac{m!! (n-1)!!}{(m+n+3)!!} [(m+n+3) - (n+1)] f_n \\ &= \frac{(m+2)!! (n-1)!!}{(m+n+3)!!} f_n \end{aligned} \quad (17)$$

($f_n := 1$ for even n and $\pi/2$ for odd n) which is exactly proposition (8) for $m \rightarrow m+2$.

This inductive step together with the proven base cases proves proposition (8) $\forall \{m, n\} \subset \mathbb{N}$.

□

S2. POWDER-AVERAGED PHASE POWERS

Listed up to eighth power:

$$\langle \Phi \rangle = 0 \quad (18)$$

$$\langle \Phi^2 \rangle = \left(\frac{\delta\omega_0}{\omega_r} \right)^2 \cdot \frac{1}{45} (3 + \eta^2) (5 + \cos \gamma_r) (1 - \cos \gamma_r) \quad (19)$$

$$\langle \Phi^3 \rangle = \left(\frac{\delta\omega_0}{\omega_r} \right)^3 \cdot \frac{4}{5 \cdot 7} (1 - \eta^2) \sin \gamma_r \sin^2 \frac{\gamma_r}{2} \quad (20)$$

$$\langle \Phi^4 \rangle = \left(\frac{\delta\omega_0}{\omega_r} \right)^4 \cdot \frac{4}{945} (3 + \eta^2)^2 (5 + \cos \gamma_r)^2 \sin^4 \frac{\gamma_r}{2} \quad (21)$$

$$\langle \Phi^5 \rangle = \left(\frac{\delta\omega_0}{\omega_r} \right)^5 \cdot \frac{32}{693} (3 + \eta^2) (1 - \eta^2) (5 + \cos \gamma_r) \sin \gamma_r \sin^4 \frac{\gamma_r}{2} \quad (22)$$

$$\begin{aligned} \langle \Phi^6 \rangle = & \left(\frac{\delta\omega_0}{\omega_r} \right)^6 \cdot \left[\frac{1}{16016} \left(5515 + \frac{16381}{3} \eta^2 + \frac{49963}{27} \eta^4 + \frac{49471}{243} \eta^6 \right) \right. \\ & - \frac{1}{286} \left(131 + \frac{1009}{7} \eta^2 + \frac{2567}{63} \eta^4 + \frac{2843}{567} \eta^6 \right) \cos \gamma_r + \frac{1}{32032} \left(2983 + 6219 \eta^2 + \frac{2477}{9} \eta^4 + \frac{12185}{81} \eta^6 \right) \cos 2\gamma_r \\ & + \frac{1}{12012} \left(397 - \frac{1237}{3} \eta^2 + \frac{8429}{27} \eta^4 + \frac{1145}{243} \eta^6 \right) \cos 3\gamma_r - \frac{1}{16016} \left(179 - \frac{235}{3} \eta^2 + \frac{3155}{27} \eta^4 + \frac{839}{243} \eta^6 \right) \cos 4\gamma_r \\ & \left. - \frac{1}{143} \left(\frac{5}{28} + \frac{19}{84} \eta^2 + \frac{37}{756} \eta^4 + \frac{7}{972} \eta^6 \right) \cos 5\gamma_r - \frac{1}{24} \frac{1}{143} \left(\frac{5}{28} + \frac{19}{84} \eta^2 + \frac{37}{756} \eta^4 + \frac{7}{972} \eta^6 \right) \cos 6\gamma_r \right] \quad (23) \end{aligned}$$

$$\langle \Phi^7 \rangle = \left(\frac{\delta\omega_0}{\omega_r} \right)^7 \cdot \frac{64}{3861} (\eta^2 - 1) (3 + \eta^2)^2 (5 + \cos \gamma_r)^2 \cos \frac{\gamma_r}{2} \sin^7 \frac{\gamma_r}{2} \quad (24)$$

$$\begin{aligned} \langle \Phi^8 \rangle = & \left(\frac{\delta\omega_0}{\omega_r} \right)^8 \cdot \frac{1}{15949791} \cdot 4 (3 + \eta^2) (5 + \cos \gamma_r) [1274778 + 282042\eta^2 + 645534\eta^4 + 34958\eta^6 \\ & + 3 (296217 - 132759\eta^2 + 194067\eta^4 + 5675\eta^6) \cos \gamma_r + 51030 \cos 2\gamma_r + 1701 \cos 3\gamma_r \\ & + \eta^2 (2997 + 279\eta^2 + 79\eta^4) (30 \cos 2\gamma_r + \cos 3\gamma_r)] \sin^8 \frac{\gamma_r}{2} \quad (25) \end{aligned}$$

S3. MATHEMATICA EXPRESSIONS FOR EVALUATION OF THE GENERAL SSB POLYNOMIAL

The following passages can be copied and pasted into Mathematica, possibly with an in-between step of pasting the text into a simple text editor to remove formatting information. Note that on some systems it seems that the curly brackets { and } are pasted as letters *f* and *g*, respectively. Since *f* and *g* do not appear in the formulae, search-and-replace can be used.

First, we define an auxiliary function with the independent variables #1, #2 and #3 being identified with n , k , and η , respectively:

```
aux = Sum[#2!/(p!q!(#2 - p - q)!)*Binomial[#1 - 2*#2, r]2^(4*#2 + r + p)/6^#1*(-1)^r*(p + r - 1)!!(q + #1 - 2*#2 - r - 1)!/(p + q + #1 - 2*#2)!!(1 + (-1)^(r - p))(1 + (-1)^(q + #1 + 2*#2 - r))/4*Sum[(-1)^(q - s + u)*Binomial[q,s]*Binomial[#2 - p - q, t]*Binomial[#1 - 2*#2 - r, u]*(2*#2)!! (p + r + 2*s + 2*t + 2*u - 1)!/(2*#2 + p + r + 2*s + 2*t + 2*u + 1)!*Sum[(-1)^v*3^(#1 - 2*#2 + p - r + 2*s + 2*t - v - w)*Binomial[p + 2*s + 2*t + u, v] Binomial[#1 - 2*#2 - r - u, w]*#3^(v + w + 2*#2 - p - 2*s - 2*t + r)*(v + w - 1)!! (2*#2 - p - 2*s - 2*t + r - 1)!/(v + w + 2*#2 - p - 2*s - 2*t + r)!!*(1 + (-1)^(v + w))*(1 + (-1)^(r - p))/4, {w, 0, #1 - 2*#2 - r - u}, {v, 0, p + 2*s + 2*t + u}, {u, 0, #1 - 2*#2 - r}, {t, 0, #2 - p - q}, {s, 0, q}, {r, 0, #1 - 2*#2}, {q, 0, #2}, {p, 0, #2}]&;
```

The general function for SSB generation, with #1, #2, #3 and #4 identified with the SSB order m , $\delta\omega_0/\omega_r$, η and the maximum order n of the polynomial, respectively, is then:

```
rsb = Sum[1/2^n*#2^n*(-1)^(n - k - #1 - b)/((n - k - #1 - 2*b)!*(3*k - n + #1 + 2b)!(n - 2*k - b)!*b!)*aux[n, k, #3], {n, #1, #4}, {k, 0, n/2}, {b, 0, n - 2*k}] &;
```

With this, one can readily generate the SSB polynomials, e.g. for the centerband ($m = 0$) up to order $n = 6$:

```
rsb[0, delta, eta, 6] // Simplify
```

S4. SPINNING SIDEBAND INTENSITIES

Equations for SSB intensities using polynomials up to 12th order in ω_0/ω_r
(abbreviations: $K_1 := 3 + \eta^2$, $K_2 := 1 - \eta^2$ and $w = \delta\omega_0/\omega_r$).

$$\begin{aligned}
I_0 = & 1 - \frac{K_1^2}{20}w^2 + \frac{227 K_1^2}{181\,440}w^4 - \frac{49\,471 K_1^3 + 4\,428 K_2^2}{2\,802\,159\,360}w^6 + \frac{K_1(1\,466\,405 K_1^3 - 709\,776 K_2^2)}{9\,146\,248\,151\,040}w^8 \\
& - \frac{K_1^2(286\,311\,167 K_1^3 - 494\,915\,400 K_2^2)}{281\,521\,518\,089\,011\,200}w^{10} \\
& + \frac{998\,271\,153\,509 K_1^6 - 2\,160 K_2^2(1\,577\,931\,893 K_1^3 + 218\,222\,883 K_2^2)}{209\,789\,835\,279\,931\,146\,240\,000}w^{12}
\end{aligned} \tag{26}$$

$$\begin{aligned}
I_{\pm 1} = & \frac{K_1}{45}w^2 \mp \frac{K_2}{105}w^3 - \frac{17 K_1^2}{22\,680}w^4 \pm \frac{23 K_1 K_2}{83\,160}w^5 + \frac{2\,843 K_1^3 - 2\,484 K_2^2}{233\,513\,280}w^6 \\
& \mp \frac{19 K_1^2 K_2}{5\,189\,184}w^7 - \frac{K_1(123\,823 K_1^3 - 285\,552 K_2^2)}{1\,028\,952\,916\,992}w^8 \pm \frac{K_2(959\,357 K_1^3 - 196\,884 K_2^2)}{32\,583\,509\,038\,080}w^9 \\
& + \frac{K_1^2(11\,362\,895 K_1^3 - 46\,559\,016 K_2^2)}{14\,076\,075\,904\,450\,560}w^{10} \mp \frac{K_1 K_2(766\,057 K_1^3 - 663\,984 K_2^2)}{4\,692\,025\,301\,483\,520}w^{11} \\
& - \frac{34\,324\,127\,551 K_1^6 - 2\,160 K_2^2(96\,357\,427 K_1^3 + 2\,033\,937 K_2^2)}{8\,741\,243\,136\,663\,797\,760\,000}w^{12}
\end{aligned} \tag{27}$$

$$\begin{aligned}
I_{\pm 2} = & \frac{K_1}{360}w^2 \pm \frac{K_2}{210}w^3 + \frac{K_1^2}{12\,960}w^4 \mp \frac{17 K_1 K_2}{83\,160}w^5 - \frac{12185 K_1^3 - 87372 K_2^2}{3736212480}w^6 \\
& \pm \frac{49 K_1^2 K_2}{14826240}w^7 + \frac{(3 + \eta^2)(966239 K_1^3 - 10569744 K_2^2)}{20579058339840}w^8 \mp \frac{K_2(990181 K_1^3 - 583956 K_2^2)}{32\,583\,509\,038\,080}w^9 \\
& - \frac{(3 + \eta^2)^2(14591857 K_1^3 - 197993592 K_2^2)}{37536202411868160}w^{10} \pm \frac{K_1 K_2(4464013 K_1^3 - 7892208 K_2^2)}{23981462652026880}w^{11} \\
& + \frac{75617921797 K_1^6 - 2\,160 K_2^2(548505769(3 + \eta^2)^3 - 72353061 K_2^2)}{34964972546655191040000}w^{12}
\end{aligned} \tag{28}$$

$$\begin{aligned}
I_{\pm 3} = & \frac{K_1^2}{22\,680}w^4 \pm \frac{K_1 K_2}{27720}w^5 - \frac{1\,145 K_1^3 + 65556 K_2^2}{4203239040}w^6 \mp \frac{163 K_1^2 K_2}{155675520}w^7 \\
& - \frac{K_1(9379 K_1^3 - 682128 K_2^2)}{1714921528320}w^8 \pm \frac{K_2(2845 K_1^3 - 5076 K_2^2)}{212964111360}w^9 \\
& + \frac{K_1^2(224699 K_1^3 - 10360440 K_2^2)}{2346012650741760}w^{10} \mp \frac{K_1 K_2(1832201 K_1^3 - 7529328 K_2^2)}{17986096989020160}w^{11} \\
& - \frac{19307643899 K_1^6 - 2\,160 K_2^2(360943523 K_1^3 - 121172787 K_2^2)}{26223729409991393280000}w^{12}
\end{aligned} \tag{29}$$

$$\begin{aligned}
I_{\pm 4} = & \frac{K_1^2}{362880}w^4 \pm \frac{K_1 K_2}{166320}w^5 + \frac{839 K_1^3 + 20844 K_2^2}{5604318720}w^6 \mp \frac{K_1^2 K_2}{77837760}w^7 \\
& - \frac{K_1(58999 K_1^3 + 5681232 K_2^2)}{41158116679680}w^8 \pm \frac{K_2(2845 K_1^3 - 5076 K_2^2)}{32583509038080}w^9 \\
& + \frac{K_1^2(34081 K_1^3 - 18031032 K_2^2)}{9384050602967040}w^{10} \pm \frac{K_1 K_2(233311 K_1^3 - 2825712 K_2^2)}{8993048494510080}w^{11} \\
& + \frac{11419571509 K_1^6 - 2\,160 K_2^2(656644693 K_1^3 - 496531917 K_2^2)}{93239926791080509440000}w^{12}
\end{aligned} \tag{30}$$

S5. 2D OSCILLATION COEFFICIENTS

A. Belonging to I_0

$$C_{00} = I_0^{(\text{iso})} + \left(\frac{\omega_0\delta}{\omega_r}\right)^2 \left(\frac{1}{12} Q_2^{(2)} \langle P_2 \rangle - \frac{31}{96} Q_4^{(2)} \langle P_4 \rangle\right) + \left(\frac{\omega_0\delta}{\omega_r}\right)^4 \left(\frac{85}{528} Q_{11} \langle P_2 \rangle + Q_{21} \langle P_4 \rangle + \frac{59}{3024} Q_3 \langle P_6 \rangle + \frac{19733}{7248384} Q_4 \langle P_8 \rangle\right) \quad (31)$$

$$C_{02} = \left(\frac{\omega_0\delta}{\omega_r}\right)^2 \frac{3 Q_2^{(2)} \langle P_2 \rangle + 5 Q_4^{(2)} \langle P_4 \rangle}{18} + \left(\frac{\omega_0\delta}{\omega_r}\right)^4 \cdot \frac{1}{12} \left(Q_{12} \langle P_2 \rangle - Q_{22} \langle P_4 \rangle + \frac{1}{2} Q_3 \langle P_6 \rangle - \frac{1}{11} Q_4 \langle P_8 \rangle\right) \quad (32)$$

$$C_{04} = -\left(\frac{\omega_0\delta}{\omega_r}\right)^2 \frac{35}{576} Q_4^{(2)} \langle P_4 \rangle + \left(\frac{\omega_0\delta}{\omega_r}\right)^4 \cdot \frac{1}{12} \left(Q_{23} \langle P_4 \rangle + \frac{1}{15} Q_3 \langle P_6 \rangle + \frac{111}{260} Q_4 \langle P_8 \rangle\right) \quad (33)$$

$$C_{06} = \left(\frac{\omega_0\delta}{\omega_r}\right)^4 \cdot \frac{11 Q_3 \langle P_6 \rangle + 6 Q_4 \langle P_8 \rangle}{360} \quad (34)$$

$$C_{08} = \left(\frac{\omega_0\delta}{\omega_r}\right)^4 \cdot \frac{Q_4 \langle P_8 \rangle}{768} \quad (35)$$

$$S_{02} = -i \frac{\omega_0\delta}{\omega_r} \frac{1}{2\sqrt{6}} E_5 \langle P_2 \rangle + i \left(\frac{\omega_0\delta}{\omega_r}\right)^3 \frac{3344\sqrt{3} (3 + \eta^2) \langle P_2 \rangle E_5 - 296 \langle P_4 \rangle Q_4^{(3)} + 875 \langle P_6 \rangle Q_6^{(3)}}{532224\sqrt{2}} \quad (36)$$

$$S_{0;4} = -i \left(\frac{\omega_0\delta}{\omega_r}\right)^3 \frac{\langle P_4 \rangle Q_4^{(3)} + 6 \langle P_6 \rangle Q_6^{(3)}}{4752\sqrt{2}} \quad (37)$$

$$S_{0;6} = i \left(\frac{\omega_0\delta}{\omega_r}\right)^3 \frac{Q_6^{(3)} \langle P_6 \rangle}{6912\sqrt{2}} \quad (38)$$

$$S_{08} = 0 \quad (39)$$

B. Belonging to $I_{\pm 1}$

$$C_{\pm 10} = I_{\pm 1}^{(\text{iso})} + \left(\frac{\omega_0\delta}{\omega_r}\right)^2 \cdot \frac{1}{18} \left[-Q_2^{(2)} \langle P_2 \rangle + 3 Q_4^{(2)} \langle P_4 \rangle\right] \pm \left(\frac{\omega_0\delta}{\omega_r}\right)^3 \frac{21 Q_4^{(3)} \langle P_4 \rangle - 50 Q_6^{(3)} \langle P_6 \rangle}{83160\sqrt{2}} - \left(\frac{\omega_0\delta}{\omega_r}\right)^4 \left[\frac{31}{264} Q_{11} \langle P_2 \rangle + Q_{24} \langle P_4 \rangle - \frac{47}{1512} Q_3 \langle P_6 \rangle + \frac{434}{10296} Q_4 \langle P_8 \rangle\right] \quad (40)$$

$$C_{\pm 1;2} = -\left(\frac{\omega_0\delta}{\omega_r}\right)^2 \cdot \frac{3 Q_2^{(2)} \langle P_2 \rangle + Q_4^{(2)} \langle P_4 \rangle}{18} \pm \left(\frac{\omega_0\delta}{\omega_r}\right)^3 \frac{44\sqrt{3} (3 + \eta^2) \langle P_2 \rangle E_5 - 5 \langle P_4 \rangle Q_4^{(3)} + 14 \langle P_6 \rangle Q_6^{(3)}}{33264\sqrt{2}} + \left(\frac{\omega_0\delta}{\omega_r}\right)^4 \frac{(Q_{14} - Q_{13}) \langle P_2 \rangle - (Q_{25} + Q_{26}) \langle P_4 \rangle + \frac{3}{2} Q_3 \langle P_6 \rangle + \frac{215}{3423} Q_4 \langle P_8 \rangle}{24} \quad (41)$$

$$C_{\pm 1;4} = \pm \left(\frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{\langle P_4 \rangle Q_4^{(3)} + 6 \langle P_6 \rangle Q_6^{(3)}}{4 \cdot 752 \sqrt{2}} + \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left[\frac{1}{24} (Q_{27} + Q_{28}) \langle P_4 \rangle + \frac{41}{360} Q_3 \langle P_6 \rangle - \frac{4}{195} Q_4 \langle P_8 \rangle \right] \quad (42)$$

$$C_{\pm 1;6} = \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \frac{1}{120} \left(\frac{11}{6} Q_3 \langle P_6 \rangle + Q_4 \langle P_8 \rangle \right) \quad (43)$$

$$C_{\pm 1;8} = 0 \quad (44)$$

$$S_{\pm 1;2} = \mp i \left(\frac{\omega_0 \delta}{\omega_r} \right)^2 \frac{3 Q_2^{(2)} \langle P_2 \rangle + Q_4^{(2)} \langle P_4 \rangle}{18} - i \left(\frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{44 \sqrt{3} (3 + \eta^2) \langle P_2 \rangle E_5 - 5 \langle P_4 \rangle Q_4^{(3)} + 14 \langle P_6 \rangle Q_6^{(3)}}{33 \cdot 264 \sqrt{2}} \\ \mp i \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \frac{1}{24} \left[(Q_{14} + Q_{13}) \langle P_2 \rangle + (Q_{25} - Q_{26}) \langle P_4 \rangle - \frac{1}{2} Q_3 \langle P_6 \rangle - \frac{19}{489} Q_4 \langle P_8 \rangle \right] \quad (45)$$

$$S_{\pm 1;4} = i \left(\frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{\langle P_4 \rangle Q_4^{(3)} + 6 \langle P_6 \rangle Q_6^{(3)}}{4 \cdot 752 \sqrt{2}} \pm i \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left[\frac{1}{24} (Q_{27} - Q_{28}) \langle P_4 \rangle + \frac{7}{72} Q_3 \langle P_6 \rangle - \frac{1}{60} Q_4 \langle P_8 \rangle \right] \quad (46)$$

$$S_{\pm 1;6} = \pm i \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \frac{11 Q_3 \langle P_6 \rangle + 6 Q_4 \langle P_8 \rangle}{720} \quad (47)$$

$$S_{\pm 18} = 0 \quad (48)$$

C. Belonging to $I_{\pm 2}$

$$C_{\pm 20} = I_2^{(\text{iso})} + \left(\frac{\omega_0 \delta}{\omega_r} \right)^2 \left[\frac{1}{72} Q_2^{(2)} \langle P_2 \rangle - \frac{1}{192} Q_4^{(2)} \langle P_4 \rangle \right] \mp \left(\frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{21 \langle P_4 \rangle Q_4^{(3)} - 50 \langle P_6 \rangle Q_6^{(3)}}{166 \cdot 320 \sqrt{2}} \\ + \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left[\frac{1}{24} Q_{11} \langle P_2 \rangle + \frac{1}{24} Q_{29} \langle P_4 \rangle - \frac{7}{216} Q_3 \langle P_6 \rangle + \frac{203}{14 \cdot 976} Q_4 \langle P_8 \rangle \right] \quad (49)$$

$$C_{\pm 2;2} = \pm \frac{\omega_0 \delta}{\omega_r} \frac{1}{4 \sqrt{6}} E_5 \langle P_2 \rangle + \left(\frac{\omega_0 \delta}{\omega_r} \right)^2 \frac{1}{36} \left(3 Q_2^{(2)} \langle P_2 \rangle + Q_4^{(2)} \langle P_4 \rangle \right) \\ \mp \left(\frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{1 \cdot 584 \sqrt{3} (3 + \eta^2) E_5 \langle P_2 \rangle - 152 \langle P_4 \rangle Q_4^{(3)} + 441 \langle P_6 \rangle Q_6^{(3)}}{532 \cdot 224 \sqrt{2}} \\ + \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \frac{1}{24} \left[\left(\frac{1}{2} Q_{12} + Q_{15} \right) \langle P_2 \rangle + (Q_{22} - Q_{210}) \langle P_4 \rangle - \frac{128}{143} Q_4 \langle P_8 \rangle \right] \quad (50)$$

$$C_{\pm 2;4} = \left(\frac{\omega_0 \delta}{\omega_r} \right)^2 \frac{1}{576} Q_4^{(2)} \langle P_4 \rangle + \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \frac{1}{24} \left[\left(\frac{1}{8} Q_{28} + Q_{211} \right) \langle P_4 \rangle + \frac{521}{120} Q_3 \langle P_6 \rangle + \frac{1 \cdot 159}{2 \cdot 080} Q_4 \langle P_8 \rangle \right] \quad (51)$$

$$C_{\pm 2;6} = \mp \left(\frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{\langle P_6 \rangle Q_6^{(3)}}{4608 \sqrt{2}} + \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left[\frac{11}{1 \cdot 440} Q_3 \langle P_6 \rangle + \frac{1}{240} Q_4 \langle P_8 \rangle \right] \quad (52)$$

$$C_{\pm 2;8} = -\frac{1}{768} \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 Q_4 \langle P_8 \rangle \quad (53)$$

$$\begin{aligned}
S_{\pm 2;2} = & i \frac{\omega_0 \delta}{\omega_r} \frac{1}{4\sqrt{6}} E_5 \langle P_2 \rangle \pm \frac{i}{36} \left(\frac{\omega_0 \delta}{\omega_r} \right)^2 \left(3 Q_2^{(2)} \langle P_2 \rangle + Q_4^{(2)} \langle P_4 \rangle \right) \\
& - i \left(\frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{840\sqrt{3} (3 + \eta^2) E_5 \langle P_2 \rangle - 72 \langle P_4 \rangle Q_4^{(3)} + 217 \langle P_6 \rangle Q_6^{(3)}}{266 \, 112\sqrt{2}} \\
& \pm \frac{i}{24} \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left[\frac{1}{2} (Q_{12} - Q_{15}) \langle P_2 \rangle + (Q_{22} + Q_{210}) \langle P_4 \rangle - \frac{1}{2} Q_3 \langle P_6 \rangle - \frac{119}{143} Q_4 \langle P_8 \rangle \right]
\end{aligned} \tag{54}$$

$$S_{\pm 2;4} = \pm i \left(\frac{\omega_0 \delta}{\omega_r} \right)^2 \frac{1}{576} Q_4^{(2)} \langle P_4 \rangle \pm \frac{i}{24} \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left[\left(Q_{211} - \frac{1}{8} Q_{28} \right) \langle P_4 \rangle + \frac{523}{120} Q_3 \langle P_6 \rangle + \frac{1 \, 157}{1 \, 040} Q_4 \langle P_8 \rangle \right] \tag{55}$$

$$S_{\pm 2;6} = -i \left(\frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{\langle P_6 \rangle Q_6^{(3)}}{4608\sqrt{2}} \pm i \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left[\frac{11}{1 \, 440} Q_3 \langle P_6 \rangle + \frac{1}{240} Q_4 \langle P_8 \rangle \right] \tag{56}$$

$$S_{\pm 2;8} = \mp \frac{i}{768} \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 Q_4 \langle P_8 \rangle \tag{57}$$

D. Belonging to $I_{\pm 3}$

$$C_{\pm 30} = I_3^{(\text{iso})} - \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left(\frac{1}{264} Q_{11} \langle P_2 \rangle + \frac{1}{24} Q_{212} \langle P_4 \rangle - \frac{17}{1 \, 512} Q_3 \langle P_6 \rangle + \frac{14}{10 \, 296} Q_4 \langle P_8 \rangle \right) \tag{58}$$

$$\begin{aligned}
C_{\pm 3;2} = & \pm \left(\frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{44\sqrt{3} (3 + \eta^2) \langle P_2 \rangle E_5 - 5 \langle P_4 \rangle Q_4^{(3)} + 14 \langle P_6 \rangle Q_6^{(3)}}{33 \, 264\sqrt{2}} \\
& + \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left[\frac{1}{24} Q_{14} \langle P_2 \rangle - \frac{1}{24} Q_{26} \langle P_4 \rangle - \frac{1}{48} Q_3 \langle P_6 \rangle + \frac{41}{3 \, 432} Q_4 \langle P_8 \rangle \right]
\end{aligned} \tag{59}$$

$$C_{\pm 3;4} = \pm \left(\frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{\langle P_4 \rangle Q_4^{(3)} + 6 \langle P_6 \rangle Q_6^{(3)}}{4 \, 752\sqrt{2}} - \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left[\frac{1}{24} Q_{27} \langle P_4 \rangle + \frac{73}{720} Q_3 \langle P_6 \rangle + \frac{29}{1 \, 560} Q_4 \langle P_8 \rangle \right] \tag{60}$$

$$C_{\pm 3;6} = - \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left[\frac{11}{360} Q_3 \langle P_6 \rangle + \frac{2}{120} Q_4 \langle P_8 \rangle \right] \tag{61}$$

$$C_{\pm 3;8} = 0 \tag{62}$$

$$\begin{aligned}
S_{\pm 3;2} = & i \left(\frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{44\sqrt{3} (3 + \eta^2) \langle P_2 \rangle E_5 - 5 \langle P_4 \rangle Q_4^{(3)} + 14 \langle P_6 \rangle Q_6^{(3)}}{33 \, 264\sqrt{2}} \\
& \pm i \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left[\frac{1}{24} Q_{14} \langle P_2 \rangle - \frac{1}{24} Q_{26} \langle P_4 \rangle - \frac{1}{48} Q_3 \langle P_6 \rangle + \frac{41}{3 \, 432} Q_4 \langle P_8 \rangle \right]
\end{aligned} \tag{63}$$

$$S_{\pm 3;4} = i \left(\frac{\omega_0 \delta}{\omega_r} \right)^3 \frac{\langle P_4 \rangle Q_4^{(3)} + 6 \langle P_6 \rangle Q_6^{(3)}}{4 \, 752\sqrt{2}} \mp i \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left[\frac{1}{24} Q_{27} \langle P_4 \rangle + \frac{73}{720} Q_3 \langle P_6 \rangle + \frac{29}{1 \, 560} Q_4 \langle P_8 \rangle \right] \tag{64}$$

$$S_{\pm 3;6} = \mp i \left(\frac{\omega_0 \delta}{\omega_r} \right)^4 \left[\frac{11}{360} Q_3 \langle P_6 \rangle + \frac{2}{120} Q_4 \langle P_8 \rangle \right] \tag{65}$$

$$S_{\pm 3;8} = 0 \quad (66)$$

The Q_α^β are geometry factors, which similar to $E_1 \dots E_5$ contain information about the orientation of the CST PAF with respect to the segment vector. Their definitions are given in the following, where $P_n(x)$ are the Legendre polynomials and $P_n^{(m)}$ are the assigned Legendre polynomials:

$$Q_2^{(2)} = \frac{3 - \eta^2}{7} P_2(\cos \alpha) - \frac{\eta}{7} P_2^{(2)}(\cos \alpha) \cos 2\psi \quad (67)$$

$$Q_4^{(2)} = -\frac{18 + \eta^2}{70} P_4(\cos \alpha) - \frac{\eta}{70} P_4^{(2)}(\cos \alpha) \cos 2\psi - \frac{\eta^2}{48 \cdot 35} P_4^{(4)}(\cos \alpha) \cos 4\psi$$

$$Q_4^{(3)} = 3\sqrt{2} (9 - 4\eta^2) P_4(\cos \alpha) - \frac{\sqrt{2}}{4} \eta (3 + \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi - \frac{\sqrt{2}}{8} \eta^2 P_4^{(4)}(\cos \alpha) \cos 4\psi \quad (68)$$

$$Q_6^{(3)} = -\frac{3\sqrt{2}}{4} (6 + \eta^2) P_6(\cos \alpha) - \frac{\sqrt{2}}{240} \eta (36 + \eta^2) P_6^{(2)}(\cos \alpha) \cos 2\psi - \frac{\sqrt{2}}{480} \eta^2 P_6^{(4)}(\cos \alpha) \cos 4\psi \\ - \frac{\sqrt{2}}{17 \cdot 280} \eta^3 P_6^{(6)}(\cos \alpha) \cos 6\psi \quad (69)$$

$$Q_{11} = \frac{1}{1134} \left[(-27 - 9\eta^2 + 4\eta^4) P_2(\cos \alpha) + \frac{1}{2} \eta (27 + 5\eta^2) P_2^{(2)}(\cos \alpha) \cos 2\psi \right] \quad (70)$$

$$Q_{12} = \frac{1}{1386} \left[(315 + 72\eta^2 - 43\eta^4) P_2(\cos \alpha) + \eta (141 + 31\eta^2) P_2^{(2)}(\cos \alpha) \cos 2\psi \right] \quad (71)$$

$$Q_{13} = \frac{1}{2079} \left[(-405 - 36\eta^2 + 49\eta^4) P_2(\cos \alpha) + \eta (153 + 43\eta^2) P_2^{(2)}(\cos \alpha) \cos 2\psi \right] \quad (72)$$

$$Q_{14} = \frac{1}{1386} \left[(9 + 36\eta^2 - 5\eta^4) P_2(\cos \alpha) + \eta (-21 + \eta^2) P_2^{(2)}(\cos \alpha) \cos 2\psi \right] \quad (73)$$

$$Q_{15} = \frac{1}{8316} \left[(81 - 72\eta^2 - \eta^4) P_2(\cos \alpha) + \eta (9 - 13\eta^2) P_2^{(2)}(\cos \alpha) \cos 2\psi \right] \quad (74)$$

$$Q_{21} = \frac{1}{960 \cdot 960} \left[(213 \cdot 678 + 111 \cdot 357\eta^2 + 817\eta^4) P_4(\cos \alpha) + \eta (17 \cdot 523 + 3 \cdot 329 \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \right. \\ \left. + \frac{\eta^2}{24} (6 \cdot 219 + 4 \cdot 585\eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \quad (75)$$

$$Q_{22} = \frac{1}{2 \cdot 772} \left[(756 + 249\eta^2 + 19\eta^4) P_4(\cos \alpha) + 3\eta (11 + 5\eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \right. \\ \left. + \frac{\eta^2}{24} (51 + 13\eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \quad (76)$$

$$Q_{23} = \frac{1}{123 \cdot 552} \left[(-2 \cdot 754 - 3 \cdot 375\eta^2 + 205\eta^4) P_4(\cos \alpha) + \frac{\eta}{5} (-3 \cdot 069 + \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \right. \\ \left. + \frac{\eta^2}{120} (1 \cdot 539 - 511\eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \quad (77)$$

$$Q_{24} = \frac{1}{720 \ 720} \left[(100 \ 278 + 57 \ 177 \ \eta^2 - 163 \ \eta^4) P_4(\cos \alpha) + \eta (9207 + 1 \ 453 \ \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \right. \\ \left. + \frac{\eta^2}{24} (1 \ 935 + 2 \ 261 \ \eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \quad (78)$$

$$Q_{25} = \frac{1}{54 \ 054} \left[(11 \ 664 + 3 \ 771 \ \eta^2 + 301 \ \eta^4) P_4(\cos \alpha) + \eta (495 + 233 \ \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \right. \\ \left. + \frac{\eta^2}{24} (801 + 199 \ \eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \quad (79)$$

$$Q_{26} = \frac{1}{36 \ 036} \left[(864 + 327 \ \eta^2 + 17 \ \eta^4) P_4(\cos \alpha) + \frac{3}{5} \eta (77 + 27 \ \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \right. \\ \left. + \frac{\eta^2}{120} (249 + 79 \ \eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \quad (80)$$

$$Q_{27} = \frac{1}{123 \ 552} \left[(3402 - 2493 \ \eta^2 + 487 \ \eta^4) P_4(\cos \alpha) + \frac{1}{5} \eta (-2871 + 739 \ \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \right. \\ \left. + \frac{\eta^2}{120} (4761 - 109 \ \eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \quad (81)$$

$$Q_{28} = \frac{1}{123 \ 552} \left[(810 + 387 \ \eta^2 + 7 \ \eta^4) P_4(\cos \alpha) + \frac{1}{5} \eta (297 + 67 \ \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \right. \\ \left. - \frac{\eta^2}{120} (153 + 83 \ \eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \quad (82)$$

$$Q_{29} = \frac{1}{1 \ 441 \ 440} \left[(-31914 - 32 \ 751 \ \eta^2 + 1 \ 669 \ \eta^4) P_4(\cos \alpha) - \eta (5 \ 841 + 139 \ \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \right. \\ \left. + \frac{\eta^2}{24} (2 \ 295 - 1 \ 043 \ \eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \quad (83)$$

$$Q_{210} = \frac{1}{216 \ 216} \left[(972 + 207 \ \eta^2 + 37 \ \eta^4) P_4(\cos \alpha) + \frac{\eta}{5} (99 + 109 \ \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \right. \\ \left. + \frac{\eta^2}{120} (441 + 71 \ \eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \quad (84)$$

$$Q_{211} = \frac{1}{494 \ 208} \left[(30 \ 942 - 9 \ 927 \ \eta^2 + 3 \ 013 \ \eta^4) P_4(\cos \alpha) + \eta (-2673 + 1061 \ \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \right. \\ \left. + \frac{\eta^2}{24} (6111 + 85 \ \eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \quad (85)$$

$$Q_{212} = \frac{1}{240 \ 240} \left[(1 \ 458 - 333 \ \eta^2 + 127 \ \eta^4) P_4(\cos \alpha) + \eta (-99 + 47 \ \eta^2) P_4^{(2)}(\cos \alpha) \cos 2\psi \right. \\ \left. + \frac{\eta^2}{24} (261 + 7 \ \eta^2) P_4^{(4)}(\cos \alpha) \cos 4\psi \right] \quad (86)$$

$$\begin{aligned}
Q_3 = \frac{1}{3 \cdot 168} & \left[(-54 + 27\eta^2 + \eta^4) P_6(\cos \alpha) + \frac{\eta^3}{2} P_6^{(2)}(\cos \alpha) \cos 2\psi + \frac{\eta^2 (9 + \eta^2)}{360} P_6^{(4)}(\cos \alpha) \cos 4\psi \right. \\
& \left. + \frac{\eta^3}{720} P_6^{(6)}(\cos \alpha) \cos 4\psi \right]
\end{aligned} \tag{87}$$

$$\begin{aligned}
Q_4 = \frac{1}{6 \cdot 912} & \left[(216 + 72\eta^2 + \eta^4) P_8(\cos \alpha) + \frac{3}{7}\eta (12 + \eta^2) P_8^{(2)}(\cos \alpha) \cos 2\psi \right. \\
& \left. + \frac{\eta^2 (54 + \eta^2)}{1 \cdot 260} P_8^{(4)}(\cos \alpha) \cos 4\psi + \frac{\eta^3}{2 \cdot 520} P_8^{(6)}(\cos \alpha) \cos 4\psi + \frac{\eta^4}{120 \cdot 960} P_8^{(8)}(\cos \alpha) \cos 4\psi \right]
\end{aligned} \tag{88}$$

S6. OSCILLATION COEFFICIENTS: EXPERIMENTAL DATA

Table I. $C7 = CH_3$; all values ± 0.0016

m	C_{m0}	C_{m2}	S_{m2}
-2		- 0.00485	0.0058
-1	0.0133	0	0
0	0.9700	0.003395	- 0.0107
1	0.0126	0	0
2		0.003395	0.0061

Table II. $C1+C2+C5 = CO_3$ and the two C_q ; all values ± 0.001

m	C_{m0}	C_{m2}	S_{m2}
-3	0.014	0	0.0024
-2	-	-0.0094	0.0087
-1	0.160	-0.0113	0.0078
0	0.597	0.0081	-0.0263
1	0.167	-0.0070	-0.0130
2	0.0375	0.0184	0.0167
3	0.0045	0.0031	0.0032

Table III. $C3 = CH$; all values ± 0.0011

m	C_{m0}	C_{m2}	S_{m2}
-3	0.0048	0	0
-2	0.0416	-0.0067	0.0067
-1	0.1153	0.0080	-0.0089
0	0.6369	-0.0061	-0.0051
1	0.1834	0.0080	0.0085
2	0.0156	0	0
3	0.0024	0	0

Table IV. $C4 = CH$; all values ± 0.0011

m	C_{m0}	C_{m2}	S_{m2}
-3	0.0083	0	0
-2	0.0607	-0.0094	0.0089
-1	0.1508	0.0127	-0.0132
0	0.6675	-0.0089	-0.0077
1	0.0868	0.0117	0.0125
2	0.0230	0	0
3	0.0028	0	0