$(CH_3)_2X$ 基の取扱い

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1. 序論

２個のメチル基を持つ分子の CH 伸縮振動に対する SFG テンソルを考えてみよう。アセトンやジメチルエーテルなどのように同じ原子に２個のメチル基がついている分子や、ブチレン、ジメチルアセチレンが代表例であるが、それ以外にも、１個の原子から２本のアルキル鎖が出ている分子で、何らかの理由で末端メチル基が一定の相対配向を取る場合には、ここで示す結果が使えるはずである。

メチル基は C_{3v} の対称を持つものとする。また、$(CH_3)_2X$ 基を想定すると、メチル基の内部回転が自由回転である場合に系は C_{2v} の対称を持つ。SFG テンソルについては、ベクトルに戻って考えることが出来るから、２つのメチル基が空間的に離れている場合でも、モデル的には $(CH_3)_2X$ 基を想定して議論することが許される。

2. 座標系とメチル基の配向

(1). メチル基に固定した座標系；(abc) 系： C_3 軸上、C 原子から H 原子に向けて c 軸を取り、３個の CH 結合の１つが ac 面の上に乗るようにする。

(2). $(CH_3)_2X$ 基に固定した座標系；(xyz) 系： ２個のメチル基の C_3 軸の２等分線に沿って z 軸を取

り、X 原子からメチル基の方向を正方向とする。２個のメ C_3 軸が作る平面の上に x 軸を取る。
(3). メチル基の配向：z 軸とメチル基の C_3 軸がなす角（即ち CXC 角の半分）を α とする。また、２個のメチル基を下付き A、B で区別するとき、それぞれのメチル基の内部回転角を ϕ_A、ϕ_B と表す。メチル基の３個の H 原子が作る正三角形の頂点が表面に向いている状態を基準に取り、このときの内部回転角を $\phi_A = 0$、$\phi_B = 0$ とする。正三角形の辺が表面に寄っている時の内部回転角は 180˚ である。CXC 面内の鋭角側に CH 結合が載る状態が $\phi= 0$、鈍角側に載る状態が $\phi = \pi$ になる。

内部回転角による違いを生じるのは「縮重振動」バンドに対する SFG テンソルだけである。よって、メチル基の相対的な配向や回転の様子は、縮重バンドの様子から知ることが出来る。
(４). オイラー角；(χ, θ, ϕ)：２個のメチル基の座標系を分子固定系に重ねるときのオイラー角は、CXC 角を 2α として、$(0, \alpha, \phi)$ と (π, α, ϕ) である（こうなるように b 軸の向きを決める）。

上の定義に従って求めたテンソル成分の一般式を付録 **A** に示す。縮重バンドの表式が内部回転角に依存する形になっていることがわかる。（傾き角 θ に関しては、表で使っている sinθ、sin2θ、sin3θ の形の三角関数ではなく、下の関係式を使って変換した sinθ、cosθ のべき乗による表式を採用した。)

$$\sin 2\theta = 2\sin\theta\cos\theta, \qquad \cos 2\theta = \cos^2\theta - \sin^2\theta = 2\cos^2\theta - 1 = 1 - 2\sin^2\theta$$
$$\sin 3\theta = 3\sin\theta - 4\sin^3\theta, \qquad \sin\theta + \sin 3\theta = 4(\sin\theta - \sin^3\theta)$$
$$\cos 3\theta = 4\cos^3\theta - 3\cos\theta, \qquad \cos\theta - \cos 3\theta = 4(\cos\theta - \cos^3\theta)$$

本文では、いくつかの典型的な相対配向について (xyz) 系でのテンソル成分を示そう。なお、$(CH_3)_2X$ としての対称性は、２つのメチル基の相互配向によって違ったものになる。

3. 振動バンド

メチル基の全対称モードと縮重モードについて、２個のメチル基の対が $(CH_3)_2X$ タイプのグループを作っている場合の挙動は、下記のように整理することが出来る。
(1). 全対称振動：２個の CH_3 基がそれぞれ持っている全対称振動モードが、互いに位相をそろえて振動する対称振動と逆位相で振動する逆対称振動を作る。前者は z 軸に沿った振動モード、後者は x 軸に沿った振動モードで、ともに CXC 面内の振動である。ただし、CXC 角が 0 または π のとき、すなわち $\alpha = 0$ または $\pi/2$ のときには、x 軸方向の対称振動と逆対称振動になる。
(2). 縮重振動：１個の CH_3 基あたりの縮重振動の自由度は２であるから、$(CH_3)_2X$ タイプになったときの振動自由度は４になる。CH_3 基に固定された (abc) 座標系での縮重振動は、a 軸方向の振動と b 軸方向の振動で構成される。２個の CH_3 基で構成される系では、a 軸方向の振動の対から、同位相振動が z 軸に沿った振動になり、逆位相振動の振動が x 軸に沿った振動になる。この２モードは、分子面の上に乗った振動である。$\alpha = 0$ または $\pi/2$ のときには、y 軸まわり、すなわち、CXC 軸対して同じ方向と互いに逆方向折れ曲がる２種類の振動運動になる。

一方、a 軸方向の振動の対から作られるのは、同位相の振動が分子面に垂直な y 軸方向の振動になり、逆位相の振動が CXC 角の２等分線のまわりでのねじれ振動になる。$(CH_3)_2X$ が C_{2v} 対称を持つ場合には、ねじれ振動は赤外吸収とラマン散乱の両方に不活性な a_2 対称になり、その振動ベクトルは３つの座標軸のどれにも乗らない（軸性ベクトルになる）。$\alpha = 0$ または $\pi/2$ のときには、上に記した a 軸方向の振動と同様になるが、上とは垂直方向への振動である。

以後の導出では、２個のメチル基が直線上に並ぶ場合（２本の C_3 軸が１本の直線に乗る場合、すなわち、$\alpha = 0$ または $\pi/2$ の場合）を除外する。CXC 部分の対称性が C_{2v} から $D_{\infty h}$ に変わることから予想できることだが、議論がほぼ２倍に膨らんでしまうからである。

4. $(CH_3)_2X$ 基の対称性

CXC 部分が折れ曲がっているとするときでも、メチル基がどのような内部回転角を取っているかによって、$(CH_3)_2X$ 基の対称性は下のように分かれる。

自由回転をしているときには C_{2v} 対称
$\phi_A = \phi_B = 0$ または π のときには C_{2v} 対称
$\phi_A = \phi_B \neq 0$ または π のときには C_2 対称（z axis）
$\phi_A = 0, \phi_B = \pi$ または $\phi_A = \pi, \phi_B = 0$ のときには C_s 対称（xz plane）
$\phi_A = -\phi_B \neq 0$ のときには C_s 対称（yz-plane）
$\phi_A \neq \pm\phi_B$ のときには対称無し（C_1 対称；おそらくは $C_{3v}{}^A \times C_{3v}{}^B$ タイプの積表現が正しい）。
（厳密に扱うには、置換・回転群（Bunker の教科書）による解析と分類が適切であろう。）

5. 分子固定 SFG テンソル

自由回転

内部回転角 ϕ_A と ϕ_B がからむ項を除いたものにすればよい。

［全対称バンド］　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ のときには、　$\beta_{aac} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$,　$\beta_{ccc} \sim (1/9)\,\beta_{\zeta\zeta\zeta}$　である。

(a$_1$)　$\beta_{xxz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{aac}\cos\alpha$
$\beta_{yyz} = +2\beta_{aac}\cos\alpha$
$\beta_{zzz} = +2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{ccc}\cos\alpha$
(b$_1$)　$\beta_{zxx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$
$\beta_{xzx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

［縮重バンド］　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ のときには、　$\beta_{caa} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$,　$\beta_{aaa} \sim 4\sqrt{2}/9\,\beta_{\zeta\zeta\zeta}$　である。

(a$_1$)　$\beta_{xxz} = -2\beta_{caa}(\cos\alpha - \cos^3\alpha)$
$\beta_{yyz} = 0$
$\beta_{zzz} = 2\beta_{caa}(\cos\alpha - \cos^3\alpha)$
(b$_1$)　$\beta_{zxx} = -\beta_{caa}(\cos\alpha - 2\cos^3\alpha)$
$\beta_{xzx} = -\beta_{caa}(\cos\alpha - 2\cos^3\alpha)$
(b$_2$)　$\beta_{zyy} = \beta_{caa}\cos\alpha$
$\beta_{yzy} = \beta_{caa}\cos\alpha$

$\phi_A = \phi_B = 0, \pi$（三角形が 2 つとも下向き又は 2 つとも上向き）

$\phi_A = \phi_B = 0$ のときには $\cos\phi_A = \cos\phi_B = \cos2\phi_A = \cos2\phi_B = \cos3\phi_A = \cos3\phi_B = +1$、$\phi_A = \phi_B = \pi$ のときには、$\cos\phi_A = \cos\phi_B = \cos3\phi_A = \cos3\phi_B = -1$、$\cos2\phi_A = \cos2\phi_B = +1$ である。

［全対称バンド］　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ のときには、　$\beta_{aac} \sim (4/9)\beta_{\zeta\zeta\zeta}$,　$\beta_{ccc} \sim (1/9)\beta_{\zeta\zeta\zeta}$　である。

(a$_1$)　$\beta_{xxz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{aac}\cos\alpha$

$\beta_{yyz} = +2\beta_{aac}\cos\alpha$

$\beta_{zzz} = +2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{ccc}\cos\alpha$

(b$_1$)　$\beta_{zxx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

$\beta_{xzx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

［縮重バンド］　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ のときには、　$\beta_{caa} \sim (4/9)\beta_{\zeta\zeta\zeta}$,　$\beta_{aaa} \sim 4\sqrt{2}/9\ \beta_{\zeta\zeta\zeta}$　である。。

（β_{zyy} と β_{yzy} には b 軸方向の振動が、他の成分には a 軸方向の振動が寄与する。）

（± 記号については、上側が $\phi_A = \phi_B = 0$ に、下側が $\phi_A = \phi_B = \pi$ に対応する。）

(a$_1$)　$\beta_{xxz} = 2[-2\beta_{caa}(\cos\alpha - \cos^3\alpha) \pm \beta_{aaa}(\sin\alpha - \sin^3\alpha)]$

$\beta_{yyz} = -(\pm 2)\beta_{aaa}\sin\alpha$

$\beta_{zzz} = 2[2\beta_{caa}(\cos\alpha - \cos^3\alpha) \pm \beta_{aaa}\sin^3\alpha]$

(b$_1$)　$\beta_{zxx} = -2[\beta_{caa}(\cos\alpha - \cos^3\alpha) \pm \beta_{aaa}(\sin\alpha - \sin^3\alpha)]$

$\beta_{xzx} = -2[\beta_{caa}(\cos\alpha - \cos^3\alpha) \pm \beta_{aaa}(\sin\alpha - \sin^3\alpha)]$

(b$_2$)　$\beta_{zyy} = 2[\beta_{caa}\cos\alpha - (\pm)\beta_{aaa}\sin\alpha]$

$\beta_{yzy} = 2[\beta_{caa}\cos\alpha - (\pm)\beta_{aaa}\sin\alpha]$

$\phi_A = \phi_B \neq 0, \pi$（2 つの三角形が反発しあうようにずれている）

$\sin(n\phi_B) = -\sin(n\phi_A)$、$\cos(n\phi_B) = \cos(n\phi_A)$ である。

［全対称バンド］　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ のときには、　$\beta_{aac} \sim (4/9)\beta_{\zeta\zeta\zeta}$、$\beta_{ccc} \sim (1/9)\beta_{\zeta\zeta\zeta}$　である。

$\beta_{xxz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{aac}\cos\alpha$

$\beta_{yyz} = +2\beta_{aac}\cos\alpha$

$\beta_{zzz} = +2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{ccc}\cos\alpha$

$\beta_{zxx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

$\beta_{xzx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

［縮重バンド］　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ のときには、　$\beta_{caa} \sim (4/9)\beta_{\zeta\zeta\zeta}$、$\beta_{aaa} \sim 4\sqrt{2}/9\ \beta_{\zeta\zeta\zeta}$　である。

（面外振動と面内振動を分ける際に便利なので、a 軸方向の振動と b 軸方向の振動を区別する。）

（± 記号の上側が a 軸方向の振動、下側が b 軸方向の振動に対応する。）

$\beta_{zxx} = -\beta_{caa}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)$

$\beta_{xzx} = -\beta_{caa}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)$

$\beta_{zyy} = \beta_{caa}\cos\alpha[1 - (\pm)\cos2\phi_A] - \beta_{aaa}\sin\alpha[\cos3\phi_A - (\pm)\cos\phi_A]$

$\beta_{yzy} = \beta_{caa}\cos\alpha[1 - (\pm)\cos2\phi_A] - \beta_{aaa}\sin\alpha[\cos3\phi_A - (\pm)\cos\phi_A]$

$\beta_{xxz} = -2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)$

$\beta_{yyz} = -\beta_{aaa}\sin\alpha(\cos3\phi_A \pm \cos\phi_A)$

$\beta_{zzz} = 2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)$

β_{yzx} = $-(\pm)\beta_{caa}\cos^2\alpha\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)$

β_{zyx} = $-(\pm)\beta_{caa}\cos^2\alpha\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)$

β_{zxy} = $-(\pm)\beta_{caa}(2\cos^2\alpha - 1)\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha[\sin3\phi_A - (\pm)\sin\phi_A]$

β_{xzy} = $-(\pm)\beta_{caa}(2\cos^2\alpha - 1)\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha[\sin3\phi_A - (\pm)\sin\phi_A]$

β_{xyz} = $\pm\beta_{caa}\sin^2\alpha\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)$

β_{yxz} = $\pm\beta_{caa}\sin^2\alpha\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)$

$\phi_A = 0, \phi_B = \pi$ または$\phi_A = \pi, \phi_B = 0$（1つの三角形は下向き、もうひとつの三角形は下向き）

［全対称バンド］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには、** $\beta_{aac} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$、$\beta_{ccc} \sim (1/9)\,\beta_{\zeta\zeta\zeta}$ **である。**

β_{xxz} = $-2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{aac}\cos\alpha$

β_{yyz} = $+2\beta_{aac}\cos\alpha$

β_{zzz} = $+2(\beta_{aac}-\beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{ccc}\cos\alpha$

β_{zxx} = $-2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

β_{xzx} = $-2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

［縮重バンド］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには、** $\beta_{caa} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$、$\beta_{aaa} \sim 4\sqrt{2}\,/\,9\,\beta_{\zeta\zeta\zeta}$ **である。**

（β_{zyy} **と** β_{yzy} **には** b **軸方向の振動が、他の成分には** a **軸方向の振動が寄与する。**）

（± **記号の上側は** $\phi_A = 0$、$\phi_B = \pi$ **に、下側は**$\phi_A = \pi$、$\phi_B = 0$ **に対応する。**）

β_{zxx} = $-2\beta_{caa}(\cos\alpha - 2\cos^3\alpha)$

β_{xzx} = $-2\beta_{caa}(\cos\alpha - 2\cos^3\alpha)$

β_{zyy} = $2\beta_{caa}\cos\alpha$

β_{yzy} = $2\beta_{caa}\cos\alpha$

β_{xxz} = $-4\beta_{caa}(\cos\alpha - \cos^3\alpha)$

β_{yyz} = 0

β_{zzz} = $4\beta_{caa}(\cos\alpha - \cos^3\alpha)$

$\phi_A = -\phi_B \neq 0, \pi$（2つの三角形が同じ側にかしいでいる。）

［全対称バンド］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには、** $\beta_{aac} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$、$\beta_{ccc} \sim (1/9)\,\beta_{\zeta\zeta\zeta}$ **である。**

β_{xxz} = $-2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{aac}\cos\alpha$

β_{yyz} = $+2\beta_{aac}\cos\alpha$

β_{zzz} = $+2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{ccc}\cos\alpha$

β_{zxx} = $-2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

β_{xzx} = $-2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

［縮重バンド］

（± **記号の上側が** a **軸方向の振動、下側が** b **軸方向の振動に対応する。**）

β_{zxx} = $-\beta_{caa}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)$

β_{xzx} = $-\beta_{caa}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)$

$ß_{zyy} = ß_{caa}\cos\alpha[1 - (\pm)\cos2\phi_A] - ß_{aaa}\sin\alpha[\cos3\phi_A - (\pm)\cos\phi_A]$

$ß_{yzy} = ß_{caa}\cos\alpha[1 - (\pm)\cos2\phi_A] - ß_{aaa}\sin\alpha[\cos3\phi_A - (\pm)\cos\phi_A]$

$ß_{xxz} = -2ß_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) + ß_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)$

$ß_{yyz} = -ß_{aaa}\sin\alpha(\cos3\phi_A \pm \cos\phi_A)$

$ß_{zzz} = 2ß_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) + ß_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)$

$ß_{yxx} = \pm ß_{caa}\sin\alpha\cos\alpha\sin2\phi_A - ß_{aaa}\cos^2\alpha(\sin3\phi_A \pm \sin\phi_A)$

$ß_{xyx} = \pm ß_{caa}\sin\alpha\cos\alpha\sin2\phi_A - ß_{aaa}\cos^2\alpha(\sin3\phi_A \pm \sin\phi_A)$

$ß_{xxy} = \pm 2ß_{caa}\sin\alpha\cos\alpha\sin2\phi_A - ß_{aaa}\cos^2\alpha[\sin3\phi_A - (\pm)\sin\phi_A]$

$ß_{yyy} = ß_{aaa}[\sin3\phi_A - (\pm)\sin\phi_A]$

$ß_{zzy} = -(\pm)2ß_{caa}\sin\alpha\cos\alpha\sin2\phi_A - ß_{aaa}\sin^2\alpha[\sin3\phi_A - (\pm)\sin\phi_A]$

$ß_{yzz} = -ß_{caa}\sin\alpha\cos\alpha\sin2\phi_A - ß_{aaa}\sin^2\alpha(\sin3\phi_A \pm \sin\phi_A)$

$ß_{zyz} = -ß_{caa}\sin\alpha\cos\alpha\sin2\phi_A - ß_{aaa}\sin^2\alpha(\sin3\phi_A \pm \sin\phi_A)$

6. 空間固定(XYZ)系におけるテンソル成分

分子固定 (xyz) 系が、オイラー角 (χ, θ, ϕ) によって空間固定 (XYZ) 系に重なるものとしよう。このときに、(XYZ) 系でのテンソル成分を一般的に求めると付録 F のようになる。

なお、式中で用いられるオイラー角と $(CH_3)_2X$ 基の配向の関係は、次のようになる。

(1) 内部回転角 ϕ：CXC 面の（表面に対する）ねじれ角である。z 軸まわりの回転で分子面を表面と垂直にするために必要な回転角、あるいは、-Z 軸の ab 面への射影に x 軸を重ねるための回転角でもある。ここでの Z 軸の向きでは、X 軸を見て y 軸が左側に来るので、CXC 面が右上がりになっている場合がプラス（< 90°）回転になる。（x 軸に沿ったベクトルと X 軸方向のベクトルの内積がプラスになる方向で重ねる。）**(a)** 分子面が表面に垂直なときには $\phi = 0$ or π、CXC 面が表面と向き合っているときには $\phi = \pi/2$ or $3\pi/2$ である。**(b)** ２個のメチル基が等価な場合は、内部回転角が ϕ の $(CH_3)_2X$ 基に対して内部回転角が $-\phi$ の $(CH_3)_2X$ 基が同数存在する。**(c)** $(CH_3)_2X$ 基が自由回転をしているかあるいはランダムな内部回転角を取っている場合には ϕ は $0 \sim 2\pi$ の任意の値を同じウェイトで取る。

(2) 傾き角・tilt 角 θ_{tilt}：通常の定義に合わせて、z 軸（CXC の２等分線）と外向きの法線の間の角と定義し、N 軸まわりの回転で z 軸を外向きの法線に重ねる方向をプラス回転とする。Z 軸は下向きの法線であるから、オイラー角 θ は $\pi - \theta_{tilt}$ である。また、$(CH_3)_2X$ 基が 2 個の CH_3 を真空側に向けているときには $\theta_{tilt} < \pi/2$ である。

(3) 面内配向角 $\chi_{in\text{-}plane}$ (χ_{ip} と略記する)： z 軸の XY 面への射影を Z 軸まわりの回転で X 軸に重ねるための回転角とする。ここでの Z 軸の向きでは、X 軸の方向に見て射影が左側にあるときがプラスになる。Z 軸を基板の内部に向けて取っているので、対応するオイラー角 χ は $\pi/2 + \chi_{ip}$ である。**(a)** 射影した CXC の２等分線が X 軸から角 α だけずれているときには、y 軸と Y 軸がなす角も α である。射影した CXC の２等分線が八の字形に X 軸から左右交互にずれているときには χ_{ip} は $+\alpha$ と $-\alpha$ で表される。**(b)** 面内配向がランダムなときには、χ_{ip} は $0 \sim 2\pi$ の任意の値を同じウェイトで取る。

本稿では、現実の系で起こりそうないくつかのケース、すなわち、メチル基が自由回転しているケース、$\phi_A = \phi_B = 0$ または π で固定されているケース、$\phi_A = \phi_B \neq 0, \pi$ で固定されているケース、さらに、$\phi_A = 0, \phi_B = \pi$ または $\phi_A = \pi, \phi_B = 0$ で固定されているケース、におけるテンソル成分を示す。４つ

のケースに共通することは、下記の事実である。

全対称振動では、$\beta_{zxx} = \beta_{xzx}$
縮重振動では、$\beta_{zxx} = \beta_{xzx}$、$\beta_{zyy} = \beta_{yzy}$、**（最後のケースでは次も）**$\beta_{yzx} = \beta_{zyx}$、$\beta_{zxy} = \beta_{xzy}$、$\beta_{xyz} = \beta_{yxz}$

なお、一般的な空間配向に対する表式は長くなるのでそれぞれ付録 B、付録 C、付録 D、付録 E に示し、本文では面内配向がランダムな場合に対する表式だけを記す。（さらに表面に対する CXC **面の配向角** (ϕ) **もランダムな場合に対しては下で** $\cos(n\phi) = 0$, $\sin(n\phi) = 0$ **と置けばよい。）**
その他の配向に対する表式は、「CH_3 **基の配向と** SFG **テンソル**」**および**「CH_2 **基の配向と** SFG **テンソル**」**を参照して求めればよい。**

自由回転・ランダム配向（一般的な配向に対する表式は付録 B **に示す。）**
［**全対称バンド**］　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには**　$\beta_{aac} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$、$\beta_{ccc} \sim (1/9)\,\beta_{\zeta\zeta\zeta}$　**である。**
原理的には振動バンドが２つに分裂するが、実際には重なっているときには、以下に示す２つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{xxz} + \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 4\beta_{aac}\cos\alpha$
$\beta_{xxz} - \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$
$\beta_{xxz} + \beta_{yyz} - 2\beta_{zzz} = -2(\beta_{aac} - \beta_{ccc})[3(\cos\alpha - \cos^3\alpha) - 2\cos\alpha]$
$\beta_{zxx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$　**であるから、**

［**対称** (a_1) **振動**］

(ppp)　$\chi_{XZX} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

$\chi_{ZXX} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

$$\chi_{XXZ} = (1/2)(\beta_{aac} - \beta_{ccc})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta) - 2(\cos\alpha - \cos^3\alpha)\cos\theta\} + 2\beta_{aac}\cos\alpha\cos\theta$$

$\chi_{ZZZ} = -(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(1 + \cos2\phi)(\cos\theta - \cos^3\theta) + 2\cos^3\alpha\cos^3\theta]$

(spp)　$\chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(ssp)　$$\chi_{YYZ} = (1/2)(\beta_{aac} - \beta_{ccc})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta) - 2(\cos\alpha - \cos^3\alpha)\cos\theta\} + 2\beta_{aac}\cos\alpha\cos\theta$$

(psp)　$\chi_{ZYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(sps)　$\chi_{YZY} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

(pps)　$\chi_{XZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

$\chi_{ZXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(pss)　$\chi_{ZYY} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

(sss)　(none)

［逆対称 (b_1) 振動］

(ppp)　$\chi_{XX} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos 2\phi)]$

　　　$\chi_{XZX} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos 2\phi)]$

　　　$\chi_{XXZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos 2\phi)$

　　　$\chi_{ZZZ} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos 2\phi)$

(spp)　(none)

(ssp)　$\chi_{YYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos 2\phi)$

(psp)　(none)

(sps)　$\chi_{YZY} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos 2\phi)]$

(pps)　(none)

(pss)　$\chi_{ZYY} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos 2\phi)]$

(sss)　(none)

［縮重バンド］　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには**　$\beta_{caa} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$、$\beta_{aaa} \sim (4\sqrt{2}/9)\,\beta_{\zeta\zeta\zeta}$　**である。**

原理的には振動バンドが３つに分裂するが、実際には重なっているときには、以下に示す３つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{xxz} + \beta_{yyz} = -2\,\beta_{caa}(\cos\alpha - \cos^3\alpha)$

$\beta_{xxz} - \beta_{yyz} = -2\,\beta_{caa}(\cos\alpha - \cos^3\alpha)$

$\beta_{xxz} + \beta_{yyz} - 2\,\beta_{zzz} = -6\,\beta_{caa}(\cos\alpha - \cos^3\alpha)$

$\beta_{zxx} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)$

$\beta_{zyy} = \beta_{caa}\cos\alpha$　**であるから、**

［対称 (a_1) 振動］

(ppp)　$\chi_{XZX} = (1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(3 + \cos 2\phi)$

　　　$\chi_{ZXX} = (1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(3 + \cos 2\phi)$

　　　$\chi_{XXZ} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)[\cos\theta - (1/2)(\cos\theta - \cos^3\theta)(3 + \cos 2\phi)]$

　　　$\chi_{ZZZ} = \beta_{caa}(\cos\alpha - \cos^3\alpha)[\cos\theta - 3\cos^3\theta + (\cos\theta - \cos^3\theta)\cos 2\phi]$

(spp)　$\chi_{YZX} = -(1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)\sin^2\theta\sin 2\phi$

(ssp)　$\chi_{YYZ} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)[\cos\theta - (1/2)(\cos\theta - \cos^3\theta)(3 + \cos 2\phi)]$

(psp)　$\chi_{ZYX} = -(1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)\sin^2\theta\sin 2\phi$

(sps)　$\chi_{YZY} = (1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(3 + \cos 2\phi)$

(pps)　$\chi_{XZY} = -(1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)\sin^2\theta\sin 2\phi$

$\chi_{ZXY} = -(1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)\sin^2\theta\sin2\phi$

(pss) $\chi_{ZYY} = (1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(3 + \cos2\phi)$

(sss) (none)

［**逆対称 (b$_1$) 振動**］

(ppp) $\chi_{ZXX} = -(1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[\cos\theta - (1 + \cos2\phi)(\cos\theta - \cos^3\theta)]$

$\chi_{XZX} = -(1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[\cos\theta - (1 + \cos2\phi)(\cos\theta - \cos^3\theta)]$

$\chi_{XXZ} = (1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)(1 + \cos2\phi)(\cos\theta - \cos^3\theta)$

$\chi_{ZZZ} = -\beta_{caa}(\cos\alpha - 2\cos^3\alpha)(1 + \cos2\phi)(\cos\theta - \cos^3\theta)$

(spp) (none)

(ssp) $\chi_{YYZ} = (1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)(1 + \cos2\phi)(\cos\theta - \cos^3\theta)$

(psp) (none)

(sps) $\chi_{YZY} = -(1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[\cos\theta - (1 + \cos2\phi)(\cos\theta - \cos^3\theta)]$

(pps) (none)

(pss) $\chi_{ZYY} = -(1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[\cos\theta - (1 + \cos2\phi)(\cos\theta - \cos^3\theta)]$

(sss) (none)

［**面外 (b$_2$) 振動**］

(ppp) $\chi_{ZXX} = (1/2)\beta_{caa}\cos\alpha[\cos\theta - (\cos\theta - \cos^3\theta)(1 - \cos2\phi)]$

$\chi_{XZX} = (1/2)\beta_{caa}\cos\alpha[\cos\theta - (\cos\theta - \cos^3\theta)(1 - \cos2\phi)]$

$\chi_{XZ} = -(1/2)\beta_{caa}\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\phi)$

$\chi_{ZZZ} = \beta_{caa}\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\phi)$

(spp) (none)

(ssp) $\chi_{YYZ} = -(1/2)\beta_{caa}\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\phi)$

(psp) (none)

(sps) $\chi_{YZY} = (1/2)\beta_{caa}\cos\alpha[\cos\theta - (\cos\theta - \cos^3\theta)(1 - \cos2\phi)]$

(pps) (none)

(pss) $\chi_{ZYY} = (1/2)\beta_{caa}\cos\alpha[\cos\theta - (\cos\theta - \cos^3\theta)(1 - \cos2\phi)]$

(sss) (none)

$\phi_A = \phi_B = 0, \pi$・ランダム配向（一般的な配向に対する表式は付録 C に示す。）

［**全対称バンド**］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには** $\beta_{aac} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$、$\beta_{ccc} \sim (1/9)\,\beta_{\zeta\zeta\zeta}$ **である。**

原理的には振動バンドが２つに分裂するが、実際には重なっているときには、以下に示す２つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{xxz} + \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 4\beta_{aac}\cos\alpha$

$\beta_{xxz} - \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

$\beta_{xxz} + \beta_{yyz} - 2\beta_{zzz} = -2(\beta_{aac} - \beta_{ccc})[3(\cos\alpha - \cos^3\alpha) - 2\cos\alpha]$

$\beta_{zxx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$　**であるから、**

［**対称 (a$_1$) 振動**］

(ppp)　$\chi_{XZX} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

$\chi_{ZXX} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

$\chi_{XXZ} = (1/2)(\beta_{aac} - \beta_{ccc})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta) - 2(\cos\alpha - \cos^3\alpha)\cos\theta\} + 2\beta_{aac}\cos\alpha\cos\theta$

$\chi_{ZZZ} = -(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(1 + \cos2\phi)(\cos\theta - \cos^3\theta) + 2\cos^3\alpha\cos^3\theta]$

(spp)　$\chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(ssp)　$\chi_{YYZ} = (1/2)(\beta_{aac} - \beta_{ccc})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta) - 2(\cos\alpha - \cos^3\alpha)\cos\theta\} + 2\beta_{aac}\cos\alpha\cos\theta$

(psp)　$\chi_{ZYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(sps)　$\chi_{YZY} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

(pps)　$\chi_{XZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

$\chi_{ZXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(pss)　$\chi_{ZYY} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

(sss)　(none)

［**逆対称 (b$_1$) 振動**］

(ppp)　$\chi_{ZXX} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

$\chi_{XZX} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

$\chi_{XXZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

$\chi_{ZZZ} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

(spp)　(none)

(ssp)　$\chi_{YYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

(psp)　(none)

(sps)　$\chi_{YZY} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

(pps)　(none)

(pss)　$\chi_{ZYY} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

(sss)　(none)

［縮重バンド］　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには**　$\beta_{caa} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$、$\beta_{aaa} \sim (4\sqrt{2}/9)\,\beta_{\zeta\zeta\zeta}$　**である。**

原理的には振動バンドが実際には３つに分裂するが、重なっているときには、以下に示す３つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{xxz} + \beta_{yyz} = -4\beta_{caa}(\cos\alpha - \cos^3\alpha) \pm 2\beta_{aaa}\sin^3\alpha$

$\beta_{xxz} - \beta_{yyz} = -4\beta_{caa}(\cos\alpha - \cos^3\alpha) \pm 2\beta_{aaa}(2\sin\alpha + \sin^3\alpha)$

$\beta_{xxz} + \beta_{yyz} - 2\beta_{zzz} = -12\beta_{caa}(\cos\alpha - \cos^3\alpha) - (\pm)2\beta_{aaa}\sin^3\alpha$

$\beta_{zxx} = -2\beta_{caa}(\cos\alpha - 2\cos^3\alpha) - (\pm)2\beta_{aaa}(\sin\alpha - \sin^3\alpha)$

$\beta_{zyy} = 2\beta_{caa}\cos\alpha - (\pm)2\beta_{aaa}\sin\alpha$　**であるから、**

［対称 (a_1) 振動］

(ppp)　$\chi_{XZX} = \beta_{caa}(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$
$\quad \pm (1/2)\beta_{aaa}[2\sin\alpha - (2\sin\alpha + \sin^3\alpha)(1 + \cos2\phi)](\cos\theta - \cos^3\theta)$

$\chi_{ZXX} = \beta_{caa}(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$
$\quad \pm (1/2)\beta_{aaa}[2\sin\alpha - (2\sin\alpha + \sin^3\alpha)(1 + \cos2\phi)](\cos\theta - \cos^3\theta)$

$\chi_{XXZ} = \beta_{caa}(\cos\alpha - \cos^3\alpha)[-2\cos\theta + (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$
$\quad \pm (1/2)\beta_{aaa}[\sin^3\alpha(\cos\theta + \cos^3\theta) - (2\sin\alpha + \sin^3\alpha)(\cos\theta - \cos^3\theta)\cos2\phi]$

$\chi_{ZZZ} = -2\beta_{caa}(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$
$\quad \pm \beta_{aaa}[2\sin\alpha + \sin^3\alpha(1 + \cos2\phi)](\cos\theta - \cos^3\theta)$

(spp)　$\chi_{YZX} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)\sin^2\theta\sin2\phi$
$\quad \pm (1/2)\beta_{aaa}(2\sin\alpha + \sin^3\alpha)]\sin^2\theta\sin2\phi$

(ssp)　$\chi_{YYZ} = \beta_{caa}(\cos\alpha - \cos^3\alpha)[-2\cos\theta + (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$
$\quad \pm (1/2)\beta_{aaa}[\sin^3\alpha(\cos\theta + \cos^3\theta) - (2\sin\alpha + \sin^3\alpha)(\cos\theta - \cos^3\theta)\cos2\phi]$

(psp)　$\chi_{ZYX} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)\sin^2\theta\sin2\phi$
$\quad \pm (1/2)\beta_{aaa}(2\sin\alpha + \sin^3\alpha)]\sin^2\theta\sin2\phi$

(sps)　$\chi_{YZY} = \beta_{caa}(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$
$\quad \pm (1/2)\beta_{aaa}[2\sin\alpha - (2\sin\alpha + \sin^3\alpha)(1 + \cos2\phi)](\cos\theta - \cos^3\theta)$

(pps)　$\chi_{XZY} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)\sin^2\theta\sin2\phi$
$\quad \pm (1/2)\beta_{aaa}(2\sin\alpha + \sin^3\alpha)]\sin^2\theta\sin2\phi$

$\chi_{ZXY} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)\sin^2\theta\sin2\phi$
$\quad \pm (1/2)\beta_{aaa}(2\sin\alpha + \sin^3\alpha)]\sin^2\theta\sin2\phi$

(pss)　$\chi_{ZYY} = \beta_{caa}(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$
$\quad \pm (1/2)\beta_{aaa}[2\sin\alpha - (2\sin\alpha + \sin^3\alpha)(1 + \cos2\phi)](\cos\theta - \cos^3\theta)$

(sss)　(none)

［**逆対称 (b_1) 振動**］

($\beta_{\xi\xi\zeta} >> \beta_{\xi\xi\zeta} \sim \beta_{\eta\eta\zeta}$ **とすると、**$\beta_{caa} = \beta_{\zeta\zeta\zeta}(\cos\alpha - \cos^3\alpha) \sim 2\sqrt{3}/9\ \beta_{\zeta\zeta\zeta}$ (Td)、$3/8\ \beta_{\zeta\zeta\zeta}$ (sp^2)**である。**)

(ppp) $\chi_{ZXX} = [-\beta_{caa}(\cos\alpha - 2\cos^3\alpha) - (\pm)\beta_{aaa}(\sin\alpha - \sin^3\alpha)][\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

$\chi_{XZX} = [-\beta_{caa}(\cos\alpha - 2\cos^3\alpha) - (\pm)\beta_{aaa}(\sin\alpha - \sin^3\alpha)][\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

$\chi_{XXZ} = -[-\beta_{caa}(\cos\alpha - 2\cos^3\alpha) - (\pm)\beta_{aaa}(\sin\alpha - \sin^3\alpha)](\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

$\chi_{ZZZ} = 2[-\beta_{caa}(\cos\alpha - 2\cos^3\alpha) - (\pm)\beta_{aaa}(\sin\alpha - \sin^3\alpha)](\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

(spp) (none)

(ssp) $\chi_{YYZ} = -[-\beta_{caa}(\cos\alpha - 2\cos^3\alpha) - (\pm)\beta_{aaa}(\sin\alpha - \sin^3\alpha)](\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

(psp) (none)

(sps) $\chi_{YZY} = [-\beta_{caa}(\cos\alpha - 2\cos^3\alpha) - (\pm)\beta_{aaa}(\sin\alpha - \sin^3\alpha)][\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

(pps) (none)

(pss) $\chi_{ZYY} = [-\beta_{caa}(\cos\alpha - 2\cos^3\alpha) - (\pm)\beta_{aaa}(\sin\alpha - \sin^3\alpha)][\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

(sss) (none)

［**面外 (b_2) 振動**］

(ppp) $\chi_{ZXX} = [\beta_{caa}\cos\alpha - (\pm)\beta_{aaa}\sin\alpha][\cos\theta - (\cos\theta - \cos^3\theta)(1 - \cos2\phi)]$

$\chi_{XZX} = [\beta_{caa}\cos\alpha - (\pm)\beta_{aaa}\sin\alpha][\cos\theta - (\cos\theta - \cos^3\theta)(1 - \cos2\phi)]$

$\chi_{XXZ} = -[\beta_{caa}\cos\alpha - (\pm)\beta_{aaa}\sin\alpha](\cos\theta - \cos^3\theta)(1 - \cos2\phi)$

$\chi_{ZZZ} = 2[\beta_{caa}\cos\alpha - (\pm)\beta_{aaa}\sin\alpha](\cos\theta - \cos^3\theta)(1 - \cos2\phi)$

(spp) (none)

(ssp) $\chi_{YYZ} = -[\beta_{caa}\cos\alpha - (\pm)\beta_{aaa}\sin\alpha](\cos\theta - \cos^3\theta)(1 - \cos2\phi)$

(psp) (none)

(sps) $\chi_{YZY} = [\beta_{caa}\cos\alpha - (\pm)\beta_{aaa}\sin\alpha][\cos\theta - (\cos\theta - \cos^3\theta)(1 - \cos2\phi)]$

(pps) (none)

(pss) $\chi_{ZYY} = [\beta_{caa}\cos\alpha - (\pm)\beta_{aaa}\sin\alpha][\cos\theta - (\cos\theta - \cos^3\theta)(1 - \cos2\phi)]$

(sss) (none)

$\phi_A = \phi_B \neq 0, \pi$・ランダム配向（一般的な配向に対する表式は付録 D に示す。）

［**全対称バンド**］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには** $\beta_{aac} \sim (4/9)\ \beta_{\zeta\zeta\zeta}$、$\beta_{ccc} \sim (1/9)\ \beta_{\zeta\zeta\zeta}$ **である。**

原理的には振動バンドが２つに分裂するが、実際には重なっているときには、以下に示す２つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{xxz} + \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 4\beta_{aac}\cos\alpha$

$\beta_{xxz} - \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

$\beta_{xxz} + \beta_{yyz} - 2\beta_{zzz} = -2(\beta_{aac} - \beta_{ccc})[3(\cos\alpha - \cos^3\alpha) - 2\cos\alpha]$

$\beta_{zxx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$ **であるから、**

［**対称(a_1) 振動**］

(ppp) $\chi_{XZX} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

$\chi_{ZXX} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

$\chi_{XXZ} = (1/2)(\beta_{aac} - \beta_{ccc})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta) - 2(\cos\alpha - \cos^3\alpha)\cos\theta\}$
$+ 2\beta_{aac}\cos\alpha\cos\theta$

$\chi_{ZZZ} = -(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(1 + \cos2\phi)(\cos\theta - \cos^3\theta) + 2\cos^3\alpha\cos^3\theta]$

(spp) $\chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(ssp) $\chi_{YYZ} = (1/2)(\beta_{aac} - \beta_{ccc})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta) - 2(\cos\alpha - \cos^3\alpha)\cos\theta\}$
$+ 2\beta_{aac}\cos\alpha\cos\theta$

(psp) $\chi_{ZYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(sps) $\chi_{YZY} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

(pps) $\chi_{XZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

$\chi_{ZXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(pss) $\chi_{ZYY} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

(sss) (none)

［**逆対称 (b_1) 振動**］

(ppp) $\chi_{ZXX} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

$\chi_{XZX} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

$\chi_{XXZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

$\chi_{ZZZ} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

(spp) (none)

(ssp) $\chi_{YYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

(psp) (none)

(sps) $\chi_{YZY} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

(pps) (none)

(pss) $\chi_{ZYY} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

(sss) (none)

［**縮重バンド**］　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには**　$\beta_{caa} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$、$\beta_{aaa} \sim (4\sqrt{2}/9)\,\beta_{\zeta\zeta\zeta}$　**である。**

原理的には振動バンドが３つに分裂するが、実際には重なっているときには、以下に示す３つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{xxz} + \beta_{yyz} = -2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1\pm \cos2\phi_A) - \beta_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)$

$\beta_{xxz} - \beta_{yyz} = -2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1\pm \cos2\phi_A) + \beta_{aaa}(2\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)$

$\beta_{xxz} + \beta_{yyz} - 2\beta_{zzz} = -6\beta_{caa}(\cos\alpha - \cos^3\alpha)(1\pm \cos2\phi_A) - 3\beta_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)$

$\beta_{zxx} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)(1\pm \cos2\phi_A) + \beta_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)$

$\beta_{zyy} = \beta_{caa}\cos\alpha(1 - (\pm)\cos2\phi_A) - \beta_{aaa}\sin\alpha\,(\cos3\phi_A - (\pm)\cos\phi_A)$

$\beta_{xyz} = \beta_{yxz} = \pm\beta_{caa}\sin^2\alpha\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)$

$\beta_{yzx} = \beta_{zyx} = -(\pm)\beta_{caa}\sin^2\alpha\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)$

$\beta_{zxy} = \beta_{xzy} = -(\pm)\beta_{caa}(2\cos^2\alpha - 1)\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A - (\pm)\sin\phi_A)$　**であるから、**

［**対称 (a_1) 振動**］

(ppp)　$\chi_{XZX} = (3/4)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - \beta_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)](\cos\theta - \cos^3\theta)$
$+ (1/4)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - \beta_{aaa}(2\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]\cos2\phi(\cos\theta - \cos^3\theta)$
$- (1/2)[\pm\beta_{caa}\sin^2\alpha\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

$\chi_{ZXX} = (3/4)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - \beta_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)](\cos\theta - \cos^3\theta)$
$+ (1/4)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - \beta_{aaa}(2\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]\cos2\phi(\cos\theta - \cos^3\theta)$
$- (1/2)[\pm\beta_{caa}\sin^2\alpha\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

$\chi_{XXZ} = -(1/2)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)]\cos\theta$
$+ (3/4)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)](\cos\theta - \cos^3\theta)$
$+ (1/4)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - \beta_{aaa}(2\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]\cos2\phi(\cos\theta - \cos^3\theta)$
$- (1/2)[\pm\beta_{caa}\sin^2\alpha\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

$\chi_{ZZZ} = -(1/2)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)]\cos\theta$
$+ (3/2)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)]\cos^3\theta$
$- (1/2)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - \beta_{aaa}(2\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]\cos2\phi(\cos\theta - \cos^3\theta)$
$+ [\pm\beta_{caa}\sin^2\alpha\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

(spp)　$\chi_{YZX} = -(1/4)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - \beta_{aaa}(2\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]\sin2\phi\sin^2\theta$
$- (1/2)[\pm\beta_{caa}\sin^2\alpha\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)]\sin^2\theta\cos2\phi$

(ssp)　$\chi_{YYZ} = -(1/2)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)]\cos\theta$
$+ (3/4)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)](\cos\theta - \cos^3\theta)$
$+ (1/4)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - \beta_{aaa}(2\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]\cos2\phi(\cos\theta - \cos^3\theta)$
$- (1/2)[\pm\beta_{caa}\sin^2\alpha\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

(psp)　$\chi_{ZYX} = -(1/4)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - \beta_{aaa}(2\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]\sin2\phi\sin^2\theta$
$- (1/2)[\pm\beta_{caa}\sin^2\alpha\sin2\phi_A - \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)]\sin^2\theta\cos2\phi$

(sps)　$\chi_{YZY} = (3/4)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)](\cos\theta - \cos^3\theta)$
$+ (1/4)[2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - \beta_{aaa}(2\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]\cos2\phi(\cos\theta - \cos^3\theta)$

$- (1/2)[\pm ß_{caa}\sin^2\alpha\sin2\phi_A - ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

(pps) $\chi_{XZY} = -(1/4)[2ß_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - ß_{aaa}(2\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]\sin2\phi\sin^2\theta$
$+ (1/2)[\pm ß_{caa}\sin^2\alpha\sin2\phi_A - ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)]\sin^2\theta\cos2\phi$

$\chi_{ZXY} = -(1/4)[2ß_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - ß_{aaa}(2\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]\sin2\phi\sin^2\theta$
$+ (1/2)[\pm ß_{caa}\sin^2\alpha\sin2\phi_A - ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)]\sin^2\theta\cos2\phi$

(pss) $\chi_{ZYY} = (3/4)[2ß_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) + ß_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)](\cos\theta - \cos^3\theta)$
$+ (1/4)[2ß_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - ß_{aaa}(2\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]\cos2\phi(\cos\theta - \cos^3\theta)$
$- (1/2)[\pm ß_{caa}\sin^2\alpha\sin2\phi_A - ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

(sss) (none)

［**逆対称 (b_1) 振動**］

($\beta_{\xi\xi\zeta} >> \beta_{\xi\xi\zeta} \sim \beta_{\eta\eta\zeta}$ **とすると、**$\beta_{caa} = \beta_{\zeta\zeta\zeta}(\cos\alpha - \cos^3\alpha) \sim 2\sqrt{3}/9\ \beta_{\zeta\zeta\zeta}$ (Td)**、**3/8 $\beta_{\zeta\zeta\zeta}$ (sp^2)**である。**)

(ppp) $\chi_{ZXX} = -(1/2)[ß_{caa}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos2\phi_A) - ß_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]$
$\times [\cos\theta - (1 + \cos2\phi)(\cos\theta - \cos^3\theta)]$
$+ (1/2)[(\pm)ß_{caa}\sin^2\alpha\sin2\phi_A + ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

$\chi_{XZX} = -(1/2)[ß_{caa}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos2\phi_A) - ß_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]$
$\times [\cos\theta - (1 + \cos2\phi)(\cos\theta - \cos^3\theta)]$
$+ (1/2)[(\pm)ß_{caa}\sin^2\alpha\sin2\phi_A + ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

$\chi_{XXZ} = (1/2)[ß_{caa}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos2\phi_A) - ß_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]$
$\times (1 + \cos2\phi)(\cos\theta - \cos^3\theta)$
$+ ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

$\chi_{ZZZ} = -[ß_{caa}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos2\phi_A) - ß_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]$
$\times (1 + \cos2\phi)(\cos\theta - \cos^3\theta)$
$- [(\pm)ß_{caa}\sin^2\alpha\sin2\phi_A + ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

(spp) $\chi_{YZX} = (1/4)[(\pm)ß_{caa}\sin^2\alpha\sin2\phi_A + ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](1 - 3\cos^2\theta - \sin^2\theta\cos2\phi)$

(ssp) $\chi_{YYZ} = (1/2)[ß_{caa}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos2\phi_A) - ß_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]$
$\times (1 + \cos2\phi)(\cos\theta - \cos^3\theta)$
$+ (1/2)[(\pm)ß_{caa}\sin^2\alpha\sin2\phi_A + ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

(psp) $\chi_{ZYX} = (1/4)[(\pm)ß_{caa}\sin^2\alpha\sin2\phi_A + ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](1 - 3\cos^2\theta - \sin^2\theta\cos2\phi)$

(sps) $\chi_{YZY} = -(1/2)[ß_{caa}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos2\phi_A) - ß_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]$
$\times [\cos\theta - (1 + \cos2\phi)(\cos\theta - \cos^3\theta)]$
$+ (1/2)[(\pm)ß_{caa}\sin^2\alpha\sin2\phi_A + ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

(pps) $\chi_{ZXY} = -(1/4)[(\pm)ß_{caa}\sin^2\alpha\sin2\phi_A + ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](1 - 3\cos^2\theta - \sin^2\theta\cos2\phi)$

$\chi_{XZY} = -(1/4)[(\pm)ß_{caa}\sin^2\alpha\sin2\phi_A + ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](1 - 3\cos^2\theta - \sin^2\theta\cos2\phi)$

(pss) $\chi_{ZYY} = -(1/2)[\beta_{caa}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos2\phi_A) - \beta_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)]$
$\times [\cos\theta - (1 + \cos2\phi)(\cos\theta - \cos^3\theta)]$
$+ (1/2)[(\pm)\beta_{caa}\sin^2\alpha\sin2\phi_A + \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

(sss) (none)

［**面外 (b$_2$) 振動**］

(ppp) $\chi_{ZXX} = (1/2)[\beta_{caa}\cos\alpha(1 - (\pm)\cos2\phi_A) - \beta_{aaa}\sin\alpha(\cos3\phi_A - (\pm)\cos\phi_A)][\cos\theta - (1 - \cos2\phi)(\cos\theta - \cos^3\theta)]$
$+ (1/2)[(\pm)\beta_{caa}(2\cos^2\alpha - 1)\sin2\phi_A + \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A - (\pm)\sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

$\chi_{XZX} = (1/2)[\beta_{caa}\cos\alpha(1 - (\pm)\cos2\phi_A) - \beta_{aaa}\sin\alpha(\cos3\phi_A - (\pm)\cos\phi_A)][\cos\theta - (1 - \cos2\phi)(\cos\theta - \cos^3\theta)]$
$+ (1/2)[(\pm)\beta_{caa}(2\cos^2\alpha - 1)\sin2\phi_A + \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A - (\pm)\sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

$\chi_{XXZ} = -(1/2)[\beta_{caa}\cos\alpha(1 - (\pm)\cos2\phi_A) - \beta_{aaa}\sin\alpha(\cos3\phi_A - (\pm)\cos\phi_A)](1 - \cos2\phi)(\cos\theta - \cos^3\theta)$
$+ (1/2)[(\pm)\beta_{caa}(2\cos^2\alpha - 1)\sin2\phi_A + \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A - (\pm)\sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

$\chi_{ZZZ} = [\beta_{caa}\cos\alpha(1 - (\pm)\cos2\phi_A) - \beta_{aaa}\sin\alpha(\cos3\phi_A - (\pm)\cos\phi_A)](1 - \cos2\phi)(\cos\theta - \cos^3\theta)$
$- [(\pm)\beta_{caa}(2\cos^2\alpha - 1)\sin2\phi_A + \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A - (\pm)\sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

(spp) $\chi_{YZX} = (1/4)[\beta_{caa}\cos\alpha(1 - (\pm)\cos2\phi_A) - \beta_{aaa}\sin\alpha(\cos3\phi_A - (\pm)\cos\phi_A)](1 - 3\cos^2\theta - \sin^2\theta\cos2\phi)$

(ssp) $\chi_{YYZ} = -(1/2)[\beta_{caa}\cos\alpha(1 - (\pm)\cos2\phi_A) - \beta_{aaa}\sin\alpha(\cos3\phi_A - (\pm)\cos\phi_A)](1 - \cos2\phi)(\cos\theta - \cos^3\theta)$
$+ (1/2)[(\pm)\beta_{caa}(2\cos^2\alpha - 1)\sin2\phi_A + \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A - (\pm)\sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

(psp) $\chi_{ZYX} = (1/4)[\beta_{caa}\cos\alpha(1 - (\pm)\cos2\phi_A) - \beta_{aaa}\sin\alpha(\cos3\phi_A - (\pm)\cos\phi_A)](1 - 3\cos^2\theta - \sin^2\theta\cos2\phi)$

(sps) $\chi_{YZY} = (1/2)[\beta_{caa}\cos\alpha(1 - (\pm)\cos2\phi_A) - \beta_{aaa}\sin\alpha(\cos3\phi_A - (\pm)\cos\phi_A)][\cos\theta - (1 - \cos2\phi)(\cos\theta - \cos^3\theta)]$
$+ (1/2)[(\pm)\beta_{caa}(2\cos^2\alpha - 1)\sin2\phi_A + \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A - (\pm)\sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

(pps) $\chi_{ZXY} = -(1/4)[\beta_{caa}\cos\alpha(1 - (\pm)\cos2\phi_A) - \beta_{aaa}\sin\alpha(\cos3\phi_A - (\pm)\cos\phi_A)](1 - 3\cos^2\theta - \sin^2\theta\cos2\phi)$

$\chi_{XZY} = -(1/4)[\beta_{caa}\cos\alpha(1 - (\pm)\cos2\phi_A) - \beta_{aaa}\sin\alpha(\cos3\phi_A - (\pm)\cos\phi_A)](1 - 3\cos^2\theta - \sin^2\theta\cos2\phi)$

(pss) $\chi_{ZYY} = (1/2)[\beta_{caa}\cos\alpha(1 - (\pm)\cos2\phi_A) - \beta_{aaa}\sin\alpha(\cos3\phi_A - (\pm)\cos\phi_A)][\cos\theta - (1 - \cos2\phi)(\cos\theta - \cos^3\theta)]$
$+ (1/2)[(\pm)\beta_{caa}(2\cos^2\alpha - 1)\sin2\phi_A + \beta_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A - (\pm)\sin\phi_A)](\cos\theta - \cos^3\theta)\sin2\phi$

(sss) (none)

$\phi_A = 0, \phi_B = \pi$ または $\phi_A = \pi, \phi_B = 0$（一般的な配向に対する表式は付録 E に示す。）

［**全対称バンド**］

原理的には振動バンドが２つに分裂するが、実際には重なっているときには、以下に示す２つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには** $\beta_{aac} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$、$\beta_{ccc} \sim (1/9)\,\beta_{\zeta\zeta\zeta}$ **である。**

$\beta_{xxz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{aac}\cos\alpha$

$\beta_{yyz} = +2\beta_{aac}\cos\alpha$

$\beta_{zzz} = +2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{ccc}\cos\alpha$

$\beta_{zxx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

$$\beta_{xzx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$$

$$\beta_{xxz} + \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 4\beta_{aac}\cos\alpha$$

$$\beta_{xxz} - \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$$

$$\beta_{xxz} + \beta_{yyz} - 2\beta_{zzz} = -2(\beta_{aac} - \beta_{ccc})[3(\cos\alpha - \cos^3\alpha) - 2\cos\alpha]$$

$\beta_{zxx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$ **であるから、**

［**対称 (a$_1$) 振動**］

(ppp) $\chi_{XZX} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

$\chi_{ZXX} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

$\chi_{XXZ} = (1/2)(\beta_{aac} - \beta_{ccc})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$
$- 2(\cos\alpha - \cos^3\alpha)\cos\theta\} + 2\beta_{aac}\cos\alpha\cos\theta$

$\chi_{ZZZ} = -(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(1 + \cos2\phi)(\cos\theta - \cos^3\theta) + 2\cos^3\alpha\cos^3\theta]$

(spp) $\chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(ssp) $\chi_{YYZ} = (1/2)(\beta_{aac} - \beta_{ccc})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$
$- 2(\cos\alpha - \cos^3\alpha)\cos\theta\} + 2\beta_{aac}\cos\alpha\cos\theta$

(psp) $\chi_{ZYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(sps) $\chi_{YZY} = (1/2)(\beta_{aac} - \beta_{ccc})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

(pps) $\chi_{XZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

$\chi_{ZXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(pss) $\chi_{ZYY} = (1/2)(\beta_{aac} - \beta_{ccc}\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\phi) - 2\cos\alpha](\cos\theta - \cos^3\theta)$

(sss) (none)

［**逆対称 (b$_1$) 振動**］

(ppp) $\chi_{ZXX} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

$\chi_{XZX} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

$\chi_{XXZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

$\chi_{ZZZ} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

(spp) (none)

(ssp) $\chi_{YYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

(psp) (none)

(sps) $\chi_{YZY} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

(pps) (none)

(pss) $\chi_{ZYY} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

(sss) (none)

［縮重バンド］　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ のときには　$\beta_{caa} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$、$\beta_{aaa} \sim (4\sqrt{2}/9)\,\beta_{\zeta\zeta\zeta}$　である。

（β_{zyy} と β_{yzy} には b 軸方向の振動が、他の成分には a 軸方向の振動が寄与する。）

（± 記号の上側は$\phi_A = 0, \phi_B = \pi$ に、下側は $\phi_A = \pi, \phi_B = 0$ に対応する。）

原理的には振動バンドが３つに分裂するが、実際には重なっているときには、以下に示す３つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{zxx} = -2\beta_{caa}(\cos\alpha - 2\cos^3\alpha)$

$\beta_{xzx} = -2\beta_{caa}(\cos\alpha - 2\cos^3\alpha)$

$\beta_{zyy} = 2\beta_{caa}\cos\alpha$

$\beta_{yzy} = 2\beta_{caa}\cos\alpha$

$\beta_{xxz} = -4\beta_{caa}(\cos\alpha - \cos^3\alpha)$

$\beta_{yyz} = 0$

$\beta_{zzz} = 4\beta_{caa}(\cos\alpha - \cos^3\alpha)$

［対称 (a_1) 振動］

(ppp)　$\chi_{XZX} = \beta_{caa}(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(3 + \cos2\phi)$

$\chi_{ZXX} = \beta_{caa}(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(3 + \cos2\phi)$

$\chi_{XXZ} = \beta_{caa}(\cos\alpha - \cos^3\alpha)[-2\cos\theta + (\cos\theta - \cos^3\theta)(3 + \cos2\phi)]$

$\chi_{ZZZ} = 2\,\beta_{caa}(\cos\alpha - \cos^3\alpha)[2\cos\theta - (\cos\theta - \cos^3\theta)(3 + \cos2\phi)]$

(spp)　$\chi_{YZX} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(ssp)　$\chi_{YYZ} = \beta_{caa}(\cos\alpha - \cos^3\alpha)\cos\theta[-2\cos\theta + (\cos\theta - \cos^3\theta)(3 + \cos2\phi)]$

(psp)　$\chi_{ZYX} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(sps)　$\chi_{YZY} = 3\beta_{caa}(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(3 + \cos2\phi)$

(pps)　$\chi_{XZY} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

$\chi_{ZXY} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)\sin2\phi\sin^2\theta$

(pss)　$\chi_{ZYY} = 3\beta_{caa}(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(3 + \cos2\phi)$

(sss)　(none)

［逆対称 (b_1) 振動］

(ppp)　$\chi_{ZXX} = -\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

$\chi_{XZX} = -\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$

$\chi_{XXZ} = \beta_{caa}(\cos\alpha - 2\cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

$\chi_{ZZZ} = -2\beta_{caa}(\cos\alpha - 2\cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

(spp)　(none)

(ssp)　$\chi_{YYZ} = \beta_{caa}(\cos\alpha - 2\cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

(psp)　(none)

(sps)　$\chi_{YZY} = -ß_{caa}(\cos\alpha - 2\cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$
(pps)　(none)

(pss)　$\chi_{ZYY} = -ß_{caa}(\cos\alpha - 2\cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)]$
(sss)　(none)

［面外 (b_2) 振動］

(ppp)　$\chi_{ZXX} = ß_{caa}\cos\alpha[\cos\theta - (\cos\theta - \cos^3\theta)(1 - \cos2\phi)]$
$\chi_{XZX} = ß_{caa}\cos\alpha[\cos\theta - (\cos\theta - \cos^3\theta)(1 - \cos2\phi)]$
$\chi_{XXZ} = -ß_{caa}\cos(\cos\theta - \cos^3\theta)(1 - \cos2\phi)$
$\chi_{ZZZ} = 2ß_{caa}\cos(\cos\theta - \cos^3\theta)(1 - \cos2\phi)$
(spp)　(none)

(ssp)　$\chi_{YYZ} = -ß_{caa}\cos(\cos\theta - \cos^3\theta)(1 - \cos2\phi)$
(psp)　(none)

(sps)　$\chi_{YZY} = ß_{caa}\cos\alpha[\cos\theta - (\cos\theta - \cos^3\theta)(1 - \cos2\phi)]$
(pps)　(none)

(pss)　$\chi_{ZYY} = ß_{caa}\cos\alpha[\cos\theta - (\cos\theta - \cos^3\theta)(1 - \cos2\phi)]$
(sss)　(none)

付録 A：$(CH_3)_2X$ 基の SFG テンソル

［座標系とメチル基の配向］

1. メチル基に固定した座標系；(a, b, c) 系：C_3 **軸を** C **原子から** H **原子の方向に向けて** c **軸を取り、３個の** CH **結合の１つが** ac **面の上に乗るようにする。**

2. $(CH_3)_2X$ 基に固定した座標系；(x, y, z) 系：２個のメチル基の C_3 **軸の２等分線に沿って** z **軸を取り、**X **原子からメチル基の方向を正方向とする。２本の** C_3 **軸が作る平面の上に** x **軸を取る。**

3. メチル基の配向：z **軸とメチル基の分子軸の間の角（即ち** CXC **角の半分）を** α **とする。また、２個のメチル基を下付き** A, B **で区別するとき、それぞれのメチル基の内部回転角を** ϕ_A, ϕ_B **と表す。メチル基の３個の** H **原子が作る正三角形の頂点が表面を向いている状態を基準に取り、このときの内部回転角を** $\phi_A = 0, \phi_B = 0$ **とする。正三角形の辺が表面に寄っている時の内部回転角は** 180° **である。**

内部回転角による違いを生じるのは「縮重振動」バンドに対する SFG **テンソルだけである。よって、縮重バンドの様子から、メチル基の相対的な配向や回転の様子を知ることが出来る。**

4. オイラー角；(χ, θ, ϕ)：２個のメチル基の座標系を分子固定系に重ねるときのオイラー角は、CXC **角を** 2α **として、**$(0, \alpha, \phi)$**と** (π, α, ϕ)**である（こうなるように** b **軸の向きを決める）。**

テンソル成分の変換式、

$\beta_{ijk} = \sum U_{ijk:abc}\beta_{abc}$ (i, j, k = x, y, z)

において、別ファイル「変換行列 (xyz)」または *Appl. Spectrosc.* **の論文の表に示されている係数** $U_{ijk:abc}$ **の一欄表を用いると、(xyz) 系での SFG テンソル成分は下のように求められる。（傾き角 θ に関しては表で使っている sinθ、sin2θ、sin3θ の形の三角関数ではなく、下の関係式で変換した sinθ、cosθ のべき乗による表式を採用する。）**

$\sin2\theta = 2\sin\theta\cos\theta$, $\cos2\theta = \cos^2\theta - \sin^2\theta = 2\cos^2\theta - 1 = 1 - 2\sin^2\theta$

$\sin3\theta = 3\sin\theta - 4\sin^3\theta$, $\sin\theta + \sin3\theta = 4(\sin\theta - \sin^3\theta)$

$\cos3\theta = 4\cos^3\theta - 3\cos\theta$, $\cos\theta - \cos3\theta = 4(\cos\theta - \cos^3\theta)$

［全対称バンド］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには** $\beta_{aac} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$, $\beta_{ccc} \sim (1/9)\,\beta_{\zeta\zeta\zeta}$ **である。**
（メチル基の相対的な配向によらず同じ表式になる。）

$\beta_{xxz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{aac}\cos\alpha$

$\beta_{yyz} = +2\beta_{aac}\cos\alpha$

$\beta_{zzz} = +2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{ccc}\cos\alpha$

$\beta_{zxx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

$\beta_{xzx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

［縮重バンド］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには** $\beta_{caa} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$, $\beta_{aaa} \sim (4\sqrt{2}/9)\,\beta_{\zeta\zeta\zeta}$ **である。**
（面外振動と面内振動を分ける際に便利なので、a 軸方向の振動と b 軸方向の振動を区別する。）
（± 記号の上側が a 軸方向の振動、下側が b 軸方向の振動に対応する。）

グループ 1

$\beta_{zxx} = -(1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[2 \pm (\cos2\phi_A + \cos2\phi_B)]$
$\quad + (1/2)\beta_{aaa}(\sin\alpha - \sin^3\alpha)[(\cos3\phi_A + \cos3\phi_B) \pm (\cos\phi_A + \cos\phi_B)]$

$\beta_{xzx} = -(1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[2 \pm (\cos2\phi_A + \cos2\phi_B)]$
$\quad + (1/2)\beta_{aaa}(\sin\alpha - \sin^3\alpha)[(\cos3\phi_A + \cos3\phi_B) \pm (\cos\phi_A + \cos\phi_B)]$

$\beta_{zyy} = (1/2)\beta_{caa}\cos\alpha[2 - (\pm)(\cos2\phi_A + \cos2\phi_B)]$
$\quad - (1/2)\beta_{aaa}\sin\alpha[(\cos3\phi_A + \cos3\phi_B) - (\pm)(\cos\phi_A + \cos\phi_B)]$

$\beta_{yzy} = (1/2)\beta_{caa}\cos\alpha[2 - (\pm)(\cos2\phi_A + \cos2\phi_B)]$
$\quad - (1/2)\beta_{aaa}\sin\alpha[(\cos3\phi_A + \cos3\phi_B) - (\pm)(\cos\phi_A + \cos\phi_B)]$

$\beta_{xxz} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)[2 \pm (\cos2\phi_A + \cos2\phi_B)]$
$\quad + (1/2)\beta_{aaa}(\sin\alpha - \sin^3\alpha)[(\cos3\phi_A + \cos3\phi_B) \pm (\cos\phi_A + \cos\phi_B)]$

$\beta_{yyz} = -(1/2)\beta_{aaa}\sin\alpha[(\cos3\phi_A + \cos3\phi_B) \pm (\cos\phi_A + \cos\phi_B)]$

$\beta_{zzz} = \beta_{caa}(\cos\alpha - \cos^3\alpha)[2 \pm (\cos2\phi_A + \cos2\phi_B)]$
$\quad + (1/2)\beta_{aaa}\sin^3\alpha[(\cos3\phi_A + \cos3\phi_B) \pm (\cos\phi_A + \cos\phi_B)]$

グループ 2

$\beta_{yzx} = -(\pm)(1/2)\beta_{caa}\cos^2\alpha(\sin2\phi_A + \sin2\phi_B)$

$\quad - (1/2)\beta_{aaa}\sin\alpha\cos\alpha[(\sin3\phi_A + \sin3\phi_B) \pm (\sin\phi_A + \sin\phi_B)]$

$\beta_{zyx} = -(\pm)(1/2)\beta_{caa}\cos^2\alpha(\sin2\phi_A + \sin2\phi_B)$

$\quad - (1/2)\beta_{aaa}\sin\alpha\cos\alpha[(\sin3\phi_A + \sin3\phi_B) \pm (\sin\phi_A + \sin\phi_B)]$

$\beta_{zxy} = -(\pm)(1/2)\beta_{caa}(2\cos^2\alpha -1)(\sin2\phi_A + \sin2\phi_B)$

$\quad - (1/2)\beta_{aaa}\sin\alpha\cos\alpha[(\sin3\phi_A + \sin3\phi_B) - (\pm)(\sin\phi_A + \sin\phi_B)]$

$\beta_{xzy} = -(\pm)(1/2)\beta_{caa}(2\cos^2\alpha -1)(\sin2\phi_A + \sin2\phi_B)$

$\quad - (1/2)\beta_{aaa}\sin\alpha\cos\alpha[(\sin3\phi_A + \sin3\phi_B) - (\pm)(\sin\phi_A + \sin\phi_B)]$

$\beta_{xyz} = \pm(1/2)\beta_{caa}\sin^2\alpha(\sin2\phi_A + \sin2\phi_B)$

$\quad - (1/2)\beta_{aaa}\sin\alpha\cos\alpha[(\sin3\phi_A + \sin3\phi_B) \pm (\sin\phi_A + \sin\phi_B)]$

$\beta_{yxz} = \pm(1/2)\beta_{caa}\sin^2\alpha(\sin2\phi_A + \sin2\phi_B)$

$\quad - (1/2)\beta_{aaa}\sin\alpha\cos\alpha[(\sin3\phi_A + \sin3\phi_B) \pm (\sin\phi_A + \sin\phi_B)]$

グループ 3

$\beta_{xxx} = -(\pm)\beta_{caa}(\sin\alpha - \sin^3\alpha)(\cos2\phi_A - \cos2\phi_B)$

$\quad - (1/2)\beta_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\phi_A - \cos3\phi_B) \pm (\cos\phi_A - \cos\phi_B)]$

$\beta_{yyx} = -(1/2)\beta_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\phi_A - \cos3\phi_B) \pm (\cos\phi_A - \cos\phi_B)]$

$\beta_{zzx} = \pm\beta_{caa}(\sin\alpha - \sin^3\alpha)(\cos2\phi_A - \cos2\phi_B)$

$\quad + (1/2)\beta_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\phi_A - \cos3\phi_B) \pm (\cos\phi_A - \cos\phi_B)]$

$\beta_{xyy} = \pm(1/2)\beta_{caa}\sin\alpha\ (\cos2\phi_A - \cos2\phi_B)$

$\quad - (1/2)\beta_{aaa}\cos\alpha\ [(\cos3\phi_A - \cos3\phi_B) - (\pm)(\cos\phi_A - \cos\phi_B)]$

$\beta_{yxy} = \pm(1/2)\beta_{caa}\sin\alpha\ (\cos2\phi_A - \cos2\phi_B)$

$\quad - (1/2)\beta_{aaa}\cos\alpha\ [(\cos3\phi_A - \cos3\phi_B) - (\pm)(\cos\phi_A - \cos\phi_B)]$

$\beta_{xzz} = \pm(1/2)\beta_{caa}(\sin\alpha - 2\sin^3\alpha)(\cos2\phi_A - \cos2\phi_B)$

$\quad + (1/2)\beta_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\phi_A - \cos3\phi_B) \pm (\cos\phi_A - \cos\phi_B)]$

$\beta_{zxz} = \pm(1/2)\beta_{caa}(\sin\alpha - 2\sin^3\alpha)(\cos2\phi_A - \cos2\phi_B)$

$\quad + (1/2)\beta_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\phi_A - \cos3\phi_B) \pm (\cos\phi_A - \cos\phi_B)]$

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$\beta_{yxx} = \pm(1/2)\beta_{caa}\sin\alpha\cos\alpha\ (\sin2\phi_A - \sin2\phi_B)$

$\quad - (1/2)\beta_{aaa}\cos^2\alpha\ [(\sin3\phi_A - \sin3\phi_B) \pm (\sin\phi_A - \sin\phi_B)]$

$\beta_{xyx} = \pm(1/2)\beta_{caa}\sin\alpha\cos\alpha\ (\sin2\phi_A - \sin2\phi_B)$

$\quad - (1/2)\beta_{aaa}\cos^2\alpha\ [(\sin3\phi_A - \sin3\phi_B) \pm (\sin\phi_A - \sin\phi_B)]$

$\beta_{xxy} = \pm\beta_{caa}\sin\alpha\cos\alpha\ (\sin2\phi_A - \sin2\phi_B)$

$\quad - (1/2)\beta_{aaa}\ \cos^2\alpha\ [(\sin3\phi_A - \sin3\phi_B) - (\pm)(\sin\phi_A - \sin\phi_B)]$

$\beta_{yyy} = (1/2)\beta_{aaa}[(\sin3\phi_A - \sin3\phi_B) - (\pm)(\sin\phi_A - \sin\phi_B)]$

$\beta_{zzy} = -(\pm)\beta_{caa}\sin\alpha\cos\alpha\ (\sin2\phi_A - \sin2\phi_B)$

$\quad - (1/2)\beta_{aaa}\sin^2\alpha\ [(\sin3\phi_A - \sin3\phi_B) - (\pm)(\sin\phi_A - \sin\phi_B)]$

$\beta_{yzz} = -(\pm1/2)\beta_{caa}\sin\alpha\cos\alpha\ (\sin2\phi_A - \sin2\phi_B)$

$- (1/2)\beta_{aaa}\sin^2\alpha\ [(\sin 3\phi_A - \sin 3\phi_B) \pm (\sin\phi_A - \sin\phi_B)]$

$\beta_{zyz} = -(\pm 1/2)\beta_{caa}\sin\alpha\cos\alpha\ (\sin 2\phi_A - \sin 2\phi_B)$

$- (1/2)\beta_{aaa}\sin^2\alpha\ [(\sin 3\phi_A - \sin 3\phi_B) \pm (\sin\phi_A - \sin\phi_B)]$

付録 B：自由回転しているときの (XYZ) 系でのテンソル成分

［全対称バンド］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには** $\beta_{aac} \sim (4/9)\ \beta_{\zeta\zeta\zeta}$、$\beta_{ccc} \sim (1/9)\ \beta_{\zeta\zeta\zeta}$ **である。**

原理的には振動バンドが２つに分裂するが、実際には重なっているときには、以下に示す２つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{xxz} + \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 4\beta_{aac}\cos\alpha$

$\beta_{xxz} - \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

$\beta_{xxz} + \beta_{yyz} - 2\beta_{zzz} = -2(\beta_{aac} - \beta_{ccc})[3(\cos\alpha - \cos^3\alpha) - 2\cos\alpha]$

$\beta_{zxx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$ **であるから、**

［**対称 (a_1) 振動**］

(ppp) $\chi_{XXX} = -2\beta_{aac}\cos\alpha\sin\theta\cos\chi$

$+ (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{4\sin\theta\cos\chi - 3\sin^3\theta(3\cos\chi + \cos 3\chi)$

$- [\sin\theta(\cos\chi - \cos 3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos 3\chi)]\cos 2\phi - 2\sin\theta\cos\theta(\sin\chi + \sin 3\chi)\sin 2\phi\}$

$+ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(3\cos\chi + \cos 3\chi)$

$\chi_{XZZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(3 + \cos 2\phi) - \sin\theta\cos\theta\sin\chi\sin 2\phi]$

$+ 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi$

$\chi_{ZXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(3 + \cos 2\phi) - \sin\theta\cos\theta\sin\chi\sin 2\phi]$

$+ 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi$

$\chi_{ZZX} = -2\beta_{aac}\cos\alpha\sin\theta\cos\chi$

$+ (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\sin\theta\cos\chi - 3(\sin\theta - \sin^3\theta)\cos\chi + \sin^3\theta\cos\chi\cos 2\phi]$

$+ 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi$

$\chi_{XZX} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)(3 + \cos 2\phi) - \sin^2\theta\sin 2\chi\sin 2\phi]$

$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)$

$\chi_{ZXX} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)(3 + \cos 2\phi) - \sin^2\theta\sin 2\chi\sin 2\phi]$

$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)$

$\chi_{XXZ} = 2\beta_{aac}\cos\alpha\cos\theta$

$+ (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)$

$+ [(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos 2\chi]\cos 2\phi + 2\cos^2\theta\sin 2\chi\sin 2\phi\}$

$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)$

$\chi_{ZZZ} = -2\beta_{aac}\cos\alpha\cos\theta$

$+ (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[-\cos\theta + 3\cos^3\theta - (\cos\theta - \cos^3\theta)\cos 2\phi]$

$- 2(\beta_{aac} - \beta_{ccc})\cos\alpha\cos^3\theta$

(spp) $\chi_{YXX} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos 2\phi](\sin\chi + \sin 3\chi)$

$$+ 2\sin\theta\cos\theta\,(\cos\chi + \cos 3\chi)\sin 2\phi\}$$
$$- (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta\,(\sin\chi + \sin 3\chi)$$
$$\chi_{YZZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos 2\phi) + \sin\theta\cos\theta\cos\chi\sin 2\phi]$$
$$- 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\sin\chi$$
$$\chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin 2\chi(3 + \cos 2\phi) + \sin^2\theta\,(1 + \cos 2\chi)\sin 2\phi]$$
$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi$$
$$\chi_{YXZ} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos 2\phi]\sin 2\chi$$
$$- 2\cos^2\theta\cos 2\chi\sin 2\phi\}$$
$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi$$

(ssp)
$$\chi_{YYX} = -2\beta_{aac}\cos\alpha\sin\theta\cos\chi$$
$$+ (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{4\sin\theta\cos\chi - 3\sin^3\theta(\cos\chi - \cos 3\chi)$$
$$- [\sin\theta(3\cos\chi + \cos 3\chi) - (\sin\theta - \sin^3\theta)(\cos\chi - \cos 3\chi)]\cos 2\phi$$
$$+ 2\sin\theta\cos\theta(\sin\chi + \sin 3\chi)\sin 2\phi\}$$
$$+ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos 3\chi)$$
$$\chi_{YYZ} = 2\beta_{aac}\cos\alpha\sin\theta\cos\chi$$
$$+ (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 - \cos 2\chi)$$
$$+ [(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos 2\chi]\cos 2\phi - 2\cos^2\theta\sin 2\chi\sin 2\phi\}$$
$$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos 2\chi)$$

(psp)
$$\chi_{XYX} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos 2\phi](\sin\chi + \sin 3\chi)$$
$$+ 2\sin\theta\cos\theta\,(\cos\chi + \cos 3\chi)\sin 2\phi\}$$
$$- (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta\,(\sin\chi + \sin 3\chi)$$
$$\chi_{ZYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos 2\phi) + \sin\theta\cos\theta\cos\chi\sin 2\phi]$$
$$- 2(\beta_{aac} - \beta_{ccc})\cos\alpha\,(\sin\theta - \sin^3\theta)\sin\chi$$
$$\chi_{XYZ} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos 2\phi]\sin 2\chi$$
$$- 2\cos^2\theta\cos 2\chi\sin 2\phi\}$$
$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi$$
$$\chi_{ZYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin 2\chi(3 + \cos 2\phi) + \sin^2\theta\,(1 + \cos 2\chi)\sin 2\phi]$$
$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi$$

(sps)
$$\chi_{YXY} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos 2\phi](\cos\chi - \cos 3\chi)$$
$$- 2\sin\theta\cos\theta\,(\sin\chi - \sin 3\chi)\sin 2\phi\}$$
$$+ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta\,(\cos\chi - \cos 3\chi)$$
$$\chi_{YZY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos 2\chi)(3 + \cos 2\phi) + \sin^2\theta\sin 2\chi\sin 2\phi]$$
$$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos 2\chi)$$

(pps)
$$\chi_{XXY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi$$
$$+ (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-4\sin\theta\sin\chi + 3\sin^3\theta(\sin\chi + \sin 3\chi)$$
$$+ [\sin\theta(3\sin\chi - \sin 3\chi) - (\sin\theta - \sin^3\theta)(\sin\chi + \sin 3\chi)]\cos 2\phi$$

$$+\ 2\sin\theta\cos\theta\ (\cos\chi - \cos3\chi)\sin2\phi\}$$

$$-\ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)$$

$$\chi_{ZZY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi$$

$$+\ (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[-\sin\theta + 3(\sin\theta - \sin^3\theta) - \sin^3\theta\cos2\phi]\sin\chi$$

$$-\ 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\sin\chi$$

$$\chi_{XZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$$

$$+\ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

$$\chi_{ZXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$$

$$+\ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

(pss)

$$\chi_{XYY} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)$$

$$-\ 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$$

$$+\ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)$$

$$\chi_{ZYY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$$

$$-\ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$$

(sss)

$$\chi_{YYY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi$$

$$+\ (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-4\sin\theta\sin\chi + 3\sin^3\theta(3\sin\chi - \sin3\chi)$$

$$+\ [\sin\theta(\sin\chi + \sin3\chi) - (\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)]\cos2\phi$$

$$-\ 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$$

$$-\ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(3\sin\chi - \sin3\chi)$$

$$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = -(4\beta_{aac} + 2\beta_{ccc})\cos\alpha\sin\theta\cos\chi$$

$$\chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = +(4\beta_{aac} + 2\beta_{ccc})\cos\alpha\sin\theta\sin\chi$$

$$\chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = +(4\beta_{aac} + 2\beta_{ccc})\cos\alpha\cos\theta$$

［逆対称 (b_1) 振動］

(ppp)

$$\chi_{XXX} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)(1 + \cos2\phi)$$

$$+\ \sin\theta(\cos\chi - \cos3\chi)(1 - \cos2\phi)] - 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$$

$$\chi_{XZZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$

$$\chi_{ZXZ} = --(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$

$$\chi_{ZZX} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$

$$\chi_{ZXX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 + \cos2\chi\cos2\phi)$$

$$-\ (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi)] + (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$

$$\chi_{XZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 + \cos2\chi\cos2\phi)$$

$$-\ (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi)] + (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$

$$\chi_{XXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[-(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$$

$$\chi_{ZZZ} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$$

(spp)

$$\chi_{YXX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi)$$

$$+ \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$$

$$\chi_{YZZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$\chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos2\phi\cos\theta]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$

$$\chi_{YXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$$

(ssp)

$$\chi_{YYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[-(\sin\theta - \sin^3\theta)(1 + \cos2\phi) + \sin\theta(1 - \cos2\phi)](\cos\chi - \cos3\chi) + 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$$

$$\chi_{YYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$$

(psp)

$$\chi_{XYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$$

$$\chi_{ZYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$\chi_{XYZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$$

$$\chi_{ZYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos2\phi\cos\theta]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$

(sps)

$$\chi_{YXY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$$

$$\chi_{YZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)] - (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$

(pps)

$$\chi_{XXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(1 + \cos2\phi) - \sin\theta(1 - \cos2\phi)](\sin\chi + \sin3\chi) + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$$

$$\chi_{ZZY} = 2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$\chi_{ZXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$

$$\chi_{XZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$

(pss)

$$\chi_{XYY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + (1 - \cos2\phi)\sin\theta(\cos\chi + \cos3\chi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$$

$$\chi_{ZYY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)] - (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$

(sss)

$$\chi_{YYY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi + \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$$

$$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0$$

［縮重バンド］　　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ のときには　$\beta_{caa} \sim (4/9)\beta_{\zeta\zeta\zeta}$、$\beta_{aaa} \sim (4\sqrt{2}/9)\beta_{\zeta\zeta\zeta}$　である。

原理的には振動バンドが３つに分裂するが、実際には重なっているときには、以下に示す３つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{xxz} + \beta_{yyz} = -2\beta_{caa}(\cos\alpha - \cos^3\alpha)$

$\beta_{xxz} - \beta_{yyz} = -2\beta_{caa}(\cos\alpha - \cos^3\alpha)$

$\beta_{xxz} + \beta_{yyz} - 2\beta_{zzz} = -6\beta_{caa}(\cos\alpha - \cos^3\alpha)$

$\beta_{zxx} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)$

$\beta_{zyy} = \beta_{caa}\cos\alpha$　であるから、

［対称 (a_1) 振動］

(ppp)

$$\chi_{XXX} = (1/4)\beta_{caa}(\cos\alpha - \cos^3\alpha)\{4\sin\theta\cos\chi - 3\sin^3\theta(3\cos\chi + \cos3\chi) - [\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\cos2\phi + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$$

$$\chi_{XZZ} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(3 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$

$$\chi_{ZXZ} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(3 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$

$$\chi_{ZZX} = \beta_{caa}(\cos\alpha - \cos^3\alpha)[\sin\theta\cos\chi - 3(\sin\theta - \sin^3\theta)\cos\chi + \sin^3\theta\cos\chi\cos2\phi]$$

$$\chi_{XZX} = (1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]$$

$$\chi_{ZXX} = (1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]$$

$$\chi_{XXZ} = (1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)\{-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 + \cos2\chi) + [(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi + 2\cos^2\theta\sin2\chi\sin2\phi)\}$$

$$\chi_{ZZZ} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)[-\cos\theta + 3\cos^3\theta - (\cos\theta - \cos^3\theta)\cos2\phi]$$

(spp)

$$\chi_{YXX} = (1/4)\beta_{caa}(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi) - 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$$

$$\chi_{YZZ} = \beta_{caa}(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$\chi_{YZX} = -(1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$$

$$\chi_{YXZ} = -(1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 - \cos2\phi) - 2\cos^2\theta\cos2\chi\sin2\phi]$$

(ssp)

$$\chi_{YYX} = (1/4)\beta_{caa}(\cos\alpha - \cos^3\alpha)\{4\sin\theta\cos\chi - 3\sin^3\theta(\cos\chi - \cos3\chi) - [\sin\theta(3\cos\chi + \cos3\chi) - (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\cos2\phi + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$$

$$\chi_{YYZ} = (1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)\{-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 - \cos2\chi) + [(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi - 2\cos^2\theta\sin2\chi\sin2\phi\}$$

(psp)

$$\chi_{XYX} = (1/4)\beta_{caa}(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi) - 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$$

$$\chi_{ZYZ} = \beta_{caa}(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$\chi_{XYZ} = (1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)[-3(\cos\theta - \cos^3\theta)\sin2\chi + (\cos\theta + \cos^3\theta)\sin2\chi\cos2\phi + 2\cos^2\theta\cos2\chi\sin2\phi]$$

$$\chi_{ZYX} = -(1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$$

(sps) $\chi_{YXY} = (1/4)\beta_{caa}(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)$
$- 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$

$\chi_{YZY} = (1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$

(pps) $\chi_{XXY} = (1/4)\beta_{caa}(\cos\alpha - \cos^3\alpha)\{-4\sin\theta\sin\chi + 3\sin^3\theta(\sin\chi + \sin3\chi)$
$+ [\sin\theta(3\sin\chi - \sin3\chi) - (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\cos2\phi + 2\sin\theta\cos\theta\ (\cos\chi - \cos3\chi)\sin2\phi\}$

$\chi_{ZZY} = \beta_{caa}(\cos\alpha - \cos^3\alpha)[2\sin\theta\sin\chi - \sin^3\theta\sin\chi\ \cos2\phi]$

$\chi_{XZY} = -(1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$

$\chi_{ZXY} = -(1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$

(pss) $\chi_{XYY} = (1/4)\beta_{caa}(\cos\alpha - \cos^3\alpha)[-3\sin^3\theta(\cos\chi - \cos3\chi) + (2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\cos2\phi$
$- 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi]$

$\chi_{ZYY} = (1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)[(\cos\theta\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$

(sss) $\chi_{YYY} = (1/4)\beta_{caa}(\cos\alpha - \cos^3\alpha)\{-\sin\theta\sin\chi + 3\sin^3\theta(3\sin\chi - \sin3\chi)$
$+ [\sin\theta(\sin\chi + \sin3\chi) - (\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)]\ \cos2\phi$
$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$

$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0$

［**逆対称 (b_1) 振動**］

(ppp) $\chi_{XXX} = (1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)(1 + \cos2\phi)$
$+ \sin\theta(\cos\chi - \cos3\chi)(1 - \cos2\phi)] - 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$

$\chi_{XZZ} = -(1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZXZ} = -(1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZZX} = -\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZXX} = -(1/4\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi)]$
$+ (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

$\chi_{XZX} = -(1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi)]$
$+ (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

$\chi_{XXZ} = -(1/2\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[-(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$

$\chi_{ZZZ} = -\beta_{caa}(\cos\alpha - 2\cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

(spp) $\chi_{YXX} = -(1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi)$
$+ \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$

$\chi_{YZZ} = (1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\chi_{YZX} = -(1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi$
$+ [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

$\chi_{YXZ} = -(1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$

(ssp) $\chi_{YYX} = -(1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{[-(\sin\theta - \sin^3\theta)(1 + \cos2\phi) + \sin\theta(1 - \cos2\phi)](\cos\chi - \cos3\chi)$
$+ 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$

$\chi_{YYZ} = (1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$

(psp) $\chi_{XYX} = -(1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi)$
$+ \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$

$\chi_{ZYZ} = (1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\chi_{XYZ} = -(1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$

$\chi_{ZYX} = -(1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi$
$+ [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

(sps) $\chi_{YXY} = (1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi)$
$+ \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$

$\chi_{YZY} = -(1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)]$
$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

(pps) $\chi_{XXY} = -(1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha))\{[(\sin\theta - \sin^3\theta)(1 + \cos2\phi) - \sin\theta(1 - \cos2\phi)](\sin\chi + \sin3\chi)$
$+ 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$

$\chi_{ZZY} = \beta_{caa}(\cos\alpha - 2\cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\chi_{ZXY} = -(1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi$
$+ [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

$\chi_{XZY} = -(1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi$
$+ [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

(pss) $\chi_{XYY} = (1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi)$
$+ \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)]$
$+ 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$

$\chi_{ZYY} = -(1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)]$
$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

(sss) $\chi_{YYY} = -(1/4)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 + \cos2\phi)$
$+ \sin\theta(\sin\chi + \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi]\}$

$$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0$$

［**面外 (b_2) 振動**］

(ppp) $\chi_{XXX} = -(1/4)\beta_{caa}\cos\alpha\{[\sin\theta(\cos\chi - \cos3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)(1 - \cos2\phi)]$
$+ 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$

$\chi_{XZZ} = (1/2)\beta_{caa}\cos\alpha[(\sin\theta - 2\sin^3\theta)\cos\chi(1 - \cos2\phi) + \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZXZ} = (1/2)\beta_{caa}\cos\alpha[(\sin\theta - 2\sin^3\theta)\cos\chi(1 - \cos2\phi) + \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZZX} = \beta_{caa}\cos\alpha[(\sin\theta - \sin^3\theta)\cos\chi(1 - \cos2\phi) + \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZXX} = (1/4)\beta_{caa}\cos\alpha\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 - \cos2\phi)] - (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

$\chi_{XZX} = (1/4)\beta_{caa}\cos\alpha\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 - \cos2\phi)] - (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

$\chi_{XXZ} = -(1/2)\beta_{caa}\cos\alpha[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 - \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$

$\chi_{ZZZ} = \beta_{caa}\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\phi)$

(spp) $\chi_{YXX} = (1/4)\beta_{caa}\cos\alpha\{[\sin\theta(\sin\chi - \sin3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 - \cos2\phi)] - 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$

$\chi_{YZZ} = -(1/2)\beta_{caa}\cos\alpha[(\sin\theta - 2\sin^3\theta)\sin\chi(1 - \cos2\phi) - \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\chi_{YZX} = (1/4)\beta_{caa}\cos\alpha\{2[(\cos\theta - \cos^3\theta)(1 - \cos2\phi) + \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta - (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

$\chi_{YXZ} = (1/2)\beta_{caa}\cos\alpha[(\cos\theta - \cos^3\theta)\sin2\chi(1 - \cos2\phi) - \sin^2\theta\cos2\chi\sin2\phi]$

(ssp) $\chi_{YYX} = (1/4)\beta_{caa}\cos\alpha\{[\sin\theta(1 + \cos2\phi) - (\sin\theta - \sin^3\theta)(1 - \cos2\phi)](\cos\chi - \cos3\chi) - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$

$\chi_{YYZ} = -(1/2)\beta_{caa}\cos\alpha[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 - \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]$

(psp) $\chi_{XYX} = (1/4)\beta_{caa}\cos\alpha\{[\sin\theta(\sin\chi - \sin3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 - \cos2\phi)] - 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$

$\chi_{ZYZ} = -(1/2)\beta_{caa}\cos\alpha[(\sin\theta - 2\sin^3\theta)\sin\chi(1 - \cos2\phi) - \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\chi_{XYZ} = (1/2)\beta_{caa}\cos\alpha[(\cos\theta - \cos^3\theta)\sin2\chi(1 - \cos2\phi) - \sin^2\theta\cos2\chi\sin2\phi]$

$\chi_{ZYX} = (1/4)\beta_{caa}\cos\alpha\{2[(\cos\theta - \cos^3\theta)(1 - \cos2\phi) + \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta - (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

(sps) $\chi_{YXY} = -(1/4)\beta_{caa}\cos\alpha\{[\sin\theta(\cos\chi + \cos3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 - \cos2\phi)] - 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$

$\chi_{YZY} = (1/4)\beta_{caa}\cos\alpha\{2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 - \cos2\phi)] + (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

(pps) $\chi_{XXY} = (1/4)\beta_{caa}\cos\alpha\{[-\sin\theta(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\phi)](\sin\chi + \sin3\chi) - \sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$

$\chi_{ZZY} = \beta_{caa}\cos\alpha[-(\sin\theta - \sin^3\theta)\sin\chi(1 - \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\chi_{ZXY} = (1/4)\beta_{caa}\cos\alpha\{2[(\cos\theta - \cos^3\theta)(1 - \cos2\phi) + \cos\theta\cos2\phi]\sin2\chi - [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

$\chi_{XZY} = (1/4)\beta_{caa}\cos\alpha\{2[(\cos\theta - \cos^3\theta)(1 - \cos2\phi) + \cos\theta\cos2\phi]\sin2\chi - [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

(pss) $\chi_{XYY} = -(1/4)\beta_{caa}\cos\alpha\{[\sin\theta(\cos\chi + \cos3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 - \cos2\phi)] - 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$

χ_{ZYY} = (1/4)β_{caa}cosα{2[cosθ(1 + cos2χcos2ϕ) - (cosθ - cos^{3}θ)(1 - cos2χ)(1 - cos2ϕ)]
+ (1 - 3cos^{2}θ)sin2χsin2ϕ}

(sss) χ_{YYY} = (1/4 β_{caa}cosα{[sinθ(sinχ + sin3χ)(1 + cos2ϕ) + (sinθ - sin^{3}θ)(3sinχ - sin3χ)(1 - cos2ϕ)]
- 2sinθcosθ(cosχ - cos3χ)sin2ϕ}

$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0$

付録 C： $\phi_A = \phi_B = 0, \pi$ のときの (XYZ) 系でのテンソル成分

［全対称バンド］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ のときには $\beta_{aac} \sim (4/9)\, \beta_{\zeta\zeta\zeta}$、$\beta_{ccc} \sim (1/9)\, \beta_{\zeta\zeta\zeta}$ である。

原理的には振動バンドが２つに分裂するが、実際には重なっているときには、以下に示す２つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{xxz} + \beta_{yyz}$ = -2(β_{aac} - β_{ccc})(cosα - cos^{3}α) + 4β_{aac}cosα
$\beta_{xxz} - \beta_{yyz}$ = -2(β_{aac} - β_{ccc})(cosα - cos^{3}α)
$\beta_{xxz} + \beta_{yyzv}$- 2$\beta_{zzz}$ = -2(β_{aac} - β_{ccc})[3(cosα - cos^{3}α) - 2cosα]
β_{zxx} = -2(β_{aac} - β_{ccc})(cosα - cos^{3}α)) であるから、

［対称 (a_1) 振動］

(ppp) χ_{XXX} = -2β_{aac}cosαsinθcosχ
+ (1/4)(β_{aac} - β_{ccc})(cosα - cos^{3}α){4sinθcosχ - 3sin^{3}θ(3cosχ + cos3χ)
- [sinθ(cosχ - cos3χ) - (sinθ - sin^{3}θ)(3cosχ + cos3χ)]cos2ϕ
- 2sinθcosθ(sinχ + sin3χ)sin2ϕ}
+ (1/2)(β_{aac} - β_{ccc})cosαsin^{3}θ(3cosχ + cos3χ)

χ_{XZZ} = -(β_{aac} - β_{ccc})(cosα - cos^{3}α)[(sinθ - sinθ)cosχ(3 + cos2ϕ) - sinθcosθsinχsin2ϕ]
+ 2(β_{aac} - β_{ccc})cosα(sinθ - sin^{3}θ)cosχ

χ_{ZXZ} = -(β_{aac} - β_{ccc})(cosα - cos^{3}α)[(sinθ - sinθ)cosχ(3 + cos2ϕ) - sinθcosθsinχsin2ϕ]
+ 2(β_{aac} - β_{ccc})cosα(sinθ - sin^{3}θ)cosχ

χ_{ZZX} = -2β_{aac}cosαsinθcosχ
+ (β_{aac} - β_{ccc})(cosα - cos^{3}α)[sinθcosχ - 3(sinθ - sin^{3}θ)cosχ + sin^{3}θcosχcos2ϕ]
+ 2(β_{aac} - β_{ccc})cosα(sinθ - sin^{3}θ)cosχ

χ_{XZX} = (1/2)(β_{aac} - β_{ccc})(cosα - cos^{3}α)[(cosθ - cos^{3}θ)(1 + cos2χ)(3 + cos2ϕ) - sin^{2}θsin2χsin2ϕ]
- (β_{aac} - β_{ccc})cosα(cosθ - cos^{3}θ)(1 + cos2χ)

χ_{ZXX} = (1/2)(β_{aac} - β_{ccc})(cosα - cos^{3}α)[(cosθ - cos^{3}θ)(1 + cos2χ)(3 + cos2ϕ) - sin^{2}θsin2χsin2ϕ]
- (β_{aac} - β_{ccc})cosα(cosθ - cos^{3}θ)(1 + cos2χ)

χ_{XXZ} = 2β_{aac}cosαcosθ
+ (1/2) (β_{aac} - β_{ccc})(cosα - cos^{3}α){-2cosθ + 3(cosθ - cos^{3}θ)(1 + cos2χ)
+ [(cosθ - cos^{3}θ) - (cosθ + cos^{3}θ)cos2χ]cos2ϕ + 2cos^{2}θsin2χsin2ϕ}

$$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$$

$$\chi_{ZZZ} = -2\beta_{aac}\cos\alpha\cos\theta$$

$$+ (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[-\cos\theta + 3\cos^3\theta - (\cos\theta - \cos^3\theta)\cos2\phi]$$

$$- 2(\beta_{aac} - \beta_{ccc})\cos\alpha\cos^3\theta$$

(spp)

$$\chi_{YXX} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)$$

$$+ 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$$

$$- (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)$$

$$\chi_{YZZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$- 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\sin\chi$$

$$\chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta\,(1 + \cos2\chi)\sin2\phi]$$

$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

$$\chi_{YXZ} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\chi$$

$$- 2\cos^2\theta\cos2\chi\sin2\phi\}$$

$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

(ssp)

$$\chi_{YYX} = -2\beta_{aac}\cos\alpha\sin\theta\cos\chi$$

$$+ (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{4\sin\theta\cos\chi - 3\sin^3\theta(\cos\chi - \cos3\chi)$$

$$- [\sin\theta(3\cos\chi + \cos3\chi) - (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\cos2\phi$$

$$+ 2\sin\theta\cos\theta\,(\sin\chi + \sin3\chi)\sin2\phi\}$$

$$+ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)$$

$$\chi_{YYZ} = 2\beta_{aac}\cos\alpha\sin\theta\cos\chi$$

$$+ (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$$

$$+ [(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi - 2\cos^2\theta\sin2\chi\sin2\phi\}$$

$$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$$

(psp)

$$\chi_{XYX} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)$$

$$+ 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$$

$$- (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)$$

$$\chi_{ZYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$- 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\sin\chi$$

$$\chi_{XYZ} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\chi$$

$$- 2\cos^2\theta\cos2\chi\sin2\phi\}$$

$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

$$\chi_{ZYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$$

$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

(sps)

$$\chi_{YXY} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)$$

$$- 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$$

$$+ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)$$

$$\chi_{YZY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$$
$$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$$

(pps)

$$\chi_{XXY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi$$
$$+ (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-4\sin\theta\sin\chi + 3\sin^3\theta(\sin\chi + \sin3\chi)$$
$$+ [\sin\theta(3\sin\chi - \sin3\chi) - (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\cos2\phi$$
$$+ 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$$
$$- (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)$$
$$\chi_{ZZY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi$$
$$+ (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[-\sin\theta + 3(\sin\theta - \sin^3\theta) - \sin^3\theta\cos2\phi]\sin\chi$$
$$- 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\sin\chi$$
$$\chi_{XZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$$
$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$
$$\chi_{ZXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$$
$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

(pss)

$$\chi_{XYY} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)$$
$$- 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$$
$$+ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)$$
$$\chi_{ZYY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$$
$$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$$

(sss)

$$\chi_{YYY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi$$
$$+ (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-4\sin\theta\sin\chi + 3\sin^3\theta(3\sin\chi - \sin3\chi)$$
$$+ [\sin\theta(\sin\chi + \sin3\chi) - (\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)]\cos2\phi$$
$$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$$
$$- (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(3\sin\chi - \sin3\chi)$$

$$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = - (4\beta_{aac} + 2\beta_{ccc})\cos\alpha\sin\theta\cos\chi$$
$$\chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = + (4\beta_{aac} + 2\beta_{ccc})\cos\alpha\sin\theta\sin\chi$$
$$\chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = + (4\beta_{aac} + 2\beta_{ccc})\cos\alpha\cos\theta$$

［逆対称 (b_1) 振動］

(ppp)

$$\chi_{XXX} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)(1 + \cos2\phi)$$
$$+ \sin\theta(\cos\chi - \cos3\chi)(1 - \cos2\phi)] - 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$$
$$\chi_{XZZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$
$$\chi_{ZXZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$
$$\chi_{ZZX} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$
$$\chi_{ZXX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 + \cos2\chi\cos2\phi)$$
$$- (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi)] + (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$

$$\chi_{XZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi)] + (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$

$$\chi_{XXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[-(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$$

$$\chi_{ZZZ} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$$

(spp)

$$\chi_{YXX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$$

$$\chi_{YZZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$\chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos2\phi\cos\theta]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$

$$\chi_{YXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$$

(ssp)

$$\chi_{YYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[-(\sin\theta - \sin^3\theta)(1 + \cos2\phi) + \sin\theta(1 - \cos2\phi)](\cos\chi - \cos3\chi) + 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$$

$$\chi_{YYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$$

(psp)

$$\chi_{XYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$$

$$\chi_{ZYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$\chi_{XYZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$$

$$\chi_{ZYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$

(sps)

$$\chi_{YXY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$$

$$\chi_{YZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)] - (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$

(pps)

$$\chi_{XXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(1 + \cos2\phi) - \sin\theta(1 - \cos2\phi)](\sin\chi + \sin3\chi) + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$$

$$\chi_{ZZY} = 2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$\chi_{ZXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$

$$\chi_{XZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$

(pss)

$$\chi_{XYY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + (1 - \cos2\phi)\sin\theta(\cos\chi + \cos3\chi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$$

$$\chi_{ZYY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)] - (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$

(sss) $\chi_{YYY} = -(1/2)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(3\sin\chi - \sin 3\chi)(1 + \cos 2\phi)$
$+ \sin\theta(\sin\chi + \sin 3\chi)(1 - \cos 2\phi)] + 2\sin\theta\cos\theta\,(\cos\chi - \cos 3\chi)\sin 2\phi\}$

$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0$

［縮重バンド］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ のときには $\beta_{caa} \sim (4/9)\,\beta_{\zeta\zeta\zeta}$, $\beta_{aaa} \sim (4\sqrt{2}/9)\,\beta_{\zeta\zeta\zeta}$ である。

原理的には振動バンドが３つに分裂するが、実際には重なっているときには、以下に示す３つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$ß_{xxz} + ß_{yyz} = -4ß_{caa}(\cos\alpha - \cos^3\alpha) \pm 2ß_{aaa}\sin^3\alpha$
$ß_{xxz} - ß_{yyz} = -4ß_{caa}(\cos\alpha - \cos^3\alpha) \pm 2ß_{aaa}(2\sin\alpha + \sin^3\alpha)$
$ß_{xxz} + ß_{yyz} - 2ß_{zzz} = -12ß_{caa}(\cos\alpha - \cos^3\alpha) - (\pm)2ß_{aaa}\sin^3\alpha$
$ß_{zxx} = -2ß_{caa}(\cos\alpha - 2\cos^3\alpha) - (\pm)2ß_{aaa}(\sin\alpha - \sin^3\alpha)$
$ß_{zyy} = 2ß_{caa}\cos\alpha - (\pm)2ß_{aaa}\sin\alpha$ であるから、

［対称 (a_1) 振動］

(ppp) $\chi_{XXX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$
$+ (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(3\cos\chi + \cos 3\chi)$
$+ (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(\cos\chi - \cos 3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos 3\chi)]\cos 2\phi$
$+ 2\sin\theta\cos\theta(\sin\chi + \sin 3\chi)\sin 2\phi\}$

$\chi_{XZZ} = (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi$
$+ (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\cos\chi - \sin 2\phi\sin\theta\cos\theta\sin\chi]\cos 2\phi$

$\chi_{ZXZ} = (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi$
$+ (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\cos\chi - \sin 2\phi\sin\theta\cos\theta\sin\chi]\cos 2\phi$

$\chi_{ZZX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$
$+ (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi$
$- (1/2)(\beta_{aac} - \beta_{bbc})\sin^3\theta\cos\chi\cos 2\phi$

$\chi_{XZX} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)$
$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 + \cos 2\chi) - \sin 2\phi\sin^2\theta\sin 2\chi]\cos 2\phi$

$\chi_{ZXX} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)$
$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 + \cos 2\chi) - \sin 2\phi\sin^2\theta\sin 2\chi]\cos 2\phi$

$\chi_{XXZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$
$- (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)$
$- (1/4)(\beta_{aac} - \beta_{bbc})\{[(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos 2\chi] + 2\sin 2\phi\cos^2\theta\sin 2\chi\}\cos 2\phi$

$\chi_{ZZZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$
$- (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\cos^3\theta$
$+ (1/2)(\beta_{aac} - \beta_{bbc})\cos 2\phi(\cos\theta - \cos^3\theta)$

(spp) $\chi_{YXX} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi)$
$+ (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi) + 2\sin2\phi\sin\theta\cos\theta(\cos\chi + \cos3\chi)]\cos2\phi$

$\chi_{YZZ} = -(1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\sin\chi$
$- (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi + \sin2\phi\sin\theta\cos\theta\cos\chi]\cos2\phi$

$\chi_{YZX} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$
$+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi + \sin2\phi\sin^2\theta(1 + \cos2\chi)]\cos2\phi$

$\chi_{YXZ} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$
$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta + \cos^3\theta)\sin2\chi + 2\sin2\phi\cos^2\theta\cos2\chi]\cos2\phi$

(ssp) $\chi_{YYX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$
$+ (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi)$
$+ (1/8)(\beta_{aac} - \beta_{bbc})\{ [\sin\theta(3\cos\chi + \cos3\chi) - (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\cos2\phi$
$- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\}\sin2\phi$

$\chi_{YYZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$
$- (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$
$- (1/4)(\beta_{aac} - \beta_{bbc})\{[(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi - 2\cos^2\theta\sin2\chi)\sin2\phi\}$

(psp) $\chi_{XYX} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi)$
$+ (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi) + 2\sin2\phi\sin\theta\cos\theta(\cos\chi + \cos3\chi)]\cos2\phi$

$\chi_{ZYZ} = -(1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\sin\chi$
$- (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi\cos2\phi + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\chi_{XYZ} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$
$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta + \cos^3\theta)\sin2\chi\cos2\phi + 2\cos^2\theta\cos2\chi\sin2\phi]$

$\chi_{ZYX} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$
$+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$

(sps) $\chi_{YXY} = (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi)$
$- (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\cos2\phi - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi]$

$\chi_{YZY} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$
$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\cos2\phi + \sin^2\theta\sin2\chi\sin2\phi]$

(pps) $\chi_{XXY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi$
$- (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi)$
$- (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(3\sin\chi - \sin3\chi) - (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\cos2\phi$
$+ 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$

$\chi_{ZZY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi$
$- (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\sin\chi$
$+ (1/2)(\beta_{aac} - \beta_{bbc})\sin^3\theta\sin\chi\cos2\phi$

$\chi_{XZY} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$
$+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$

$$\chi_{ZXY} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$$
$$+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$$

(pss)
$$\chi_{XYY} = (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi)$$
$$- (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\cos2\phi - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi]$$
$$\chi_{ZYY} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$$
$$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\cos2\phi + \sin^2\theta\sin2\chi\sin2\phi]$$

(sss)
$$\chi_{YYY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi$$
$$- (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(3\sin\chi - \sin3\chi)$$
$$- (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(\sin\chi + \sin3\chi) - (\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)]\cos2\phi$$
$$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$$

$$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = -(\beta_{aac} + \beta_{bbc} + \beta_{ccc})\sin\theta\cos\chi$$
$$\chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = +(\beta_{aac} + \beta_{bbc} + \beta_{ccc})\sin\theta\sin\chi$$
$$\chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = +(\beta_{aac} + \beta_{bbc} + \beta_{ccc})\cos\theta$$

［逆対称 (b_1) 振動］

(ppp)
$$\chi_{XXX} = -(1/4)\beta_{caa}\{[(1 + \cos2\phi)(\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi) + (1 - \cos2\phi)\sin\theta(\cos\chi - \cos3\chi)]$$
$$- 2\sin2\phi\sin\theta\cos\theta(\sin\chi + \sin3\chi)\}$$
$$\chi_{XZZ} = (1/2)\beta_{caa}[(1 + \cos2\phi)(\sin\theta - 2\sin^3\theta)\cos\chi - \sin2\phi\sin\theta\cos\theta\sin\chi]$$
$$\chi_{ZXZ} = (1/2)\beta_{caa}[(1 + \cos2\phi)(\sin\theta - 2\sin^3\theta)\cos\chi - \sin2\phi\sin\theta\cos\theta\sin\chi]$$
$$\chi_{ZZX} = \beta_{caa}[(1 + \cos2\phi)(\sin\theta - \sin^3\theta)\cos\chi - \sin2\phi\sin\theta\cos\theta\sin\chi]$$
$$\chi_{ZXX} = (1/4)\beta_{caa}\{2[\cos\theta(1 + \cos2\phi\cos2\chi) - (1 + \cos2\phi)(\cos\theta - \cos^3\theta)(1 + \cos2\chi)]$$
$$+ \sin2\phi(1 - 3\cos^2\theta)\sin2\chi\}$$
$$\chi_{XZX} = (1/4)\beta_{caa}\{2[\cos\theta(1 + \cos2\phi\cos2\chi) - (1 + \cos2\phi)(\cos\theta - \cos^3\theta)(1 + \cos2\chi)]$$
$$+ \sin2\phi(1 - 3\cos^2\theta)\sin2\chi\}$$
$$\chi_{XXZ} = (1/2)\beta_{caa}[-(1 + \cos2\phi)(\cos\theta - \cos^3\theta)(1 + \cos2\chi) + \sin2\phi\sin^2\theta\sin2\chi]$$
$$\chi_{ZZZ} = \beta_{caa}(1 + \cos2\phi)(\cos\theta - \cos^3\theta)$$

(spp)
$$\chi_{YXX} = (1/4)\beta_{caa}\{[(1 + \cos2\phi)(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi) + (1 - \cos2\phi)\sin\theta(\sin\chi - \sin3\chi)]$$
$$+ 2\sin2\phi\sin\theta\cos\theta\cos3\chi\}$$
$$\chi_{YZZ} = -(1/2)\beta_{caa}[(1 + \cos2\phi)(\sin\theta - 2\sin^3\theta)\sin\chi + \sin2\phi\sin\theta\cos\theta\cos\chi]$$
$$\chi_{YZX} = (1/4)\beta_{caa}\{2[(1 + \cos2\phi)(\cos\theta - \cos^3\theta) - \cos2\phi\cos\theta]\sin2\chi + \sin2\phi[-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\}$$
$$\chi_{YXZ} = (1/2)\beta_{caa}[(1 + \cos2\phi)(\cos\theta - \cos^3\theta)\sin2\chi + \sin2\phi\sin^2\theta\cos2\chi]$$

(ssp)
$$\chi_{YYX} = (1/4)\beta_{caa}\{[-(1 + \cos2\phi)(\sin\theta - \sin^3\theta) + (1 - \cos2\phi)\sin\theta](\cos\chi - \cos3\chi)$$
$$+ 2\sin2\phi\sin\theta\cos\theta(\sin\chi - \sin3\chi)\}$$
$$\chi_{YYZ} = -(1/2)\beta_{caa}[(1 + \cos2\phi)(\cos\theta - \cos^3\theta)(1 - \cos2\chi) + \sin2\phi\sin^2\theta\sin2\chi]$$

(psp) $\chi_{XYX} = (1/4)\beta_{caa}\{[(1 + \cos2\phi)(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi) + (1 - \cos2\phi)\sin\theta(\sin\chi - \sin3\chi)] + 2\sin2\phi\sin\theta\cos\theta\cos3\chi\}$

$\chi_{ZYZ} = -(1/2)\beta_{caa}[(1 + \cos2\phi)(\sin\theta - 2\sin^3\theta)\sin\chi + \sin2\phi\sin\theta\cos\theta\cos\chi]$

$\chi_{XYZ} = (1/2)\beta_{caa}[(1 + \cos2\phi)(\cos\theta - \cos^3\theta)\sin2\chi + \sin2\phi\sin^2\theta\cos2\chi]$

$\chi_{ZYX} = (1/4)\beta_{caa}\{2[(1 + \cos2\phi)(\cos\theta - \cos^3\theta) - \cos2\phi\cos\theta]\sin2\chi + \sin2\phi[-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\}$

(sps) $\chi_{YXY} = -(1/4)\beta_{caa}\{[(1 + \cos2\phi)(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi) + (1 - \cos2\phi)\sin\theta(\cos\chi + \cos3\chi)] + 2\sin2\phi\sin\theta\cos\theta\sin3\chi\}$

$\chi_{YZY} = (1/4)\beta_{caa}\{2[\cos\theta(1 - \cos2\phi\cos2\chi) - (1 + \cos2\phi)(\cos\theta - \cos^3\theta)(1 - \cos2\chi)] - \sin2\phi(1 - 3\cos^2\theta)\sin2\chi\}$

(pps) $\chi_{XXY} = (1/4)\beta_{caa}\{[(1 + \cos2\phi)(\sin\theta - \sin^3\theta) - (1 - \cos2\phi)\sin\theta](\sin\chi + \sin3\chi) + 2\sin2\phi\sin\theta\cos\theta(\cos\chi + \cos3\chi)\}$

$\chi_{ZZY} = -\beta_{caa}[(1 + \cos2\phi)(\sin\theta - \sin^3\theta)\sin\chi + \sin2\phi\sin\theta\cos\theta\cos\chi]$

$\chi_{ZXY} = (1/4)\beta_{caa}\{2[(1 + \cos2\phi)(\cos\theta - \cos^3\theta) - \cos2\phi\cos\theta]\sin2\chi + \sin2\phi[\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\}$

$\chi_{XZY} = (1/4)\beta_{caa}\{2[(1 + \cos2\phi)(\cos\theta - \cos^3\theta) - \cos2\phi\cos\theta]\sin2\chi + \sin2\phi[\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\}$

(pss) $\chi_{XYY} = -(1/4)\beta_{caa}\{[(1 + \cos2\phi)(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi) + (1 - \cos2\phi)\sin\theta(\cos\chi + \cos3\chi)] + 2\sin2\phi\sin\theta\cos\theta\sin3\chi\}$

$\chi_{ZYY} = (1/4)\beta_{caa}\{2[\cos\theta(1 - \cos2\phi\cos2\chi) - (1 + \cos2\phi)(\cos\theta - \cos^3\theta)(1 - \cos2\chi)] - \sin2\phi(1 - 3\cos^2\theta)\sin2\chi\}$

(sss) $\chi_{YYY} = (1/4)\beta_{caa}\{[(1 + \cos2\phi)(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi) + (1 - \cos2\phi)\sin\theta(\sin\chi + \sin3\chi)] + 2\sin2\phi\sin\theta\cos\theta(\cos\chi - \cos3\chi)]\}$

$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0$

［**面外 (b_2) 振動**］

(ppp) $\chi_{XXX} = -(1/4)\beta_{cbb}\{[(1 + \cos2\phi)\sin\theta(\cos\chi - \cos3\chi) + (1 - \cos2\phi)(\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)] + 2\sin2\phi\sin\theta\cos\theta(\sin\chi + \sin3\chi)\}$

$\chi_{XZZ} = (1/2)\beta_{cbb}[(1 - \cos2\phi)(\sin\theta - 2\sin^3\theta)\cos\chi + \sin2\phi\sin\theta\cos\theta\sin\chi]$

$\chi_{ZXZ} = (1/2)\beta_{cbb}[(1 - \cos2\phi)(\sin\theta - 2\sin^3\theta)\cos\chi + \sin2\phi\sin\theta\cos\theta\sin\chi]$

$\chi_{ZZX} = \beta_{cbb}[(1 - \cos2\phi)(\sin\theta - \sin^3\theta)\cos\chi + \sin2\phi\sin\theta\cos\theta\sin\chi]$

$\chi_{ZXX} = (1/4)\beta_{cbb}\{2[\cos\theta(1 - \cos2\phi\cos2\chi) - (1 - \cos2\phi)(\cos\theta - \cos^3\theta)(1 + \cos2\chi)] - \sin2\phi(1 - 3\cos^2\theta)\sin2\chi\}$

$\chi_{XZX} = (1/4)\beta_{cbb}\{2[\cos\theta(1 - \cos2\phi\cos2\chi) - (1 - \cos2\phi)(\cos\theta - \cos^3\theta)(1 + \cos2\chi)] - \sin2\phi(1 - 3\cos^2\theta)\sin2\chi\}$

$\chi_{XXZ} = -(1/2)\beta_{cbb}[(1 - \cos2\phi)(\cos\theta - \cos^3\theta)(1 + \cos2\chi) + \sin2\phi\sin^2\theta\sin2\chi]$

$\chi_{ZZZ} = \beta_{cbb}(1 - \cos2\phi)(\cos\theta - \cos^3\theta)$

(spp) $\chi_{YXX} = (1/4)\beta_{cbb}\{[(1 + \cos2\phi)\sin\theta(\sin\chi - \sin3\chi) + (1 - \cos2\phi)(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)] - 2\sin2\phi\sin\theta\cos\theta\cos3\chi\}$

$\chi_{YZZ} = -(1/2)\beta_{cbb}[(1 - \cos2\phi)(\sin\theta - 2\sin^3\theta)\sin\chi - \sin2\phi\sin\theta\cos\theta\cos\chi]$

$\chi_{YZX} = (1/4)\beta_{cbb}\{2[(1 - \cos2\phi)(\cos\theta - \cos^3\theta) + \cos2\phi\cos\theta]\sin2\chi + \sin2\phi[\sin^2\theta - (1 - 3\cos^2\theta)\cos2\chi]\}$

$\chi_{YXZ} = (1/2)\beta_{cbb}[(1 - \cos2\phi)(\cos\theta - \cos^3\theta)\sin2\chi - \sin2\phi\sin^2\theta\cos2\chi]$

(ssp) $\chi_{YYX} = (1/4)\beta_{cbb}\{[(1 + \cos2\phi)\sin\theta - (1 - \cos2\phi)(\sin\theta - \sin^3\theta)](\cos\chi - \cos3\chi) - 2\sin2\phi\sin\theta\cos\theta(\sin\chi - \sin3\chi)\}$

$\chi_{YYZ} = -(1/2)\beta_{cbb}[(1 - \cos2\phi)(\cos\theta - \cos^3\theta)(1 - \cos2\chi) - \sin2\phi\sin^2\theta\sin2\chi]$

(psp) $\chi_{XYX} = (1/4)\beta_{cbb}\{[(1 + \cos2\phi)\sin\theta(\sin\chi - \sin3\chi) + (1 - \cos2\phi)(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)] - 2\sin2\phi\sin\theta\cos\theta\cos3\chi\}$

$\chi_{ZYZ} = -(1/2)\beta_{cbb}[(1 - \cos2\phi)(\sin\theta - 2\sin^3\theta)\sin\chi - \sin2\phi\sin\theta\cos\theta\cos\chi]$

$\chi_{XYZ} = (1/2)\beta_{cbb}[(1 - \cos2\phi)(\cos\theta - \cos^3\theta)\sin2\chi - \sin2\phi\sin^2\theta\cos2\chi]$

$\chi_{ZYX} = (1/4)\beta_{cbb}\{2[(1 - \cos2\phi)(\cos\theta - \cos^3\theta) + \cos2\phi\cos\theta]\sin2\chi + \sin2\phi[\sin^2\theta - (1 - 3\cos^2\theta)\cos2\chi]\}$

(sps) $\chi_{YXY} = -(1/4)\beta_{cbb}\{[(1 + \cos2\phi)\sin\theta(\cos\chi + \cos3\chi) + (1 - \cos2\phi)(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)] - 2\sin2\phi\sin\theta\cos\theta\sin3\chi\}$

$\chi_{YZY} = (1/4)\beta_{cbb}\{2[\cos\theta(1 + \cos2\phi\cos2\chi) - (1 - \cos2\phi)(\cos\theta - \cos^3\theta)(1 - \cos2\chi)] + \sin2\phi(1 - 3\cos^2\theta)\sin2\chi\}$

(pps) $\chi_{XXY} = (1/4)\beta_{cbb}\{[-(1 + \cos2\phi)\sin\theta + (1 - \cos2\phi)(\sin\theta - \sin^3\theta)](\sin\chi + \sin3\chi) - \sin2\phi\sin\theta\cos\theta(\cos\chi + \cos3\chi)\}$

$\chi_{ZZY} = \beta_{cbb}[-(1 - \cos2\phi)(\sin\theta - \sin^3\theta)\sin\chi + \sin2\phi\sin\theta\cos\theta\cos\chi]$

$\chi_{ZXY} = (1/4)\beta_{cbb}\{2[(1 - \cos2\phi)(\cos\theta - \cos^3\theta) + \cos2\phi\cos\theta]\sin2\chi - \sin2\phi[\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\}$

$\chi_{XZY} = (1/4)\beta_{cbb}\{2[(1 - \cos2\phi)(\cos\theta - \cos^3\theta) + \cos2\phi\cos\theta]\sin2\chi - \sin2\phi[\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\}$

(pss) $\chi_{XYY} = -(1/4)\beta_{cbb}\{[(1 + \cos2\phi)\sin\theta(\cos\chi + \cos3\chi) + (1 - \cos2\phi)(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)] - 2\sin2\phi\sin\theta\cos\theta\sin3\chi\}$

$\chi_{ZYY} = (1/4)\beta_{cbb}\{2[\cos\theta(1 + \cos2\phi\cos2\chi) - (1 - \cos2\phi)(\cos\theta - \cos^3\theta)(1 - \cos2\chi)] + \sin2\phi(1 - 3\cos^2\theta)\sin2\chi\}$

(sss) $\chi_{YYY} = (1/4)\beta_{cbb}\{[(1 + \cos2\phi)\sin\theta(\sin\chi + \sin3\chi) + (1 - \cos2\phi)(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)] - 2\sin2\phi\sin\theta\cos\theta(\cos\chi - \cos3\chi)]\}$

$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0$

付録 D： $\phi_A = \phi_B \neq 0, \pi$ のときの (XYZ)系でのテンソル成分

［全対称バンド］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ のときには $\beta_{aac} \sim (4/9)\beta_{\zeta\zeta\zeta}$、$\beta_{ccc} \sim (1/9)\beta_{\zeta\zeta\zeta}$ である。

原理的には振動バンドが２つに分裂するが、実際には重なっているときには、以下に示す２つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{xxz} + \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 4\beta_{aac}\cos\alpha$

$\beta_{xxz} - \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

$\beta_{xxz} + \beta_{yyz} - 2\beta_{zzz} = -2(\beta_{aac} - \beta_{ccc})[3(\cos\alpha - \cos^3\alpha) - 2\cos\alpha]$

$\beta_{zxx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$　**であるから、**

［**対称 (a_1) 振動**］

(ppp)

$$\chi_{XXX} = -2\beta_{aac}\cos\alpha\sin\theta\cos\chi$$
$$+ (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{4\sin\theta\cos\chi - 3\sin^3\theta(3\cos\chi + \cos3\chi)$$
$$-[\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\cos2\phi$$
$$-2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$$
$$+ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(3\cos\chi + \cos3\chi)$$

$$\chi_{XZZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(3 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$
$$+ 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi$$

$$\chi_{ZXZ} =-(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(3 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$
$$+ 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi$$

$$\chi_{ZZX} = -2\beta_{aac}\cos\alpha\sin\theta\cos\chi$$
$$+ (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\sin\theta\cos\chi - 3(\sin\theta - \sin^3\theta)\cos\chi + \sin^3\theta\cos\chi\cos2\phi]$$
$$+ 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi$$

$$\chi_{XZX} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]$$
$$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$$

$$\chi_{ZXX} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]$$
$$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$$

$$\chi_{XXZ} = 2\beta_{aac}\cos\alpha\cos\theta$$
$$+ (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$$
$$+ [(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi + 2\cos^2\theta\sin2\chi\sin2\phi\}$$
$$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$$

$$\chi_{ZZZ} = -2\beta_{aac}\cos\alpha\cos\theta$$
$$+ (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[-\cos\theta + 3\cos^3\theta - (\cos\theta - \cos^3\theta)\cos2\phi]$$
$$- 2(\beta_{aac} - \beta_{ccc})\cos\alpha\cos^3\theta$$

(spp)

$$\chi_{YXX} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)$$
$$+ 2\sin\theta\cos\theta\,(\cos\chi + \cos3\chi)\sin2\phi\}$$
$$- (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)$$

$$\chi_{YZZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$
$$- 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\sin\chi$$

$$\chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$$
$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

$\chi_{YXZ} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\chi$

$\quad -2\cos^2\theta\cos2\chi\sin2\phi\}$

$\quad + (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$

(ssp) $\chi_{YYX} = -2\beta_{aac}\cos\alpha\sin\theta\cos\chi$

$\quad + (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{4\sin\theta\cos\chi - 3\sin^3\theta(\cos\chi - \cos3\chi)$

$\quad - [\sin\theta(3\cos\chi + \cos3\chi) - (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\cos2\phi$

$\quad + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$

$\quad + (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)$

$\chi_{YYZ} = 2\beta_{aac}\cos\alpha\sin\theta\cos\chi$

$\quad + (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$

$\quad + [(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi - 2\cos^2\theta\sin2\chi\sin2\phi\}$

$\quad - (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$

(psp) $\chi_{XYX} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)$

$\quad + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$

$\quad - (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)$

$\chi_{ZYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\quad - 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\sin\chi$

$\chi_{XYZ} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\chi$

$\quad -2\cos^2\theta\cos2\chi\sin2\phi\}$

$\quad + (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$

$\chi_{ZYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$

$\quad + (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$

(sps) $\chi_{YXY} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)$

$\quad - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$

$\quad + (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)$

$\chi_{YZY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$

$\quad - (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$

(pps) $\chi_{XXY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi$

$\quad + (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-4\sin\theta\sin\chi + 3\sin^3\theta(\sin\chi + \sin3\chi)$

$\quad + [\sin\theta(3\sin\chi - \sin3\chi) - (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\cos2\phi$

$\quad + 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$

$\quad - (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\,\mathrm{in}^3\theta(\sin\chi + \sin3\chi)$

$\chi_{ZZY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi$

$\quad + (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[-\sin\theta + 3(\sin\theta - \sin^3\theta) - \sin^3\theta\cos2\phi]\sin\chi$

$\quad - 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\sin\chi$

$\chi_{XZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$

$$+(\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi$$

$$\chi_{ZXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin 2\chi(3 + \cos 2\phi) - \sin^2\theta(1 - \cos 2\chi)\sin 2\phi]$$
$$+(\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi$$

(pss)
$$\chi_{XYY} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos 2\phi](\cos\chi - \cos 3\chi)$$
$$- 2\sin\theta\cos\theta(\sin\chi - \sin 3\chi)\sin 2\phi\}$$
$$+ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos 3\chi)$$

$$\chi_{ZYY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos 2\chi)(3 + \cos 2\phi) + \sin^2\theta\sin 2\chi\sin 2\phi]$$
$$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos 2\chi)$$

(sss)
$$\chi_{YYY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi$$
$$+ (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-4\sin\theta\sin\chi + 3\sin^3\theta(3\sin\chi - \sin 3\chi)$$
$$+ [\sin\theta(\sin\chi + \sin 3\chi) - (\sin\theta - \sin^3\theta)(3\sin\chi - \sin 3\chi)]\cos 2\phi$$
$$- 2\sin\theta\cos\theta(\cos\chi - \cos 3\chi)\sin 2\phi\}$$
$$- (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(3\sin\chi - \sin 3\chi)$$

$$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = - (4\beta_{aac} + 2\beta_{ccc})\cos\alpha\sin\theta\cos\chi$$
$$\chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = + (4\beta_{aac} + 2\beta_{ccc})\cos\alpha\sin\theta\sin\chi$$
$$\chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = + (4\beta_{aac} + 2\beta_{ccc})\cos\alpha\cos\theta$$

［**逆対称 (b_1) 振動**］

(ppp)
$$\chi_{XXX} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(3\cos\chi + \cos 3\chi)(1 + \cos 2\phi)$$
$$+ \sin\theta(\cos\chi - \cos 3\chi)(1 - \cos 2\phi)] - 2\sin\theta\cos\theta(\sin\chi + \sin 3\chi)\sin 2\phi\}$$

$$\chi_{XZZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos 2\phi) - \sin\theta\cos\theta\sin\chi\sin 2\phi]$$

$$\chi_{ZXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos 2\phi) - \sin\theta\cos\theta\sin\chi\sin 2\phi]$$

$$\chi_{ZZX} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(1 + \cos 2\phi) - \sin\theta\cos\theta\sin\chi\sin 2\phi]$$

$$\chi_{ZXX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 + \cos 2\chi\cos 2\phi)$$
$$- (\cos\theta - \cos^3\theta)(1 + \cos 2\chi)(1 + \cos 2\phi)] + (1 - 3\cos^2\theta)\sin 2\chi\sin 2\phi\}$$

$$\chi_{XZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 + \cos 2\chi\cos 2\phi)$$
$$- (\cos\theta - \cos^3\theta)(1 + \cos 2\chi)(1 + \cos 2\phi)] + (1 - 3\cos^2\theta)\sin 2\chi\sin 2\phi\}$$

$$\chi_{XXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[-(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)(1 + \cos 2\phi) + \sin^2\theta\sin 2\chi\sin 2\phi]$$

$$\chi_{ZZZ} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos 2\phi)$$

(spp)
$$\chi_{YXX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin 3\chi)(1 + \cos 2\phi)$$
$$+ \sin\theta(\sin\chi - \sin 3\chi)(1 - \cos 2\phi)] + 2\sin\theta\cos\theta\cos 3\chi\sin 2\phi\}$$

$$\chi_{YZZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos 2\phi) + \sin\theta\cos\theta\cos\chi\sin 2\phi]$$

$$\chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos 2\phi)$$
$$- \cos\theta\cos 2\phi]\sin 2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos 2\chi]\sin 2\phi\}$$

$$\chi_{YXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin 2\chi(1 + \cos 2\phi) + \sin^2\theta\cos 2\chi\sin 2\phi]$$

(ssp) $\chi_{YYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[-(\sin\theta - \sin^3\theta)(1 + \cos2\phi) + \sin\theta(1 - \cos2\phi)](\cos\chi - \cos3\chi)$
$+ 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$

$\chi_{YYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$

(psp) $\chi_{XYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi)$
$+ \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$

$\chi_{ZYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\chi_{XYZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$

$\chi_{ZYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$
$-\cos\theta\ \cos2\phi]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\ \sin2\phi\}$

(sps) $\chi_{YXY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi)$
$+ \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$

$\chi_{YZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)]$
$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

(pps) $\chi_{XXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(1 + \cos2\phi) - \sin\theta(1 - \cos2\phi)](\sin\chi + \sin3\chi)$
$+ 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$

$\chi_{ZZY} = 2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\chi_{ZXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$
$- \cos\theta\ \cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\ \sin2\phi\}$

$\chi_{XZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$
$- \cos\theta\ \cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\ \sin2\phi\}$

(pss) $\chi_{XYY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi)$
$+ \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$

$\chi_{ZYY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)]$
$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

(sss) $\chi_{YYY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 + \cos2\phi)$
$+ \sin\theta(\sin\chi + \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$

$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0$

［縮重バンド］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには** $\beta_{caa} \sim (4/9)\ \beta_{\zeta\zeta\zeta}$、$\beta_{aaa} \sim (4\sqrt{2}/9)\ \beta_{\zeta\zeta\zeta}$ **である。**

原理的には振動バンドが３つに分裂するが、実際には重なっているときには、以下に示す３つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{xxz} + \beta_{yyz} = -2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - \beta_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)$

$\beta_{xxz} - \beta_{yyz} = -2\beta_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) + \beta_{aaa}(2\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)$

$ß_{xxz} + ß_{yyz} - 2ß_{zzz} = -6ß_{caa}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\phi_A) - 3ß_{aaa}\sin^3\alpha(\cos3\phi_A \pm \cos\phi_A)$

$ß_{zxx} = -ß_{caa}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos2\phi_A) + ß_{aaa}(\sin\alpha - \sin^3\alpha)(\cos3\phi_A \pm \cos\phi_A)$

$ß_{zyy} = ß_{caa}\cos\alpha(1 - (\pm)\cos2\phi_A) - ß_{aaa}\sin\alpha(\cos3\phi_A - (\pm)\cos\phi_A)$

$ß_{xyz} = ß_{yxz} = \pm ß_{caa}\sin^2\alpha\sin2\phi_A - ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)$

$ß_{yzx} = ß_{zyx} = -(\pm)ß_{caa}\sin^2\alpha\sin2\phi_A - ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)$

$ß_{zxy} = ß_{xzy} = -(\pm)ß_{caa}(2\cos^2\alpha - 1)\sin2\phi_A - ß_{aaa}\sin\alpha\cos\alpha(\sin3\phi_A - (\pm)\sin\phi_A)$ **であるから、**

［**対称 (a_1) 振動**］

(ppp) $\chi_{XXX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$
$+ (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(3\cos\chi + \cos3\chi)$
$+ (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\cos2\phi$
$+ 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$
$+ (1/4)\beta_{abc}\{[\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\sin2\phi$
$- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\cos2\phi\}$

$\chi_{XZZ} = (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi$
$+ (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\cos\chi\cos2\phi - \sin\theta\cos\theta\sin\chi\sin2\phi]$
$+ \beta_{abc}[(\sin\theta - \sin^3\theta)\cos\chi\sin2\phi + \sin\theta\cos\theta\sin\chi\cos2\phi]$

$\chi_{ZXZ} = (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi$
$+ (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\cos\chi\cos2\phi - \sin\theta\cos\theta\sin\chi\sin2\phi]$
$+ \beta_{abc}[(\sin\theta - \sin^3\theta)\cos\chi\sin2\phi + \sin\theta\cos\theta\sin\chi\cos2\phi]$

$\chi_{ZZX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$
$+ (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi$
$- (1/2)(\beta_{aac} - \beta_{bbc})\sin^3\theta\cos\chi\cos2\phi$
$- \beta_{abc}(2\sin\theta - \sin^3\theta)\cos\chi\sin2\phi$

$\chi_{XZX} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$
$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\cos2\phi - \sin^2\theta\sin2\chi\sin2\phi]$
$- (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\sin2\phi + \sin^2\theta\sin2\chi\cos2\phi]$

$\chi_{ZXX} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$
$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\cos2\phi - \sin^2\theta\sin2\chi\sin2\phi]$
$- (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\sin2\phi + \sin^2\theta\sin2\chi\cos2\phi]$

$\chi_{XXZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$
$- (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$
$- (1/4)(\beta_{aac} - \beta_{bbc})\{[(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi + 2\cos^2\theta\sin2\chi\sin2\phi\}$
$- (1/2)\beta_{abc}\{[(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\chi]\sin2\phi - 2\cos^2\theta\sin2\chi\cos2\phi\}$

$\chi_{ZZZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$
$- (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\cos^3\theta$
$+ (1/2)(\beta_{aac} - \beta_{bbc})\cos2\phi(\cos\theta - \cos^3\theta)$
$+ \beta_{abc}(\cos\theta - \cos^3\theta)\sin2\phi$

(spp) $\chi_{YXX} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi)$

$+ (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\cos2\phi + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi]$

$+ (1/4)\beta_{abc}[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\sin2\phi - 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\cos2\phi]$

$\chi_{YZZ} = -(1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\sin\chi$

$- (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi\cos2\phi + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$- \beta_{abc}[(\sin\theta - \sin^3\theta)\sin\chi\sin2\phi - \sin\theta\cos\theta\cos\chi\cos2\phi]$

$\chi_{YZX} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$

$+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$

$+ (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi - \sin^2\theta(1 + \cos2\chi)\cos2\phi]$

$\chi_{YXZ} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$

$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta + \cos^3\theta)\sin2\chi\cos2\phi + 2\cos^2\theta\cos2\chi\sin2\phi]$

$- (1/2)\beta_{abc}[(\cos\theta + \cos^3\theta)\sin2\chi\sin2\phi - 2\cos^2\theta\cos2\chi\cos2\phi]$

(ssp) $\chi_{YYX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$

$+ (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi)$

$+ (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(3\cos\chi + \cos3\chi) - (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\cos2\phi$

$- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$

$+ (1/4)\beta_{abc}\{[4\sin\theta\cos\chi - (2\sin\theta - \sin^3\theta)]\sin2\phi + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\cos2\phi\}$

$\chi_{YYZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$

$- (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$

$- (1/4)(\beta_{aac} - \beta_{bbc})\{[(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi - 2\cos^2\theta\sin2\chi\sin2\phi\}$

$- (1/2)\beta_{abc}\{[(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos2\chi]\sin2\phi + \cos^2\theta\sin2\chi\cos2\phi\}$

(psp) $\chi_{XYX} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi)$

$+ (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\cos2\phi + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi]$

$+ (1/4)\beta_{abc}[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\sin2\phi - 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\cos2\phi]$

$\chi_{ZYZ} = -(1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\sin\chi$

$- (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi\cos2\phi + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$- \beta_{abc}[(\sin\theta - \sin^3\theta)\sin\chi\sin2\phi - \sin\theta\cos\theta\cos\chi\cos2\phi]$

$\chi_{XYZ} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$

$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta + \cos^3\theta)\sin2\chi\cos2\phi + 2\cos^2\theta\cos2\chi\sin2\phi]$

$- (1/2)\beta_{abc}[(\cos\theta + \cos^3\theta)\sin2\chi\sin2\phi - 2\cos^2\theta\cos2\chi\cos2\phi]$

$\chi_{ZYX} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$

$+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$

$+ (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi - \sin^2\theta(1 + \cos2\chi)\cos2\phi]$

(sps) $\chi_{YXY} = (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi)$

$- (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\cos2\phi - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi]$

$- (1/4)\beta_{abc}[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\sin2\phi + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\cos2\phi]$

$\chi_{YZY} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$

$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\cos2\phi + \sin^2\theta\sin2\chi\sin2\phi]$

$- (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\sin2\phi - \sin^2\theta\sin2\chi\cos2\phi]$

(pps) $\chi_{XXY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi$

$- (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi)$

$+ (1/8)(\beta_{aac} - \beta_{bbc})\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi) - \sin\theta(3\sin\chi - \sin3\chi)\cos2\phi]$

$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$

$+ (1/4)\beta_{abc}\{[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi) - 4\sin\theta\cos\chi]\sin2\phi + 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\cos2\phi\}$

$\chi_{ZZY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi$

$- (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\sin\chi$

$+ (1/2)(\beta_{aac} - \beta_{bbc})\sin^3\theta\sin\chi\cos2\phi$

$+ \beta_{abc}\sin^3\theta\sin\chi\sin2\phi$

$\chi_{XZY} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$

$+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$

$+ (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi + \sin^2\theta(1 - \cos2\chi)\cos2\phi]$

$\chi_{ZXY} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$

$+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$

$+ (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi + \sin^2\theta(1 - \cos2\chi)\cos2\phi]$

(pss) $\chi_{XYY} = (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi)$

$- (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\cos2\phi - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi]$

$- (1/4)\beta_{abc}[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\sin2\phi + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\cos2\phi]$

$\chi_{ZYY} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$

$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\cos2\phi + \sin^2\theta\sin2\chi\sin2\phi]$

$- (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\sin2\phi - \sin^2\theta\sin2\chi\cos2\phi]$

(sss) $\chi_{YYY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi$

$- (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(3\sin\chi - \sin3\chi)$

$- (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(\sin\chi + \sin3\chi) - (\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)]\cos2\phi$

$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$

$+ (1/4)\beta_{abc}\{[4(\sin\theta - \sin^3\theta)\sin\chi - (2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\sin2\phi$

$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\cos2\phi\}$

$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = -(\beta_{aac} + \beta_{bbc} + \beta_{ccc})\sin\theta\cos\chi$

$\chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = +(\beta_{aac} + \beta_{bbc} + \beta_{ccc})\sin\theta\sin\chi$

$\chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = +(\beta_{aac} + \beta_{bbc} + \beta_{ccc})\cos\theta$

［**逆対称 (b_1) 振動**］

(ppp) $\chi_{XXX} = -(1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi - \cos3\chi)(1 - \cos2\phi)]$

$- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$

$+ (1/4)\beta_{bca}\{[\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\sin2\phi$

$- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\cos2\phi\}$

$$\chi_{XZZ} = (1/2)\beta_{caa}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\chi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$
$$+ (1/2)\beta_{bca}[(\sin\theta - 2\sin^3\theta)\cos\chi\sin2\phi + \sin\theta\cos\theta\sin\chi(1 + \cos2\phi)]$$

$$\chi_{ZXZ} = (1/2)\beta_{caa}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\chi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$
$$+ (1/2)\beta_{bca}[(\sin\theta - 2\sin^3\theta)\cos\chi\sin2\phi + \sin\theta\cos\theta\sin\chi(1 + \cos2\phi)]$$

$$\chi_{ZZX} = \beta_{caa}[(\sin\theta - \sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$
$$+ \beta_{bca}[(\sin\theta - 2\sin^3\theta)\cos\chi\sin2\phi - \sin\theta\cos\theta\sin\chi(1 - \cos2\phi)]$$

$$\chi_{ZXX} = (1/4)\beta_{caa}\{2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi)]$$
$$+ (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$
$$- (1/4)\beta_{bca}\{2[(\cos\theta - \cos^3\theta) - \cos^3\theta\cos2\chi]\sin2\phi - [\sin^2\theta - (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$$

$$\chi_{XZX} = (1/4)\beta_{caa}\{2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi)]$$
$$+ (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$
$$- (1/4)\beta_{bca}\{2[(\cos\theta - \cos^3\theta) - \cos^3\theta\cos2\chi]\sin2\phi - [\sin^2\theta - (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$$

$$\chi_{XXZ} = -(1/2)\beta_{caa}[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]$$
$$- (1/2)\beta_{bca}[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\sin2\phi + \sin^2\theta\sin2\chi(1 + \cos2\phi)]$$

$$\chi_{ZZZ} = \beta_{caa}(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$$
$$+ \beta_{bca}(\cos\theta - \cos^3\theta)\sin2\phi$$

(spp)

$$\chi_{YXX} = (1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)]$$
$$+ 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$$
$$- (1/4)\beta_{bca}\{[2\sin\theta\sin\chi - (2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\sin2\phi + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi\cos2\phi)\}$$

$$\chi_{YZZ} = -(1/2)\beta_{caa}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$
$$- (1/2)\beta_{bca}[(\sin\theta - 2\sin^3\theta)\sin2\chi\sin2\phi - \sin\theta\cos\theta\cos\chi(1 + \cos2\phi)]$$

$$\chi_{YZX} = (1/4)\beta_{caa}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi] \sin2\phi\}$$
$$+ (1/4)\beta_{bca}[2\cos^3\theta\sin2\chi\sin2\phi - \sin^2\theta(1 - \cos2\chi)(1 - \cos2\phi) + 2\cos^2\theta(1 + \cos2\chi\cos2\phi)]$$

$$\chi_{YXZ} = (1/2)\beta_{caa}[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$$
$$+ (1/2)\beta_{bca}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi - \sin^2\theta\cos2\chi(1 + \cos2\phi)]$$

(ssp)

$$\chi_{YYX} = (1/4)\beta_{caa}\{[-(\sin\theta - \sin^3\theta)(1 + \cos2\phi) + \sin\theta(1 - \cos2\phi)](\cos\chi - \cos3\chi)$$
$$+ 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$$
$$- (1/4)\beta_{bca}[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\sin2\phi - 2\sin2\theta(\sin\chi + \sin3\chi)\cos2\phi\}$$

$$\chi_{YYZ} = -(1/2)\beta_{caa}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$$
$$- (1/2)\beta_{bca}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\sin2\phi - \sin^2\theta\sin2\chi(1 + \cos2\phi)]$$

(psp)

$$\chi_{XYX} = (1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)]$$
$$+ 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$$
$$- (1/4)\beta_{bca}\{[2\sin\theta\sin\chi - (2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\sin2\phi + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi\cos2\phi)\}$$

$$\chi_{ZYZ} = -(1/2)\beta_{caa}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$
$$- (1/2)\beta_{bca}[(\sin\theta - 2\sin^3\theta)\sin2\chi\sin2\phi - \sin\theta\cos\theta\cos\chi(1 + \cos2\phi)]$$

$$\chi_{XYZ} = (1/2)\beta_{caa}[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$$
$$+ (1/2)\beta_{bca}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi - \sin^2\theta\cos2\chi(1 + \cos2\phi)]$$

$\chi_{ZYX} = (1/4)\beta_{caa}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

$\quad + (1/4)\beta_{bca}[2\cos^3\theta\sin2\chi\sin2\phi - \sin^2\theta(1 - \cos2\chi)(1 - \cos2\phi) + 2\cos^2\theta(1 + \cos2\chi\cos2\phi)]$

(sps) $\chi_{YXY} = -(1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)]$

$\quad + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$

$\quad + (1/4)\beta_{bca}\{[2\sin\theta\cos\chi - (2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\sin2\phi - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\cos2\phi\}$

$\chi_{YZY} = (1/4)\beta_{caa}\{2[\cos\theta(1 - \cos2\phi\cos2\chi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)]$

$\quad - (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

$\quad - (1/4)\beta_{bca}\{2[(\cos\theta - \cos^3\theta) - \cos^3\theta\cos2\chi]\sin2\phi + [\sin^2\theta - (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$

(pps) $\chi_{XXY} = (1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(1 + \cos2\phi) - \sin\theta(1 - \cos2\phi)](\sin\chi + \sin3\chi)$

$\quad + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$

$\quad + (1/4)\beta_{bca}[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\sin2\phi + 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\cos2\phi]$

$\chi_{ZZY} = -\beta_{caa}[(\sin\theta - \sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\quad -\beta_{bca}[(\sin\theta - \sin^3\theta)\sin\chi\sin2\phi + \sin\theta\cos\theta\cos\chi(1 - \cos2\phi)]$

$\chi_{ZXY} = (1/4)\beta_{caa}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

$\quad + (1/4)\beta_{bca}[2\cos^3\theta\sin2\chi\sin2\phi + \sin^2\theta(1 + \cos2\chi)(1 - \cos2\phi) - 2(1 - \cos2\chi\cos2\phi)]$

$\chi_{XZY} = (1/4)\beta_{caa}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

$\quad + (1/4)\beta_{bca}[2\cos^3\theta\sin2\chi\sin2\phi + \sin^2\theta(1 + \cos2\chi)(1 - \cos2\phi) - 2(1 - \cos2\chi\cos2\phi)]$

(pss) $\chi_{XYY} = -(1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)]$

$\quad + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$

$\quad + (1/4)\beta_{bca}\{[2\sin\theta\cos\chi - (2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\sin2\phi - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\cos2\phi\}$

$\chi_{ZYY} = (1/4)\beta_{caa}\{2[\cos\theta(1 - \cos2\phi\cos2\chi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)]$

$\quad - (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

$\quad - (1/4)\beta_{bca}\{2[(\cos\theta - \cos^3\theta) - \cos^3\theta\cos2\chi]\sin2\phi + [\sin^2\theta - (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$

(sss) $\chi_{YYY} = (1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi + \sin3\chi)(1 - \cos2\phi)]$

$\quad + 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$

$\quad + (1/4)\beta_{bca}\{[4(\sin\theta - \sin^3\theta)\sin\chi - (2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\sin2\phi$

$\quad - 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\cos2\phi\}$

$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0$

［面外 (b_2) 振動］

(ppp) $\chi_{XXX} = -(1/4)\beta_{cbb}\{[\sin\theta(\cos\chi - \cos3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)(1 - \cos2\phi)]$

$\quad + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$

$\quad + (1/4)\beta_{cab}\{[\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\sin2\phi$

$\quad - 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\cos2\phi\}$

$\chi_{XZZ} = (1/2)\beta_{cbb}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 - \cos2\phi) + \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\quad + (1/2)\beta_{cab}[(\sin\theta - 2\sin^3\theta)\cos\chi\sin2\phi - \sin\theta\cos\theta\sin\chi(1 - \cos2\phi)]$

$$\chi_{ZXZ} = (1/2)\beta_{cbb}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 - \cos2\phi) + \sin\theta\cos\theta\sin\chi\sin2\phi]$$
$$+ (1/2)\beta_{cab}[(\sin\theta - 2\sin^3\theta)\cos\chi\sin2\phi - \sin\theta\cos\theta\sin\chi(1 - \cos2\phi)]$$
$$\chi_{ZZX} = \beta_{cbb}[(\sin\theta - \sin^3\theta)\cos\chi(1 - \cos2\phi) + \sin\theta\cos\theta\sin\chi\sin2\phi]$$
$$+ \beta_{cab}[(\sin\theta - \sin^3\theta)\cos\chi\sin2\phi + \sin\theta\cos\theta\sin\chi(1 + \cos2\phi)]$$
$$\chi_{ZXX} = (1/4)\beta_{cbb}\{2[\cos\theta(1 - \cos2\phi\cos2\chi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 - \cos2\phi)]$$
$$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$
$$- (1/4)\beta_{cab}\{2[(\cos\theta - \cos^3\theta) - \cos^3\theta\cos2\chi]\sin2\phi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$$
$$\chi_{XZX} = (1/4)\beta_{cbb}\{2[\cos\theta(1 - \cos2\phi\cos2\chi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 - \cos2\phi)]$$
$$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$
$$- (1/4)\beta_{cab}\{2[(\cos\theta - \cos^3\theta) - \cos^3\theta\cos2\chi]\sin2\phi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$$
$$\chi_{XXZ} = -(1/2)\beta_{cbb}[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 - \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$$
$$- (1/2)\beta_{cab}[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\sin2\phi - \sin^2\theta\sin2\chi(1 - \cos2\phi)]$$
$$\chi_{ZZZ} = \beta_{cbb}(\cos\theta - \cos^3\theta)(1 - \cos2\phi)$$
$$+ \beta_{cab}(\cos\theta - \cos^3\theta)\sin2\phi$$

(spp)
$$\chi_{YXX} = (1/4)\beta_{cbb}\{[\sin\theta(\sin\chi - \sin3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 - \cos2\phi)]$$
$$- 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$$
$$- (1/4)\beta_{cab}\{[\sin\theta(\sin\chi - \sin3\chi) + (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\sin2\phi$$
$$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi\cos2\phi)\}$$
$$\chi_{YZZ} = -(1/2)\beta_{cbb}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 - \cos2\phi) - \sin\theta\cos\theta\cos\chi\sin2\phi]$$
$$- (1/2)\beta_{cab}[(\sin\theta - 2\sin^3\theta)\sin\chi\sin2\phi + \sin\theta\cos\theta\cos\chi(1 - \cos2\phi)]$$
$$\chi_{YZX} = (1/4)\beta_{cbb}\{2[(\cos\theta - \cos^3\theta)(1 - \cos2\phi) + \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta - (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$
$$- (1/4)\beta_{cab}[2\cos^3\theta\sin2\chi\sin2\phi - \sin^2\theta(1 - \cos2\chi)(1 + \cos2\phi) + 2\cos^2\theta(1 - \cos2\chi\cos2\phi)]$$
$$\chi_{YXZ} = (1/2)\beta_{cbb}[(\cos\theta - \cos^3\theta)\sin2\chi(1 - \cos2\phi) - \sin^2\theta\cos2\chi\sin2\phi]$$
$$+ (1/2)\beta_{cab}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi + \sin^2\theta\cos2\chi(1 - \cos2\phi)]$$

(ssp)
$$\chi_{YYX} = (1/4)\beta_{cbb}\{[\sin\theta(1 + \cos2\phi) - (\sin\theta - \sin^3\theta)(1 - \cos2\phi)](\cos\chi - \cos3\chi)$$
$$- 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$$
$$- (1/4)\beta_{cab}\{(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\sin2\phi + 2\sin\theta\cos\theta[2\sin\chi - (\sin\chi - \sin3\chi)\cos2\phi]\}$$
$$\chi_{YYZ} = -(1/2)\beta_{cbb}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 - \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]$$
$$- (1/2)\beta_{cab}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\sin2\phi + \sin^2\theta\sin2\chi(1 - \cos2\phi)]$$

(psp)
$$\chi_{XYX} = (1/4)\beta_{cbb}\{[\sin\theta(\sin\chi - \sin3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 - \cos2\phi)]$$
$$- 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$$
$$- (1/4)\beta_{cab}\{[\sin\theta(\sin\chi - \sin3\chi) + (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\sin2\phi$$
$$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi\cos2\phi)\}$$
$$\chi_{ZYZ} = -(1/2)\beta_{cbb}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 - \cos2\phi) - \sin\theta\cos\theta\cos\chi\sin2\phi]$$
$$- (1/2)\beta_{cab}[(\sin\theta - 2\sin^3\theta)\sin\chi\sin2\phi + \sin\theta\cos\theta\cos\chi(1 - \cos2\phi)]$$
$$\chi_{XYZ} = (1/2)\beta_{cbb}[(\cos\theta - \cos^3\theta)\sin2\chi(1 - \cos2\phi) - \sin^2\theta\cos2\chi\sin2\phi]$$
$$+ (1/2)\beta_{cab}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi + \sin^2\theta\cos2\chi(1 - \cos2\phi)]$$

$$\chi_{ZYX} = (1/4)\beta_{cbb}\{2[(\cos\theta - \cos^3\theta)(1 - \cos2\phi) + \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta - (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$
$$- (1/4)\beta_{cab}[2\cos^3\theta\sin2\chi\sin2\phi - \sin^2\theta(1 - \cos2\chi)(1 + \cos2\phi) + 2\cos^2\theta(1 - \cos2\chi\cos2\phi)]$$

(sps)
$$\chi_{YXY} = -(1/4)\beta_{cbb}\{[\sin\theta(\cos\chi + \cos3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 - \cos2\phi)]$$
$$- 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$$
$$+ (1/4)\beta_{cab}\{[2\sin\theta\cos\chi - (2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\sin2\phi + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi\cos2\phi)\}$$
$$\chi_{YZY} = (1/4)\beta_{cbb}\{2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 - \cos2\phi)]$$
$$+ (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$
$$- (1/4)\beta_{cab}\{2[(\cos\theta - \cos^3\theta) + \cos^3\theta\cos2\chi]\sin2\phi - [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$$

(pps)
$$\chi_{XXY} = (1/4)\beta_{cbb}\{[-\sin\theta(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\phi)](\sin\chi + \sin3\chi)$$
$$- \sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$$
$$+ (1/4)\beta_{cab}\{(2\sin\theta - \sin^3\theta)\sin2\phi - 2\sin\theta\cos\theta\ [2\cos\chi - (\cos\chi + \cos3\chi)\cos2\phi]\}$$
$$\chi_{ZZY} = \beta_{cbb}[-(\sin\theta - \sin^3\theta)\sin\chi(1 - \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$
$$- \beta_{cab}[(\sin\theta - \sin^3\theta)\sin\chi\sin2\phi - \sin\theta\cos\theta\cos\chi(1 + \cos2\phi)]$$
$$\chi_{ZXY} = (1/4)\beta_{cbb}\{2[(\cos\theta - \cos^3\theta)(1 - \cos2\phi) + \cos\theta\cos2\phi]\sin2\chi - [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$
$$- (1/4)\beta_{cab}[2\ \cos^3\theta\sin2\chi\sin2\phi + \sin^2\theta(1 + \cos2\chi)(1 + \cos2\phi) - 2\cos^2\theta(1 + \cos2\chi\cos2\phi)]$$
$$\chi_{XZY} = (1/4)\beta_{cbb}\{2[(\cos\theta - \cos^3\theta)(1 - \cos2\phi) + \cos\theta\cos2\phi]\sin2\chi - [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$
$$- (1/4)\beta_{cab}[2\ \cos^3\theta\sin2\chi\sin2\phi + \sin^2\theta(1 + \cos2\chi)(1 + \cos2\phi) - 2\cos^2\theta(1 + \cos2\chi\cos2\phi)]$$

(pss)
$$\chi_{XYY} = -(1/4)\beta_{cbb}\{[\sin\theta(\cos\chi + \cos3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 - \cos2\phi)]$$
$$- 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$$
$$+ (1/4)\beta_{cab}\{[2\sin\theta\cos\chi - (2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\sin2\phi + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi\cos2\phi)\}$$
$$\chi_{ZYY} = (1/4)\beta_{cbb}\{2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 - \cos2\phi)]$$
$$+ (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$
$$- (1/4)\beta_{cab}\{2[(\cos\theta - \cos^3\theta) + \cos^3\theta\cos2\chi]\sin2\phi - [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$$

(sss)
$$\chi_{YYY} = (1/4)\beta_{cbb}\{[\sin\theta(\sin\chi + \sin3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 - \cos2\phi)]$$
$$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$$
$$+ (1/4)\beta_{cab}\{[4(\sin\theta - \sin^3\theta)\sin\chi - (2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\sin2\phi$$
$$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\cos2\phi\}$$

$$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0$$

付録 E： $\phi_A = 0, \phi_B = \pi$ または $\phi_A = \pi$, $\phi_B = 0$ のときの (XYZ)系でのテンソル成分

［全対称バンド］　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには**　$\beta_{aac} \sim (4/9)\ \beta_{\zeta\zeta\zeta}$、$\beta_{ccc} \sim (1/9)\ \beta_{\zeta\zeta\zeta}$　**である。**

原理的には振動バンドが２つに分裂するが、実際には重なっているときには、以下に示す２つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{xxz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{aac}\cos\alpha$

$\beta_{yyz} = +2\beta_{aac}\cos\alpha$

$\beta_{zzz} = +2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 2\beta_{ccc}\cos\alpha$

$\beta_{zxx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

$\beta_{xzx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

［**対称 (a_1) 振動**］

(ppp)

$$\begin{aligned}\chi_{XXX} = &-2\beta_{aac}\cos\alpha\sin\theta\cos\chi\\ &+ (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{4\sin\theta\cos\chi - 3\sin^3\theta(3\cos\chi + \cos3\chi)\\ &\quad - [\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\cos2\phi\\ &\quad - 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}\\ &+ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(3\cos\chi + \cos3\chi)\end{aligned}$$

$$\begin{aligned}\chi_{XZZ} = &-(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(3 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]\\ &+ 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi\end{aligned}$$

$$\begin{aligned}\chi_{ZXZ} = &-(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(3 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]\\ &+ 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi\end{aligned}$$

$$\begin{aligned}\chi_{ZZX} = &-2\beta_{aac}\cos\alpha\sin\theta\cos\chi\\ &+ (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\sin\theta\cos\chi - 3(\sin\theta - \sin^3\theta)\cos\chi + \sin^3\theta\cos\chi\cos2\phi]\\ &+ 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi\end{aligned}$$

$$\begin{aligned}\chi_{XZX} = &(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]\\ &- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\end{aligned}$$

$$\begin{aligned}\chi_{ZXX} = &(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]\\ &- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\end{aligned}$$

$$\begin{aligned}\chi_{XXZ} = &2\beta_{aac}\cos\alpha\cos\theta\\ &+ (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\\ &\quad + [(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi + 2\cos^2\theta\sin2\chi\sin2\phi\}\\ &- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\end{aligned}$$

$$\begin{aligned}\chi_{ZZZ} = &-2\beta_{aac}\cos\alpha\cos\theta\\ &+ (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[-\cos\theta + 3\cos^3\theta - (\cos\theta - \cos^3\theta)\cos2\phi]\\ &- 2(\beta_{aac} - \beta_{ccc})\cos\alpha\cos^3\theta\end{aligned}$$

(spp)

$$\begin{aligned}\chi_{YXX} = &(1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)\\ &\quad + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}\\ &- (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)\end{aligned}$$

$$\begin{aligned}\chi_{YZZ} = &(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]\\ &- 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\sin\chi\end{aligned}$$

$$\begin{aligned}\chi_{YZX} = &-(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi]\\ &+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi\end{aligned}$$

$$\begin{aligned}\chi_{YXZ} = &-(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\chi\\ &\quad - 2\cos^2\theta\cos2\chi\sin2\phi\}\end{aligned}$$

$+ (ß_{aac} - ß_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$

(ssp) $\chi_{YYX} = -2ß_{aac}\cos\alpha\sin\theta\cos\chi$

$+ (1/4)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)\{4\sin\theta\cos\chi - 3\sin^3\theta(\cos\chi - \cos3\chi)$

$- [\sin\theta(3\cos\chi + \cos3\chi) - (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\cos2\phi$

$+ 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$

$+ (1/2)(ß_{aac} - ß_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)$

$\chi_{YYZ} = 2ß_{aac}\cos\alpha\sin\theta\cos\chi$

$+ (1/2)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)\{ - 2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$

$+ [(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos2\chi] \cos2\phi - 2\cos^2\theta\sin2\chi\sin2\phi\}$

$- (ß_{aac} - ß_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$

(psp) $\chi_{XYX} = (1/4)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)$

$+ 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$

$- (1/2)(ß_{aac} - ß_{ccc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)$

$\chi_{ZYZ} = (ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$- 2(ß_{aac} - ß_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\sin\chi$

$\chi_{XYZ} = -(1/2)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\chi$

$- 2\cos^2\theta\cos2\chi\sin2\phi\}$

$+ (ß_{aac} - ß_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$

$\chi_{ZYX} = -(1/2)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$

$+ (ß_{aac} - ß_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$

(sps) $\chi_{YXY} = (1/4)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)$

$- 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$

$+ (1/2)(ß_{aac} - ß_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)$

$\chi_{YZY} = (1/2)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$

$- (ß_{aac} - ß_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$

(pps) $\chi_{XXY} = 2ß_{aac}\cos\alpha\sin\theta\sin\chi$

$+ (1/4)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)\{-4\sin\theta\sin\chi + 3\sin^3\theta(\sin\chi + \sin3\chi)$

$+ [\sin\theta(3\sin\chi - \sin3\chi) - (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\cos2\phi$

$+ 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$

$- (1/2)(ß_{aac} - ß_{ccc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)$

$\chi_{ZZY} = 2ß_{aac}\cos\alpha\sin\theta\sin\chi$

$+(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[-\sin\theta + 3(\sin\theta - \sin^3\theta) - \sin^3\theta\cos2\phi]\sin\chi$

$- 2(ß_{aac} - ß_{ccc})\cos\alpha(\sin\theta -\sin^3\theta)\sin\chi$

$\chi_{XZY} = -(1/2)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$

$+ (ß_{aac} - ß_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$

$\chi_{ZXY} = -(1/2)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$

$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi$$

(pss) $$\chi_{XYY} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos 2\phi](\cos\chi - \cos 3\chi)$$
$$- 2\sin\theta\cos\theta(\sin\chi - \sin 3\chi)\sin 2\phi\}$$
$$+ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos 3\chi)$$
$$\chi_{ZYY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos 2\chi)(3 + \cos 2\phi) + \sin^2\theta\sin 2\chi\sin 2\phi]$$
$$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos 2\chi)$$

(sss) $$\chi_{YYY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi$$
$$+ (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-4\sin\theta\sin\chi + 3\sin^3\theta(3\sin\chi - \sin 3\chi)$$
$$+ [\sin\theta(\sin\chi + \sin 3\chi) - (\sin\theta - \sin^3\theta)(3\sin\chi - \sin 3\chi)]\cos 2\phi$$
$$- 2\sin\theta\cos\theta(\cos\chi - \cos 3\chi)\sin 2\phi\}$$
$$- (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(3\sin\chi - \sin 3\chi)$$

$$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = -(4\beta_{aac} + 2\beta_{ccc})\cos\alpha\sin\theta\cos\chi$$
$$\chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = +(4\beta_{aac} + 2\beta_{ccc})\cos\alpha\sin\theta\sin\chi$$
$$\chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = +(4\beta_{aac} + 2\beta_{ccc})\cos\alpha\cos\theta$$

［**逆対称 (b_1) 振動**］

(ppp) $$\chi_{XXX} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(3\cos\chi + \cos 3\chi)(1 + \cos 2\phi)$$
$$+ \sin\theta(\cos\chi - \cos 3\chi)(1 - \cos 2\phi)] - 2\sin\theta\cos\theta(\sin\chi + \sin 3\chi)\sin 2\phi\}$$
$$\chi_{XZZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos 2\phi) - \sin\theta\cos\theta\sin\chi\sin 2\phi]$$
$$\chi_{ZXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos 2\phi) - \sin\theta\cos\theta\sin\chi\sin 2\phi]$$
$$\chi_{ZZX} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(1 + \cos 2\phi) - \sin\theta\cos\theta\sin\chi\sin 2\phi]$$
$$\chi_{ZXX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 + \cos 2\chi\cos 2\phi)$$
$$- (\cos\theta - \cos^3\theta)(1 + \cos 2\chi)(1 + \cos 2\phi)] + (1 - 3\cos^2\theta)\sin 2\chi\sin 2\phi\}$$
$$\chi_{XZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 + \cos 2\chi\cos 2\phi)$$
$$- (\cos\theta - \cos^3\theta)(1 + \cos 2\chi)(1 + \cos 2\phi)] + (1 - 3\cos^2\theta)\sin 2\chi\sin 2\phi\}$$
$$\chi_{XXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[-(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)(1 + \cos 2\phi) + \sin^2\theta\sin 2\chi\sin 2\phi]$$
$$\chi_{ZZZ} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos 2\phi)$$

(spp) $$\chi_{YXX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin 3\chi)(1 + \cos 2\phi)$$
$$+ \sin\theta(\sin\chi - \sin 3\chi)(1 - \cos 2\phi)] + 2\sin\theta\cos\theta\cos 3\chi\sin 2\phi\}$$
$$\chi_{YZZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos 2\phi) + \sin\theta\cos\theta\cos\chi\sin 2\phi]$$
$$\chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos 2\phi)$$
$$- \cos 2\phi\cos\theta]\sin 2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos 2\chi]\sin 2\phi\}$$
$$\chi_{YXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin 2\chi(1 + \cos 2\phi) + \sin^2\theta\cos 2\chi\sin 2\phi]$$

(ssp) $$\chi_{YYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[-(\sin\theta - \sin^3\theta)(1 + \cos 2\phi) + \sin\theta(1 - \cos 2\phi)](\cos\chi - \cos 3\chi)$$
$$+ 2\sin\theta\cos\theta(\sin\chi - \sin 3\chi)\sin 2\phi\}$$

$$\chi_{YYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$$

(psp)

$$\chi_{XYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi)$$
$$+ \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$$
$$\chi_{ZYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$
$$\chi_{XYZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$$
$$\chi_{ZYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$$
$$- \cos2\phi\cos\theta]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$

(sps)

$$\chi_{YXY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi)$$
$$+ \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$$
$$\chi_{YZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)]$$
$$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$

(pps)

$$\chi_{XXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(1 + \cos2\phi) - \sin\theta(1 - \cos2\phi)](\sin\chi + \sin3\chi)$$
$$+ 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$$
$$\chi_{ZZY} = 2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$
$$\chi_{ZXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$$
$$- \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$
$$\chi_{XZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$$
$$- \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$

(pss)

$$\chi_{XYY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi)$$
$$+ \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$$
$$\chi_{ZYY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)]$$
$$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$

(sss)

$$\chi_{YYY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 + \cos2\phi)$$
$$+ \sin\theta(\sin\chi + \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$$

$$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0$$

［縮重バンド］　$\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには**　$\beta_{caa} \sim (4/9)\beta_{\zeta\zeta\zeta}$、$\beta_{aaa} \sim (4\sqrt{2}/9)\beta_{\zeta\zeta\zeta}$　**である。**

原理的には振動バンドが３つに分裂するが、実際には重なっているときには、以下に示す３つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

（β_{zyy} **と** β_{yzy} **には b 軸方向の振動が寄与し、他の成分には a 軸方向の振動が寄与する。**）

（± **記号の上側は** $\phi_A = 0$、$\phi_B = \pi$ **に対応し、下側は** $\phi_A = \pi$、$\phi_B = 0$ **に対応する。**）

$\beta_{zxx} = -2\beta_{caa}(\cos\alpha - 2\cos^3\alpha)$

$\beta_{xzx} = -2\beta_{caa}(\cos\alpha - 2\cos^3\alpha)$

$\beta_{zyy} = 2\beta_{caa}\cos\alpha$

$\beta_{yzy} = 2\beta_{caa}\cos\alpha$

$\beta_{xxz} = -4\beta_{caa}(\cos\alpha - \cos^3\alpha)$

$\beta_{yyz} = 0$

$\beta_{zzz} = 4\beta_{caa}(\cos\alpha - \cos^3\alpha)$

［対称 (a$_1$) 振動］

(ppp) $\chi_{XXX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$
$+ (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(3\cos\chi + \cos3\chi)$
$+ (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\cos2\phi$
$+ 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$

$\chi_{XZZ} = (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi$
$+ (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\cos\chi\cos2\phi - \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZXZ} = (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi$
$+ (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\cos\chi\cos2\phi - \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZZX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$
$+ (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi$
$- (1/2)(\beta_{aac} - \beta_{bbc})\sin^3\theta\cos\chi\cos2\phi$

$\chi_{XZX} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$
$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\cos2\phi - \sin^2\theta\sin2\chi\sin2\phi]$

$\chi_{ZXX} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$
$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\cos2\phi - \sin^2\theta\sin2\chi\sin2\phi]$

$\chi_{XXZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$
$- (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$
$- (1/4)(\beta_{aac} - \beta_{bbc})\{ [(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi + 2\cos^2\theta\sin2\chi)\sin2\phi\}$

$\chi_{ZZZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$
$- (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\cos^3\theta$
$+ (1/2)(\beta_{aac} - \beta_{bbc})(\cos\theta - \cos^3\theta)\cos2\phi$

(spp) $\chi_{YXX} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi)$
$+ (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\cos2\phi + 2\sin\theta\cos\theta (\cos\chi + \cos3\chi)\sin2\phi]$

$\chi_{YZZ} = -(1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\sin\chi$
$- (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi\cos2\phi + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\chi_{YZX} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$
$+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$

$\chi_{YXZ} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$
$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta + \cos^3\theta)\sin2\chi\cos2\phi + 2\cos^2\theta\cos2\chi\sin2\phi]$

(ssp) $\chi_{YYX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$
$+ (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi)$

$$+ (1/8)(\beta_{aac} - \beta_{bbc})\{\cos2\phi[\sin\theta(3\cos\chi + \cos3\chi) - (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)] - 2\sin2\phi\sin\theta\cos\theta(\sin\chi + \sin3\chi)\}$$

$$\chi_{YYZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta - (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos2\chi) - (1/4)(\beta_{aac} - \beta_{bbc})[\cos2\phi[(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos2\chi] - 2\sin2\phi\cos^2\theta\sin2\chi)]$$

(psp)

$$\chi_{XYX} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi) + (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\cos2\phi + 2\sin\theta\cos\theta\,(\cos\chi + \cos3\chi)\sin2\phi]$$

$$\chi_{ZYZ} = -(1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\sin\chi - (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi\cos2\phi + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$\chi_{XYZ} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi - (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta + \cos^3\theta)\sin2\chi\cos2\phi + 2\cos^2\theta\cos2\chi\sin2\phi]$$

$$\chi_{ZYX} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi + (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$$

(sps)

$$\chi_{YXY} = (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi) - (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\cos2\phi - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi]$$

$$\chi_{YZY} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos2\chi) - (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\cos2\phi + \sin^2\theta\sin2\chi\sin2\phi]$$

(pps)

$$\chi_{XXY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi - (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi) - (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(3\sin\chi - \sin3\chi)\cos2\phi - (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)] + 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$$

$$\chi_{ZZY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi - (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\sin\chi + (1/2)(\beta_{aac} - \beta_{bbc})\sin^3\theta\sin\chi\cos2\phi$$

$$\chi_{XZY} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi + (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$$

$$\chi_{ZXY} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi + (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$$

(pss)

$$\chi_{XYY} = (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi) - (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\cos2\phi - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi]$$

$$\chi_{ZYY} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos2\chi) - (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\cos2\phi + \sin^2\theta\sin2\chi\sin2\phi]$$

(sss)

$$\chi_{YYY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi - (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(3\sin\chi - \sin3\chi) - (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta\,(\sin\chi + \sin3\chi)\cos2\phi - (\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)]$$

$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$

$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = -(\beta_{aac} + \beta_{bbc} + \beta_{ccc})\sin\theta\cos\chi$
$\chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = +(\beta_{aac} + \beta_{bbc} + \beta_{ccc})\sin\theta\sin\chi$
$\chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = +(\beta_{aac} + \beta_{bbc} + \beta_{ccc})\cos\theta$

［**逆対称 (b_1) 振動**］

(ppp) $\chi_{XXX} = -(1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi - \cos3\chi)(1 - \cos2\phi)]$
$- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$
$\chi_{XZZ} = (1/2)\beta_{caa}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$
$\chi_{ZXZ} = (1/2)\beta_{caa}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$
$\chi_{ZZX} = \beta_{caa}[(\sin\theta - \sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$
$\chi_{ZXX} = (1/4)\beta_{caa}\{2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi)]$
$+ (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$
$\chi_{XZX} = (1/4)\beta_{caa}\{2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi)]$
$+ (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$
$\chi_{XXZ} = (1/2)\beta_{caa}[-(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$
$\chi_{ZZZ} = \beta_{caa}(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

(spp) $\chi_{YXX} = (1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)]$
$+ 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$
$\chi_{YZZ} = -(1/2)\beta_{caa}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \mathrm{in}\theta\cos\theta\cos\chi\sin2\phi]$
$\chi_{YZX} = (1/4)\beta_{caa}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$
$\chi_{YXZ} = (1/2)\beta_{caa}[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$

(ssp) $\chi_{YYX} = (1/4)\beta_{caa}\{[-(\sin\theta - \sin^3\theta)(1 + \cos2\phi) + \sin\theta(1 - \cos2\phi)](\cos\chi - \cos3\chi)$
$+ 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$
$\chi_{YYZ} = -(1/2)\beta_{caa}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi) + \sin2\chi\sin^2\theta\sin2\phi]$

(psp) $\chi_{XYX} = (1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)]$
$+ 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$
$\chi_{ZYZ} = -(1/2)\beta_{caa}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$
$\chi_{XYZ} = (1/2)\beta_{caa}(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$
$\chi_{ZYX} = (1/4)\beta_{caa}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

(sps) $\chi_{YXY} = -(1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)]$
$+ 2\sin\theta\cos\theta\sin3\chi\ \sin2\phi\}$
$\chi_{YZY} = (1/4)\beta_{caa}\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)]$
$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

(pps) $\chi_{XXY} = (1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(1 + \cos2\phi) - \sin\theta(1 - \cos2\phi)](\sin\chi + \sin3\chi)$
$+ 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$

$\chi_{ZZY} = -\beta_{caa}[(\sin\theta - \sin^3\theta)\sin\chi\ (1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\ \sin2\phi]$

$\chi_{ZXY} = (1/4)\beta_{caa}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

$\chi_{XZY} = (1/4)\beta_{caa}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

(pss) $\chi_{XYY} = -(1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + (1 - \cos2\phi)\sin\theta(\cos\chi + \cos3\chi)]$
$+ 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$

$\chi_{ZYY} = (1/4)\beta_{caa}\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)]$
$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

(sss) $\chi_{YYY} = (1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi + \sin3\chi)(1 - \cos2\phi)]$
$+ 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$

$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0$

［**面外 (b_2) 振動**］

(ppp) $\chi_{XXX} = -(1/4)\beta_{cbb}\{[\sin\theta(\cos\chi - \cos3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)(1 - \cos2\phi)]$
$+ 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$

$\chi_{XZZ} = (1/2)\beta_{cbb}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 - \cos2\phi) + \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZXZ} = (1/2)\beta_{cbb}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 - \cos2\phi) + \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZZX} = \beta_{cbb}[(\sin\theta - \sin^3\theta)\cos\chi(1 - \cos2\phi) + \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZXX} = (1/4)\beta_{cbb}\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 - \cos2\phi)]$
$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

$\chi_{XZX} = (1/4)\beta_{cbb}\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 - \cos2\phi)]$
$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

$\chi_{XXZ} = -(1/2)\beta_{cbb}[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 - \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$

$\chi_{ZZZ} = \beta_{cbb}(\cos\theta - \cos^3\theta)(1 - \cos2\phi)$

(spp) $\chi_{YXX} = (1/4)\beta_{cbb}\{[\sin\theta(\sin\chi - \sin3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 - \cos2\phi)]$
$- 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$

$\chi_{YZZ} = -(1/2)\beta_{cbb}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 - \cos2\phi) - \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\chi_{YZX} = (1/4)\beta_{cbb}\{2[(\cos\theta - \cos^3\theta)(1 - \cos2\phi) + \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta - (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

$\chi_{YXZ} = (1/2)\beta_{cbb}[(\cos\theta - \cos^3\theta)\sin2\chi(1 - \cos2\phi) - \sin^2\theta\cos2\chi\sin2\phi]$

(ssp) $\chi_{YYX} = (1/4)\beta_{cbb}\{[\sin\theta(1 - \cos2\phi) - (\sin\theta - \sin^3\theta)(1 - \cos2\phi)](\cos\chi - \cos3\chi)$
$- 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$

$\chi_{YYZ} = -(1/2)\beta_{cbb}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 - \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]$

(psp) $\chi_{XYX} = (1/4)\beta_{cbb}\{[\sin\theta(\sin\chi - \sin3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 - \cos2\phi)]$

$- 2\sin\theta\cos\theta\cos 3\chi\sin 2\phi\}$

$\chi_{ZYZ} = -(1/2)\beta_{cbb}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 - \cos 2\phi) - \sin\theta\cos\theta\cos\chi\sin 2\phi]$

$\chi_{XYZ} = (1/2)\beta_{cbb}[(\cos\theta - \cos^3\theta)\sin 2\chi(1 - \cos 2\phi) - \sin^2\theta\cos 2\chi\sin 2\phi]$

$\chi_{ZYX} = (1/4)\beta_{cbb}\{2[(\cos\theta - \cos^3\theta)(1 - \cos 2\phi) + \cos\theta\cos 2\phi]\sin 2\chi + [\sin^2\theta - (1 - 3\cos^2\theta)\cos 2\chi]\sin 2\phi\}$

(sps) $\chi_{YXY} = -(1/4)\beta_{cbb}\{[\sin\theta(\cos\chi + \cos 3\chi)(1 - \cos 2\phi) + (\sin\theta - \sin^3\theta)(\cos\chi - \cos 3\chi)(1 - \cos 2\phi)]$

$- 2\sin\theta\cos\theta\sin 3\sin 2\phi\chi\}$

$\chi_{YZY} = (1/4)\beta_{cbb}\{2[\cos\theta(1 + \cos 2\chi\cos 2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos 2\chi)(1 - \cos 2\phi)]$

$+ (1 - 3\cos^2\theta)\sin 2\chi\sin 2\phi\}$

(pps) $\chi_{XXY} = (1/4)\beta_{cbb}\{[-\sin\theta(1 + \cos 2\phi) + (\sin\theta - \sin^3\theta)(1 - \cos 2\phi)](\sin\chi + \sin 3\chi)$

$- \sin\theta\cos\theta(\cos\chi + \cos 3\chi)\sin 2\phi\}$

$\chi_{ZZY} = \beta_{cbb}[-(\sin\theta - \sin^3\theta)\sin\chi(1 - \cos 2\phi) + \sin\theta\cos\theta\cos\chi\sin 2\phi]$

$\chi_{ZXY} = (1/4)\beta_{cbb}\{2[(\cos\theta - \cos^3\theta)(1 - \cos 2\phi) + \cos\theta\cos 2\phi]\sin 2\chi - [\sin^2\theta + (1 - 3\cos^2\theta)\cos 2\chi]\sin 2\phi\}$

$\chi_{XZY} = (1/4)\beta_{cbb}\{2[(\cos\theta - \cos^3\theta)(1 - \cos 2\phi) + \cos\theta\cos 2\phi]\sin 2\chi - [\sin^2\theta + (1 - 3\cos^2\theta)\cos 2\chi]\sin 2\phi\}$

(pss) $\chi_{XYY} = -(1/4)\beta_{cbb}\{[\sin\theta(\cos\chi + \cos 3\chi)(1 - \cos 2\phi) + (\sin\theta - \sin^3\theta)(\cos\chi - \cos 3\chi)(1 - \cos 2\phi)]$

$- 2\sin\theta\cos\theta\sin 3\chi\sin 2\phi\}$

$\chi_{ZYY} = (1/4)\beta_{cbb}\{2[\cos\theta(1 + \cos 2\chi\cos 2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos 2\chi)(1 - \cos 2\phi)]$

$+ (1 - 3\cos^2\theta)\sin 2\chi\sin 2\phi\}$

(sss) $\chi_{YYY} = (1/4)\beta_{cbb}\{[\sin\theta(\sin\chi + \sin 3\chi)(1 + \cos 2\phi) + (\sin\theta - \sin^3\theta)(3\sin\chi - \sin 3\chi)(1 - \cos 2\phi)]$

$- 2\sin\theta\cos\theta(\cos\chi - \cos 3\chi)\sin 2\phi\}$

$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0$

付録 F：空間固定 (XYZ)系でのテンソル成分（一般式）

［全対称バンド］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには** $\beta_{aac} \sim (4/9)\beta_{\zeta\zeta\zeta}$、$\beta_{ccc} \sim (1/9)\beta_{\zeta\zeta\zeta}$ **である。**

原理的には振動バンドが２つに分裂するが、実際には重なっているときには、以下に示す２つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

$\beta_{xxz} + \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) + 4\beta_{aac}\cos\alpha$

$\beta_{xxz} - \beta_{yyz} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$

$\beta_{xxz} + \beta_{yyz} - 2\beta_{zzz} = -2(\beta_{aac} - \beta_{ccc})[3(\cos\alpha - \cos^3\alpha) - 2\cos\alpha]$

$\beta_{zxx} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)$ **であるから、**

［対称 (a_1) 振動］

(ppp) $\chi_{XXX} = -2\beta_{aac}\cos\alpha\sin\theta\cos\chi$

$$+ (1/4)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)\{4\sin\theta\cos\chi - 3\sin^3\theta(3\cos\chi + \cos3\chi)$$
$$- [\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\cos2\phi$$
$$- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$$
$$+ (1/2)(ß_{aac} - ß_{ccc})\cos\alpha\sin^3\theta(3\cos\chi + \cos3\chi)$$

$$\chi_{XZZ} = -(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(3 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$
$$+ 2(ß_{aac} - ß_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi$$

$$\chi_{ZXZ} = -(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(3 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$$
$$+ 2(ß_{aac} - ß_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi$$

$$\chi_{ZZX} = -2ß_{aac}\cos\alpha\sin\theta\cos\chi$$
$$+ (ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[\sin\theta\cos\chi - 3(\sin\theta - \sin^3\theta)\cos\chi + \sin^3\theta\cos\chi\cos2\phi]$$
$$+ 2(ß_{aac} - ß_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi$$

$$\chi_{XZX} = (1/2)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]$$
$$- (ß_{aac} - ß_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$$

$$\chi_{ZXX} = (1/2)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]$$
$$- (ß_{aac} - ß_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$$

$$\chi_{XXZ} = 2ß_{aac}\cos\alpha\cos\theta$$
$$+ (1/2)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)\{-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$$
$$+ [(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi + 2\cos^2\theta\sin2\chi\sin2\phi\}$$
$$- (ß_{aac} - ß_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$$

$$\chi_{ZZZ} = -2ß_{aac}\cos\alpha\cos\theta$$
$$+ (ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[-\cos\theta + 3\cos^3\theta - (\cos\theta - \cos^3\theta)\cos2\phi]$$
$$- 2(ß_{aac} - ß_{ccc})\cos\alpha\cos^3\theta$$

(spp)

$$\chi_{YXX} = (1/4)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)$$
$$+ 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$$
$$- (1/2)(ß_{aac} - ß_{ccc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)$$

$$\chi_{YZZ} = (ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$
$$- 2(ß_{aac} - ß_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\sin\chi$$

$$\chi_{YZX} = -(1/2)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$$
$$+ (ß_{aac} - ß_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

$$\chi_{YXZ} = -(1/2)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\chi$$
$$- 2\cos^2\theta\cos2\chi\sin2\phi\}$$
$$+ (ß_{aac} - ß_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

(ssp)

$$\chi_{YYX} = -2ß_{aac}\cos\alpha\sin\theta\cos\chi$$
$$+ (1/4)(ß_{aac} - ß_{ccc})(\cos\alpha - \cos^3\alpha)\{4\sin\theta\cos\chi - 3\sin^3\theta(\cos\chi - \cos3\chi)$$
$$- [\sin\theta(3\cos\chi + \cos3\chi) - (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\cos2\phi$$
$$+ 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$$
$$+ (1/2)(ß_{aac} - ß_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)$$

$$\chi_{YYZ} = 2ß_{aac}\cos\alpha\sin\theta\cos\chi$$

$$+ (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$$

$$+ [(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos2\chi] \cos2\phi - 2\cos^2\theta\sin2\chi\sin2\phi\}$$

$$- (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$$

(psp) $$\chi_{XYX} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)$$

$$+ 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$$

$$- (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)$$

$$\chi_{ZYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$- 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta - \sin^3\theta)\sin\chi$$

$$\chi_{XYZ} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\chi$$

$$- 2\cos^2\theta\cos2\chi\sin2\phi\}$$

$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

$$\chi_{ZYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$$

$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

(sps) $$\chi_{YXY} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)$$

$$- 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$$

$$+ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)$$

$$\chi_{YZY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$$

$$-(\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$$

(pps) $$\chi_{XXY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi$$

$$+ (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-4\sin\theta\sin\chi + 3\sin^3\theta(\sin\chi + \sin3\chi)$$

$$+ [\sin\theta(3\sin\chi - \sin3\chi) - (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\cos2\phi$$

$$+ 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$$

$$- (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)$$

$$\chi_{ZZY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi$$

$$+ (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[-\sin\theta + 3(\sin\theta - \sin^3\theta) - \sin^3\theta\cos2\phi]\sin\chi$$

$$- 2(\beta_{aac} - \beta_{ccc})\cos\alpha(\sin\theta -\sin^3\theta)\sin\chi$$

$$\chi_{XZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$$

$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

$$\chi_{ZXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$$

$$+ (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi$$

(pss) $$\chi_{XYY} = (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)$$

$$- 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$$

$$+ (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)$$

$$\chi_{ZYY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$$

$$-(\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$$

(sss) $\chi_{YYY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi$

$+ (1/4)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{-4\sin\theta\sin\chi + 3\sin^3\theta(3\sin\chi - \sin3\chi)$

$+ [\sin\theta(\sin\chi + \sin3\chi) - (\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)]\cos2\phi$

$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$

$- (1/2)(\beta_{aac} - \beta_{ccc})\cos\alpha\sin^3\theta(3\sin\chi - \sin3\chi)$

$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = -(4\beta_{aac} + 2\beta_{ccc})\cos\alpha\sin\theta\cos\chi$

$\chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = +(4\beta_{aac} + 2\beta_{ccc})\cos\alpha\sin\theta\sin\chi$

$\chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = +(4\beta_{aac} + 2\beta_{ccc})\cos\alpha\cos\theta$

［逆対称 (b_1) 振動］

(ppp) $\chi_{XXX} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)(1 + \cos2\phi)$

$+ \sin\theta(\cos\chi - \cos3\chi)(1 - \cos2\phi)] - 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$

$\chi_{XZZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZZX} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\chi_{ZXX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 + \cos2\chi\cos2\phi)$

$- (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi)] + (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

$\chi_{XZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 + \cos2\chi\cos2\phi)$

$- (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi)] + (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$

$\chi_{XXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[-(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$

$\chi_{ZZZ} = -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi)$

(spp) $\chi_{YXX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi)$

$+ \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$

$\chi_{YZZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos2\phi\cos\theta]\sin2\chi$

$+ [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

$\chi_{YXZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$

(ssp) $\chi_{YYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[-(\sin\theta - \sin^3\theta)(1 + \cos2\phi) + \sin\theta(1 - \cos2\phi)](\cos\chi - \cos3\chi)$

$+ 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$

$\chi_{YYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$

(psp) $\chi_{XYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi)$

$+ \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$

$\chi_{ZYZ} = (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$\chi_{XYZ} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$

$\chi_{ZYX} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos2\phi\cos\theta]\sin2\chi$

$$+ [-\sin^2\theta + (1 - 3\cos^2\theta)\cos 2\chi] \sin 2\phi\}$$

(sps) $$\chi_{YXY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos 3\chi)(1 + \cos 2\phi) + \sin\theta(\cos\chi + \cos 3\chi)(1 - \cos 2\phi)] + 2\sin\theta\cos\theta\sin 3\chi\sin 2\phi\}$$

$$\chi_{YZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 - \cos 2\chi\cos 2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos 2\chi)(1 + \cos 2\phi)] - (1 - 3\cos^2\theta)\sin 2\chi\sin 2\phi\}$$

(pps) $$\chi_{XXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(1 + \cos 2\phi) - \sin\theta(1 - \cos 2\phi)](\sin\chi + \sin 3\chi) + 2\sin\theta\cos\theta(\cos\chi + \cos 3\chi)\sin 2\phi\}$$

$$\chi_{ZZY} = 2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(1 + \cos 2\phi) + \sin\theta\cos\theta\cos\chi\sin 2\phi]$$

$$\chi_{ZXY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos 2\phi) - \cos\theta \cos 2\phi]\sin 2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos 2\chi] \sin 2\phi\}$$

$$\chi_{XZY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos 2\phi) - \cos\theta \cos 2\phi]\sin 2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos 2\chi] \sin 2\phi\}$$

(pss) $$\chi_{XYY} = (1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos 3\chi)(1 + \cos 2\phi) + \sin\theta(\cos\chi + \cos 3\chi)(1 - \cos 2\phi)] + 2\sin\theta\cos\theta\sin 3\chi\sin 2\phi\}$$

$$\chi_{ZYY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta(1 - \cos 2\chi\cos 2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos 2\chi)(1 + \cos 2\phi)] - (1 - 3\cos^2\theta)\sin 2\chi\sin 2\phi\}$$

(sss) $$\chi_{YYY} = -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(3\sin\chi - \sin 3\chi)(1 + \cos 2\phi) + \sin\theta(\sin\chi + \sin 3\chi)(1 - \cos 2\phi)] + 2\sin\theta\cos\theta(\cos\chi - \cos 3\chi)\sin 2\phi\}$$

$$\chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \varpi_{ZZZ} = 0$$

［縮重バンド］ $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ **のときには** $\beta_{caa} \sim (4/9)\ \beta_{\zeta\zeta\zeta}$、$\beta_{aaa} \sim (4\sqrt{2}/9)\ \beta_{\zeta\zeta\zeta}$ **である。**

原理的には振動バンドが３つに分裂するが、実際には重なっているときには、以下に示す３つのバンドに対する表式について和を取ったものが測定されたスペクトルの解析に当てはめるべき式になる。

ここに示すテンソルの XYZ **成分の表式は、分子固定系での下付きの左２つを入れ替えたものが等しいとき（**$\beta_{ijk} = \beta_{jik}$**）にあてはまる一般式である。**

$$\beta_{xxz} + \beta_{yyz} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)[2\pm(\cos 2\phi_A + \cos 2\phi_B)] - (1/2)\beta_{aaa}\sin^3\alpha[(\cos 3\phi_A + \cos 3\phi_B)\pm(\cos\phi_A + \cos\phi_B)]$$

$$\beta_{xxz} - \beta_{yyz} = -\beta_{caa}(\cos\alpha - \cos^3\alpha)[2\pm(\cos 2\phi_A + \cos 2\phi_B)] + (1/2)\beta_{aaa}(2\sin\alpha - \sin^3\alpha)[(\cos 3\phi_A + \cos 3\phi_B) \pm (\cos\phi_A + \cos\phi_B)]$$

$$\beta_{xxz} + \beta_{yyz} - 2\beta_{zzz} = -6\beta_{caa}(\cos\alpha - \cos^3\alpha)[2 \pm (\cos 2\phi_A + \cos 2\phi_B)] - (3/2)\beta_{aaa}\sin^3\alpha[(\cos 3\phi_A + \cos 3\phi_B) \pm (\cos\phi_A + \cos\phi_B)]$$

$$\beta_{zxx} = \beta_{xzx} = -(1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[2 \pm (\cos 2\phi_A + \cos 2\phi_B)] + (1/2)\beta_{aaa}(\sin\alpha - \sin^3\alpha)[(\cos 3\phi_A + \cos 3\phi_B) \pm (\cos\phi_A + \cos\phi_B)]$$

$ß_{zyy} = ß_{yzy} = (1/2)ß_{caa}\cos\alpha[2 - (\pm)(\cos2\phi_A + \cos2\phi_B)]$

$\quad - (1/2)ß_{aaa}\sin\alpha[(\cos3\phi_A + \cos3\phi_B) - (\pm)(\cos\phi_A + \cos\phi_B)]$

$ß_{xyz} = ß_{yxz} = \pm(1/2)ß_{caa}\sin^2\alpha(\sin2\phi_A + \sin2\phi_B)$

$\quad - (1/2)ß_{aaa}\sin\alpha\cos\alpha[(\sin3\phi_A + \sin3\phi_B) \pm (\sin\phi_A + \sin\phi_B)]$

$ß_{yzx} = ß_{zyx} = -(\pm1/2)ß_{caa}\sin^2\alpha(\sin2\phi_A + \sin2\phi_B)$

$\quad - (1/2)ß_{aaa}\sin\alpha\cos\alpha[(\sin3\phi_A + \sin3\phi_B) \pm (\sin\phi_A + \sin\phi_B)]$

$ß_{zxy} = ß_{xzy} = -(\pm1/2)ß_{caa}(2\cos^2\alpha - 1)s(\sin2\phi_A + \sin2\phi_B)$

$\quad - (1/2)ß_{aaa}\sin\alpha\cos\alpha[(\sin3\phi_A + \sin3\phi_B) - (\pm)(\sin\phi_A + \sin\phi_B)]$

$ß_{xyy} = ß_{yxy} = \pm(1/2)ß_{caa}\sin\alpha(\cos2\phi_A - \cos2\phi_B)$

$\quad - (1/2)ß_{aaa}\cos\alpha[(\cos3\phi_A - \cos3\phi_B) - (\pm)(\cos\phi_A - \cos\phi_B)]$

$ß_{xzz} = ß_{zxz} = \pm(1/2)ß_{caa}(\sin\alpha - 2\sin^3\alpha)(\cos2\phi_A - \cos2\phi_B)$

$\quad + (1/2)ß_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\phi_A - \cos3\phi_B) \pm (\cos\phi_A - \cos\phi_B)]$

$ß_{xxx} = -(\pm)ß_{caa}(\sin\alpha - \sin^3\alpha)(\cos2\phi_A - \cos2\phi_B)$

$\quad - (1/2)ß_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\phi_A - \cos3\phi_B) \pm (\cos\phi_A - \cos\phi_B)]$

$ß_{yyx} = -(1/2)ß_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\phi_A - \cos3\phi_B) \pm (\cos\phi_A - \cos\phi_B)]$

$ß_{zzx} = \pm ß_{caa}(\sin\alpha - \sin^3\alpha)(\cos2\phi_A - \cos2\phi_B)$

$\quad + (1/2)ß_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\phi_A - \cos3\phi_B) \pm (\cos\phi_A - \cos\phi_B)]$

$ß_{yxx} = ß_{xyx} = \pm(1/2)ß_{caa}\sin\alpha\cos\alpha(\sin2\phi_A - \sin2\phi_B)$

$\quad + (1/2)ß_{aaa}\cos^2\alpha[(\sin3\phi_A - \sin3\phi_B) \pm (\sin\phi_A - \sin\phi_B)]$

$ß_{yzz} = ß_{zyz} = -(\pm1/2)ß_{caa}\sin\alpha\cos\alpha(\sin2\phi_A - \sin2\phi_B)$

$\quad - (1/2)ß_{aaa}\sin^2\alpha[(\sin3\phi_A - \sin3\phi_B)\pm(\sin\phi_A - \sin\phi_B)]$

$ß_{yyy} = -(1/2)ß_{aaa}[(\sin3\phi_A - \sin3\phi_B) - (\pm)(\sin\phi_A - \sin\phi_B)]$

$ß_{xxy} = \pm ß_{caa}\sin\alpha\cos\alpha(\sin2\phi_A - \sin2\phi_B)$

$\quad -(1/2)ß_{aaa}\cos^2\alpha[(\sin3\phi_A - \sin3\phi_B) \pm (\sin\phi_A - \sin\phi_B)]$

$ß_{zzy} = -(\pm1/2)ß_{caa}\sin\alpha\cos\alpha(\sin2\phi_A - \sin2\phi_B)$

$\quad - (1/2)ß_{aaa}\sin^2\alpha[(\sin3\phi_A - \sin3\phi_B) - (\pm)(\sin\phi_A - \sin\phi_B)]$

を下に代入すると、2 個のメチル基の表式になる。（abc を xyz と変えた上で）

［対称 (a_1) 振動、c 軸に沿った振動］

(ppp) $\chi_{XXX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$

$\quad + (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(3\cos\chi + \cos3\chi)$

$\quad + (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\cos2\phi$

$\qquad + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$

$\quad + (1/4)\beta_{abc}\{[\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\sin2\phi$

$\qquad - 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\cos2\phi\}$

$\quad + (1/2)\beta_{acc}[(\cos\theta - \cos^3\theta)(3\cos\chi + \cos3\chi)\cos\phi - \sin^2\theta(\sin\chi + \sin3\chi)\sin\phi]$

$\quad + (1/2)\beta_{bcc}[(\cos\theta - \cos^3\theta)(3\cos\chi + \cos3\chi)\sin\phi + \sin^2\theta(\sin\chi + \sin3\chi)\cos\phi]$

$\chi_{XZZ} = (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi$

$\quad + (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\cos\chi\cos2\phi - \sin\theta\cos\theta\sin\chi\sin2\phi]$

$\quad + \beta_{abc}[(\sin\theta - \sin^3\theta)\cos\chi\sin2\phi + \sin\theta\cos\theta\sin\chi\cos2\phi]$

$- \beta_{acc}[(\cos\theta - 2\cos^3\theta)\cos\chi\cos\phi - \sin^2\theta\sin\chi\sin\phi]$

$- \beta_{bcc}[(\cos\theta - 2\cos^3\theta)\cos\chi\sin\phi - \sin^2\theta\sin\chi\cos\phi]$

$\chi_{ZXZ} = (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi$

$+ (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\cos\chi\cos2\phi - \sin\theta\cos\theta\sin\chi\sin2\phi]$

$+ \beta_{abc}[(\sin\theta - \sin^3\theta)\cos\chi\sin2\phi + \sin\theta\cos\theta\sin\chi\cos2\phi]$

$- \beta_{acc}[(\cos\theta - 2\cos^3\theta)\cos\chi\cos\phi - \sin^2\theta\sin\chi\sin\phi]$

$- \beta_{bcc}[(\cos\theta - 2\cos^3\theta)\cos\chi\sin\phi - \sin^2\theta\sin\chi\cos\phi]$

$\chi_{ZZX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$

$+ (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi$

$- (1/2)(\beta_{aac} - \beta_{bbc})\cos\chi\sin^3\theta\cos2\phi$

$- \beta_{abc}(2\sin\theta - \sin^3\theta)\cos\chi\sin2\phi$

$- 2\beta_{acc}(\cos\theta - 2\cos^3\theta)\cos\chi\cos\phi$

$- 2\beta_{bcc}(\cos\theta - 2\cos^3\theta)\cos\chi\sin\phi$

$\chi_{XZX} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$

$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\cos2\phi - \sin^2\theta\sin2\chi\sin2\phi]$

$- (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\sin2\phi + \sin^2\theta\sin2\chi\cos2\phi]$

$- (1/2)\beta_{acc}[(\sin\theta - 2\sin^3\theta)(1 + \cos2\chi)\cos\phi - \sin\theta\cos\theta\sin2\chi\sin\phi]$

$- (1/2)\beta_{bcc}[(\sin\theta - 2\sin^3\theta)(1 + \cos2\chi)\sin\phi + \sin\theta\cos\theta\sin2\chi\cos\phi]$

$\chi_{ZXX} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$

$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\cos2\phi - \sin^2\theta\sin2\chi\sin2\phi]$

$- (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\sin2\phi + \sin^2\theta\sin2\chi\cos2\phi]$

$- (1/2)\beta_{acc}[(\sin\theta - 2\sin^3\theta)(1 + \cos2\chi)\cos\phi - \sin\theta\cos\theta\sin2\chi\sin\phi]$

$- (1/2)\beta_{bcc}[(\sin\theta - 2\sin^3\theta)(1 + \cos2\chi)\sin\phi + \sin\theta\cos\theta\sin2\chi\cos\phi]$

$\chi_{XXZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$

$- (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$

$- (1/4)(\beta_{aac} - \beta_{bbc})\{[(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi + 2\cos^2\theta\sin2\chi\sin2\phi\}$

$- (1/2)\beta_{abc}\{[(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\chi]\sin2\phi - 2\cos^2\theta\sin2\chi\cos2\phi]\}$

$- \beta_{acc}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)\cos\phi - \sin\theta\cos\theta\sin2\chi\sin\phi]$

$- \beta_{bcc}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)\sin\phi + \sin\theta\cos\theta\sin2\chi\cos\phi]$

$\chi_{ZZZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$

$- (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\cos^3\theta$

$+ (1/2)(\beta_{aac} - \beta_{bbc})(\cos\theta - \cos^3\theta)\cos2\phi$

$+ \beta_{abc}(\cos\theta - \cos^3\theta)\sin2\phi$

$+ 2\beta_{acc}(\sin\theta - \sin^3\theta)\cos\phi$

$+ 2\beta_{bcc}(\sin\theta - \sin^3\theta)\sin\phi$

(spp) $\chi_{YXX} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi)$

$+ (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\cos2\phi + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi]$

$+ (1/2)\beta_{abc}[2(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\sin2\phi - \sin\theta\cos\theta(\cos\chi + \cos3\chi)\cos2\phi]$

$- (1/2)\beta_{acc}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\cos\phi + \sin^2\theta(\cos\chi + \cos3\chi)\sin\phi]$

$- (1/2)\beta_{bcc}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\sin\phi - \sin^2\theta(\cos\chi + \cos3\chi)\cos\phi]$

$\chi_{YZZ} = -(1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\sin\chi$

$- (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi\cos2\phi + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$- \beta_{abc}[(\sin\theta - \sin^3\theta)\sin\chi\sin2\phi - \sin\theta\cos\theta\cos\chi\cos2\phi]$

$+ \beta_{acc}[(\cos\theta - 2\cos^3\theta)\sin\chi\cos\phi - \cos^2\theta\cos\chi\sin\phi]$

$+ \beta_{bcc}[(\cos\theta - 2\cos^3\theta)\sin\chi\sin\phi + \cos^2\theta\cos\chi\cos\phi]$

$\chi_{YZX} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$

$+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$

$+ (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi - \sin^2\theta(1 + \cos2\chi)\cos2\phi]$

$+ (1/2)\beta_{acc}[(\sin\theta - 2\sin^3\theta)\cos2\chi\cos\phi + \sin2\theta(1 + \cos2\chi)\sin\phi]$

$+ (1/2)\beta_{bcc}[(\sin\theta - 2\sin^3\theta)\cos2\chi\sin\phi - \sin2\theta(1 + \cos2\chi)\cos\phi]$

$\chi_{YXZ} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$

$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta + \cos^3\theta)\sin2\chi\cos2\phi + 2\cos^2\theta\cos2\chi\sin2\phi]$

$- (1/2)\beta_{abc}[(\cos\theta + \cos^3\theta)\sin2\chi\sin2\phi - 2\cos^2\theta\cos2\chi\cos2\phi]$

$+ \beta_{acc}[(\sin\theta - \sin^3\theta)\sin2\chi\cos\phi + \sin\theta\cos\theta\cos2\chi\sin\phi]$

$+ \beta_{bcc}[(\sin\theta - \sin^3\theta)\sin2\chi\sin\phi - \sin\theta\cos\theta\cos2\chi\cos\phi]$

(ssp) $\chi_{YYX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$

$+ (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi)$

$+ (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(3\cos\chi + \cos3\chi) - (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\cos2\phi$

$- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$

$+ (1/4)\beta_{abc}\{[4\sin\theta\cos\chi - (2\sin\theta - \sin^3\theta)]\sin2\phi + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\cos2\phi\}$

$+ (1/2)\beta_{acc}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)\cos\phi + \sin^2\theta(\sin\chi + \sin3\chi)\sin\phi]$

$+ (1/2)\beta_{bcc}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)\sin\phi - \sin^2\theta(\sin\chi + \sin3\chi)\cos\phi]$

$\chi_{YYZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$

$- (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$

$- (1/4)(\beta_{aac} - \beta_{bbc})\{[(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi - 2\cos^2\theta\sin2\chi\sin2\phi\}$

$- (1/2)\beta_{abc}\{[(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos2\chi]\sin2\phi + \cos^2\theta\sin2\chi\cos2\phi\}$

$- \beta_{acc}[(\sin\theta - \sin^3\theta)(1 - \cos2\chi)\cos\phi + \sin\theta\cos\theta\sin2\chi\sin\phi]$

$- \beta_{bcc}[(\sin\theta - \sin^3\theta)(1 - \cos2\chi)\sin\phi - \sin\theta\cos\theta\sin2\chi\cos\phi]$

(psp) $\chi_{XYX} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi)$

$+ (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\cos2\phi + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi]$

$+ (1/4)\beta_{abc}[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\sin2\phi - 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\cos2\phi]$

$- (1/2)\beta_{acc}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\cos\phi + \sin^2\theta(\cos\chi + \cos3\chi)\sin\phi]$

$- (1/2)\beta_{bcc}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\sin\phi - \sin^2\theta(\cos\chi + \cos3\chi)\cos\phi]$

$\chi_{ZYZ} = -(1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\sin\chi$

$- (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi\cos2\phi + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$- \beta_{abc}[(\sin\theta - \sin^3\theta)\sin\chi\sin2\phi - \sin\theta\cos\theta\cos\chi\cos2\phi]$

$+ \beta_{acc}[(\cos\theta - 2\cos^3\theta)\sin\chi\cos\phi - \cos^2\theta\cos\chi\sin\phi]$

$+ \beta_{bcc}[(\cos\theta - 2\cos^3\theta)\sin\chi\sin\phi + \cos^2\theta\cos\chi\cos\phi]$

$$\chi_{XYZ} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$$
$$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta + \cos^3\theta)\sin2\chi\cos2\phi + 2\cos^2\theta\cos2\chi\sin2\phi]$$
$$- (1/2)\beta_{abc}[(\cos\theta + \cos^3\theta)\sin2\chi\sin2\phi - 2\cos^2\theta\cos2\chi\cos2\phi]$$
$$+ \beta_{acc}[(\sin\theta - \sin^3\theta)\sin2\chi\cos\phi + \sin\theta\cos\theta\cos2\chi\sin\phi]$$
$$+ \beta_{bcc}[(\sin\theta - \sin^3\theta)\sin2\chi\sin\phi - \sin\theta\cos\theta\cos2\chi\cos\phi]$$
$$\chi_{ZYX} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$$
$$+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi + \sin^2\theta(1 + \cos2\chi)\sin2\phi]$$
$$+ (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi - \sin^2\theta(1 + \cos2\chi)\cos2\phi]$$
$$+ \beta_{acc}[(\sin\theta - \sin^3\theta)\sin2\chi\cos\phi + \sin\theta\cos\theta\cos2\chi\sin\phi]$$
$$+ \beta_{bcc}[(\sin\theta - \sin^3\theta)\sin2\chi\sin\phi - \sin\theta\cos\theta\cos2\chi\cos\phi]$$

(sps) $$\chi_{YXY} = (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi)$$
$$- (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\cos2\phi - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi]$$
$$- (1/4)\beta_{abc}[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\sin2\phi + 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\cos2\phi]$$
$$+ (1/2)\beta_{acc}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)\cos\phi - \sin^2\theta(\sin\chi - \sin3\chi)\sin\phi]$$
$$+ (1/2)\beta_{bcc}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)\sin\phi + \sin^2\theta(\sin\chi - \sin3\chi)\cos\phi]$$
$$\chi_{YZY} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$$
$$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\cos2\phi + \sin^2\theta\sin2\chi\sin2\phi]$$
$$- (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\sin2\phi - \sin^2\theta\sin2\chi\cos2\phi]$$
$$- (1/2)\beta_{acc}[(\sin\theta - 2\sin^3\theta)(1 - \cos2\chi)\cos\phi + \sin\theta\cos\theta\sin2\chi\sin2\phi]$$
$$- (1/2)\beta_{bcc}[(\sin\theta - 2\sin^3\theta)(1 - \cos2\chi)\sin\phi - \sin\theta\cos\theta\sin2\chi\cos2\phi]$$

(pps) $$\chi_{XXY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi$$
$$- (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi)$$
$$+ (1/8)(\beta_{aac} - \beta_{bbc})\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi) - \sin\theta(3\sin\chi - \sin3\chi)\cos2\phi]$$
$$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$$
$$+ (1/4)\beta_{abc}\{[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi) - 4\sin\theta\cos\chi]\sin2\phi$$
$$+ 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\cos2\phi\}$$
$$- (1/2)\beta_{acc}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\cos\phi - \sin^2\theta(\cos\chi - \cos3\chi)\sin\phi]$$
$$- (1/2)\beta_{bcc}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\sin\phi + \sin^2\theta(\cos\chi - \cos3\chi)\cos\phi]$$
$$\chi_{ZZY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi$$
$$- (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\sin\chi$$
$$+ (1/2)(\beta_{aac} - \beta_{bbc})\sin^3\theta\sin\chi\cos2\phi$$
$$+ \beta_{abc} \sin^3\theta\sin\chi\sin2\phi$$
$$+ 2\beta_{acc}(\cos\theta - \cos^3\theta)\sin\chi\cos\phi$$
$$+ 2\beta_{bcc}(\cos\theta - \cos^3\theta)\sin\chi\sin\phi$$
$$\chi_{XZY} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$$
$$+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$$
$$+ (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi + \sin^2\theta(1 - \cos2\chi)\cos2\phi]$$
$$+ (1/2)\beta_{acc}[(\sin\theta - 2\sin^3\theta)\sin2\chi\cos\phi - \sin\theta\cos\theta(1 - \cos2\chi)\sin\phi]$$

$+ (1/2)\beta_{bcc}[(\sin\theta - 2\sin^3\theta)\sin2\chi\sin\phi + \sin\theta\cos\theta(1 - \cos2\chi)\cos\phi]$

$\chi_{ZXY} = (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)\sin2\chi$

$+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi - \sin^2\theta(1 - \cos2\chi)\sin2\phi]$

$+ (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi + \sin^2\theta(1 - \cos2\chi)\cos2\phi]$

$+ (1/2)\beta_{acc}[(\sin\theta - 2\sin^3\theta)\sin2\chi\cos\phi - \sin\theta\cos\theta(1 - \cos2\chi)\sin\phi]$

$+ (1/2)\beta_{bcc}[(\sin\theta - 2\sin^3\theta)\sin2\chi\sin\phi + \sin\theta\cos\theta(1 - \cos2\chi)\cos\phi]$

(pss) $\chi_{XYY} = (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi)$

$- (1/8)(\beta_{aac} - \beta_{bbc})[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\cos2\phi - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi]$

$- (1/4)\beta_{abc}[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)\sin2\phi + 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\cos2\phi]$

$+ (1/2)\beta_{acc}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)\cos\phi - \sin^2\theta(\sin\chi - \sin3\chi)\sin\phi]$

$+ (1/2)\beta_{bcc}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)\sin\phi + \sin^2\theta(\sin\chi - \sin3\chi)\cos\phi]$

$\chi_{ZYY} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$

$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\cos2\phi + \sin^2\theta\sin2\chi\sin2\phi]$

$- (1/2)\beta_{abc}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\sin2\phi - \sin^2\theta\sin2\chi\cos2\phi]$

$- (1/2)\beta_{acc}[(\sin\theta - 2\sin^3\theta)(1 - \cos2\chi)\cos\phi + \sin\theta\cos\theta\sin2\chi\sin\phi]$

$- (1/2)\beta_{bcc}[(\sin\theta - 2\sin^3\theta)(1 - \cos2\chi)\sin\phi - \sin\theta\cos\theta\sin2\chi\cos\phi]$

(sss) $\chi_{YYY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi$

$- (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(3\sin\chi - \sin3\chi)$

$- (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(\sin\chi + \sin3\chi) - (\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)]\cos2\phi$

$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$

$+ (1/4)\beta_{abc}\{[4(\sin\theta - \sin^3\theta)\sin\chi - (2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\sin2\phi$

$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\cos2\phi\}$

$- (1/2)\beta_{acc}[(\cos\theta - \cos^3\theta)(3\sin\chi - \sin3\chi)\cos\phi + \sin^2\theta(\cos\chi - \cos3\chi)\sin\phi]$

$- (1/2)\beta_{bcc}[(\cos\theta - \cos^3\theta)(3\sin\chi - \sin3\chi)\sin\phi - \sin^2\theta(\cos\chi - \cos3\chi)\cos\phi]$

［逆対称 (b_1) 振動、a 軸に沿った振動］

(ppp) $\chi_{XXX} = -(1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi - \cos3\chi)(1 - \cos2\phi)]$

$- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$

$+ (1/4)\beta_{bca}\{[\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\sin2\phi$

$- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\cos2\phi\}$

$+ (1/16)\beta_{aaa}[-(\cos\theta - \cos^3\theta)(3\cos\chi + \cos3\chi)(3\cos\phi + \cos3\phi)$

$+ 4\cos\theta(3\cos\chi\cos\phi + \cos3\chi\cos3\phi) - 4(3\sin\chi\sin\phi + \sin3\chi\sin3\phi)$

$+ 3\sin^2\theta(\sin\chi + \sin3\chi)(\sin\phi + \sin3\phi)]$

$+ (1/16)\beta_{bba}[-(\cos\theta - \cos^3\theta)(3\cos\chi + \cos3\chi)(\cos\phi - \cos3\phi)$

$+ 4\cos\theta(\cos\chi\cos\phi - \cos3\chi\cos3\phi) - 4(\sin\chi\sin\phi - \sin3\chi\sin3\phi)$

$+ \sin^2\theta(\sin\chi + \sin3\chi)(\sin\phi - 3\sin3\phi)]$

$+ (1/4)\beta_{cca}[(\cos\theta - \cos^3\theta)(3\cos\chi + \cos3\chi)\cos\phi - \sin^2\theta(\sin\chi + \sin3\chi)\sin\phi]$

$\chi_{XZZ} = (1/2)\beta_{caa}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]$

$$+ (1/2)\beta_{bca}[(\sin\theta - 2\sin^3\theta)\cos\chi\sin 2\phi + \sin\theta\cos\theta\sin\chi(1 + \cos 2\phi)]$$
$$+ (1/4)\beta_{aaa}[(\cos\theta - \cos^3\theta)\cos\chi(3\cos\phi + \cos 3\phi) - \sin^2\theta\sin\chi(\sin\phi + \sin 3\phi)]$$
$$+ (1/4)\beta_{bba}[(\cos\theta - \cos^3\theta)\cos\chi(\cos\phi - \cos 3\phi) + \sin^2\theta\sin\chi(\sin\phi + \sin 3\phi)]$$
$$- \beta_{cca}(\cos\theta - \cos^3\theta)\cos\chi\cos\phi$$

$$\chi_{ZXZ} = (1/2)\beta_{caa}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos 2\phi) - \sin\theta\cos\theta\sin\chi\sin 2\phi]$$
$$+ (1/2)\beta_{bca}[(\sin\theta - 2\sin^3\theta)\cos\chi\sin 2\phi + \sin\theta\cos\theta\sin\chi(1 + \cos 2\phi)]$$
$$+ (1/4)\beta_{aaa}[(\cos\theta - \cos^3\theta)\cos\chi(3\cos\phi + \cos 3\phi) - \sin^2\theta\sin\chi(\sin\phi + \sin 3\phi)]$$
$$+ (1/4)\beta_{bba}[(\cos\theta - \cos^3\theta)\cos\chi(\cos\phi - \cos 3\phi) + \sin^2\theta\sin\chi(\sin\phi + \sin 3\phi)]$$
$$- \beta_{cca}(\cos\theta - \cos^3\theta)\cos\chi\cos\phi$$

$$\chi_{ZZX} = \beta_{caa}[(\sin\theta - \sin^3\theta)\cos\chi(1 + \cos 2\phi) - \sin\theta\cos\theta\sin\chi\sin 2\phi]$$
$$+ \beta_{bca}[(\sin\theta - \sin^3\theta)\cos\chi\sin 2\phi - \sin\theta\cos\theta\sin\chi(1 - \cos 2\phi)]$$
$$+ (1/4)\beta_{aaa}[(\cos\theta - \cos^3\theta)\cos\chi(3\cos\phi + \cos 3\phi) - \sin^2\theta\sin\chi(\sin\phi + \sin 3\phi)]$$
$$+ (1/4)\beta_{bba}[(\cos\theta - \cos^3\theta)\cos\chi(\cos\phi - \cos 3\phi) - \sin^2\theta\sin\chi(3\sin\phi - \sin 3\phi)]$$
$$+ \beta_{cca}[\cos^3\theta\cos\chi\cos\phi - \cos^2\theta\sin\chi\sin\phi]$$

$$\chi_{ZXX} = (1/4)\beta_{caa}\{2[\cos\theta(1 + \cos 2\chi\cos 2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos 2\chi)(1 + \cos 2\phi)]$$
$$+ (1 - 3\cos^2\theta)\sin 2\chi\sin 2\phi\}$$
$$- (1/4)\beta_{bca}\{2[(\cos\theta - \cos^3\theta) - \cos^3\theta\cos 2\chi]\sin 2\phi - [\sin^2\theta - (1 - 3\cos^2\theta)\cos 2\phi]\sin 2\chi\}$$
$$+ (1/8)\beta_{aaa}[(\sin\theta - \sin^3\theta)(1 + \cos 2\chi)(3\cos\phi + \cos 3\phi) + \sin\theta(1 - \cos 2\chi)(\cos\phi - \cos 3\phi)$$
$$- 2\sin\theta\cos\theta\sin 2\chi(\sin\phi + \sin 3\phi)]$$
$$+ (1/8)\beta_{bba}[(\sin\theta - \sin^3\theta)(1 + \cos 2\chi)(\cos\phi - \cos 3\phi) - \sin\theta(1 - \cos 2\chi)(\cos\phi - \cos 3\phi)$$
$$- 2\sin\theta\cos\theta\sin 2\chi(\sin\phi - \sin 3\phi)]$$
$$+ (1/2)\beta_{cca}[-(\sin\theta - \sin^3\theta)(1 + \cos 2\chi)\cos\phi + \sin\theta\cos\theta\sin 2\chi\sin\phi]$$

$$\chi_{XZX} = (1/4)\beta_{caa}\{2[\cos\theta(1 + \cos 2\chi\cos 2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos 2\chi)(1 + \cos 2\phi)]$$
$$+ (1 - 3\cos^2\theta)\sin 2\chi\sin 2\phi\}$$
$$- (1/4)\beta_{bca}\{2[(\cos\theta - \cos^3\theta) - \cos^3\theta\cos 2\chi]\sin 2\phi - [\sin^2\theta - (1 - 3\cos^2\theta)\cos 2\phi]\sin 2\chi\}$$
$$+ (1/8)\beta_{aaa}[(\sin\theta - \sin^3\theta)(1 + \cos 2\chi)(3\cos\phi + \cos 3\phi) + \sin\theta(1 - \cos 2\chi)(\cos\phi - \cos 3\phi)$$
$$- 2\sin\theta\cos\theta\sin 2\chi(\sin\phi + \sin 3\phi)]$$
$$+ (1/8)\beta_{bba}[(\sin\theta - \sin^3\theta)(1 + \cos 2\chi)(\cos\phi - \cos 3\phi) - \sin\theta(1 - \cos 2\chi)(\cos\phi - \cos 3\phi)$$
$$- 2\sin\theta\cos\theta\sin 2\chi(\sin\phi - \sin 3\phi)]$$
$$+ (1/2)\beta_{cca}[-(\sin\theta - \sin^3\theta)(1 + \cos 2\chi)\cos\phi + \sin\theta\cos\theta\sin 2\chi\sin\phi]$$

$$\chi_{XXZ} = -(1/2)\beta_{caa}[(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)(1 + \cos 2\phi) - \sin^2\theta\sin 2\chi\sin 2\phi]$$
$$- (1/2)\beta_{bca}[(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)\sin 2\phi + \sin^2\theta\sin 2\chi(1 + \cos 2\phi)]$$
$$+ (1/8)\beta_{aaa}[\sin\theta(1 - \cos 2\chi)(\cos\phi - \cos 3\phi) + (\sin\theta - \sin^3\theta)(1 + \cos 2\chi)(3\cos\phi + \cos 3\phi)$$
$$- 2\sin\theta\cos\theta\sin 2\chi\,(\sin\phi + \sin 3\phi)]$$
$$+ (1/8)\beta_{bba}[\sin\theta(1 - \cos 2\chi)(3\cos\phi + \cos 3\phi) + (\sin\theta - \sin^3\theta)(1 + \cos 2\chi)(\cos\phi - \cos 3\phi)$$
$$+ 2\sin\theta\cos\theta\sin 2\chi\,(\sin\phi + \sin 3\phi)]$$
$$+ (1/2)\beta_{cca}\sin^3\theta(1 + \cos 2\chi)\cos\phi$$

$$\chi_{ZZZ} = \beta_{caa}(\cos\theta - \cos^3\theta)(1 + \cos 2\phi)$$
$$+ \beta_{bca}[(\cos\theta - \cos^3\theta)\sin 2\phi$$
$$+ (1/4)\beta_{aaa}\sin^3\theta(3\cos\phi + \cos 3\phi)$$

$+ (1/4)\beta_{bba} \sin^3\theta(\cos\phi - \cos3\phi)$

$+\beta_{cca}(\sin\theta - \sin^3\theta)\cos\phi$

(spp) $\chi_{YXX} = (1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)]$

$+ 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$

$- (1/4)\beta_{bca}\{[2\sin\theta\sin\chi - (2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\sin2\phi + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi\cos2\phi)\}$

$+ (1/16)\beta_{aaa}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)(3\cos\phi + \cos3\phi) - 4\cos\theta(\sin\chi\cos\phi + \sin3\chi\cos3\phi)$

$+ \sin^2\theta(\cos\chi + 3\cos3\chi)(\sin\phi + \sin3\phi) - 4(\cos\chi\sin\phi + \cos3\chi\sin3\phi)]$

$+ (1/16)\beta_{bba}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)(\cos\phi - \cos3\phi) + 4\cos\theta(\sin\chi\cos\phi + \sin3\chi\cos3\phi)$

$- \sin^2\theta(\cos\chi - \cos3\chi)(\sin\phi + \sin3\phi) + 4\cos^2\theta(\cos\chi\sin\phi + \cos3\chi\sin3\phi)]$

$+ (1/4)\beta_{cca}[-(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\cos\phi + \sin^2\theta(\cos\chi - \cos3\chi)\sin\phi]$

$\chi_{YZZ} = -(1/2)\beta_{caa}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$

$- (1/2)\beta_{bca}[(\sin\theta - 2\sin^3\theta)\sin2\chi\sin2\phi - \sin\theta\cos\theta\cos\chi(1 + \cos2\phi)]$

$- (1/4)\beta_{aaa}[(\cos\theta - \cos^3\theta)\sin\chi(3\cos\phi + \cos3\phi) + \sin^2\theta\cos\chi(\sin\phi + \sin3\phi)]$

$- (1/4)\beta_{bba}[(\cos\theta - \cos^3\theta)\sin\chi(\cos\phi - \cos3\phi) - \sin^2\theta\cos\chi(\sin\phi + \sin3\phi)]$

$+ \beta_{cca}(\cos\theta - \cos^3\theta)\sin\chi\cos\phi$

$\chi_{YZX} = (1/4)\beta_{caa}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$

$+ (1/4)\beta_{bca}[2\cos^3\theta\sin2\chi\sin2\phi - \sin^2\theta(1 - \cos2\chi)(1 - \cos2\phi) + 2\cos^2\theta(1 + \cos2\chi\cos2\phi)]$

$+ (1/8)\beta_{aaa}[\sin\theta\sin2\chi(\cos\phi - \cos3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(3\cos\phi + \cos3\phi)]$

$- (1/8)\beta_{bba}(2\sin\theta - \sin^3\theta)\sin2\chi(\cos\phi - \cos3\phi)$

$+ (1/2)\beta_{cca}[(\sin\theta - \sin^3\theta)\sin2\chi\cos\phi - \sin\theta\cos\theta(1 - \cos2\chi)\sin\phi]$

$\chi_{YXZ} = (1/2)\beta_{caa}[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$

$+ (1/2)\beta_{bca}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi - \sin^2\theta\cos2\chi(1 + \cos2\phi)]$

$+ (1/8)\beta_{aaa}[\sin\theta\sin2\chi(\cos\phi - \cos3\phi) - [(\sin\theta - \sin^3\theta)\sin2\chi(3\cos\phi + \cos3\phi)$

$- 2\sin\theta\cos\theta\cos2\chi(\sin\phi + \sin3\phi)]$

$+ (1/8)\beta_{bba}[\sin\theta\sin2\chi(3\cos\phi + \cos3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(\cos\phi - \cos3\phi)$

$+ 2\sin\theta\cos\theta\cos2\chi(\sin\phi + \sin3\phi)]$

$- (1/2)\beta_{cca}\sin^3\theta\sin2\chi\cos\phi$

(ssp) $\chi_{YYX} = (1/4)\beta_{caa}\{[-(\sin\theta - \sin^3\theta)(1 + \cos2\phi) + \sin\theta(1 - \cos2\phi)](\cos\chi - \cos3\chi)$

$+ 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\}$

$- (1/4)\beta_{bca}\{[(2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\sin2\phi - 2\sin^2\theta(\sin\chi + \sin3\chi)\cos2\phi\}$

$+ (1/16)\beta_{aaa}[-(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)(3\cos\phi + \cos3\phi) + 4\cos\theta(\cos\chi\cos\phi - \cos3\chi\cos3\phi)$

$+ \sin^2\theta(\sin\chi - 3\sin3\chi)(\sin\phi + \sin3\phi) - (\sin\chi\sin\phi - \sin3\chi\sin3\phi)]$

$+ (1/16)\beta_{bba}[-(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)(\cos\phi - \cos3\phi) + 4\cos\theta(3\cos\chi\cos\phi + \cos3\chi\cos3\phi)$

$- \sin^2\theta(\sin\chi + \sin3\chi)(\sin\phi + \sin3\phi) - \cos^2\theta(3\sin\chi\sin\phi + \sin3\chi\sin3\phi)]$

$+ (1/4)\beta_{cca}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)\cos\phi - \sin^2\theta(3\sin\chi - \sin3\chi)\sin\phi]$

$\chi_{YYZ} = -(1/2)\beta_{caa}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$

$- (1/2)\beta_{bca}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\sin2\phi - \sin^2\theta\sin2\chi(1 + \cos2\phi)]$

$+ (1/8)\beta_{aaa}[\sin\theta(1 + \cos2\chi)(\cos\phi - \cos3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\chi)(3\cos\phi + \cos3\phi)$

$$+ 2\sin\theta\cos\theta\sin2\chi(\sin\phi + \sin3\phi)]$$

$$+ (1/8)\beta_{bba}[\sin\theta(1 + \cos2\chi)(3\cos\phi + \cos3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\chi)(\cos\phi - \cos3\phi)$$

$$- 2\sin\theta\cos\theta\sin2\chi(\sin\phi + \sin3\phi)]$$

$$+ (1/2)\beta_{cca}\sin^3\theta(1 - \cos2\chi)\cos\phi$$

(psp) $$\chi_{XYX} = (1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)]$$

$$+ 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}$$

$$- (1/4)\beta_{bca}\{[2\sin\theta\sin\chi - (2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\sin2\phi + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi\cos2\phi)\}$$

$$+ (1/16)\beta_{aaa}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)(3\cos\phi + \cos3\phi) - 4\cos\theta(\sin\chi\cos\phi + \sin3\chi\cos3\phi)$$

$$+ \sin^2\theta(\cos\chi + 3\cos3\chi)(\sin\phi + \sin3\phi) - 4(\cos\chi\sin\phi + \cos3\chi\sin3\phi)]$$

$$+ (1/16)\beta_{bba}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)(\cos\phi - \cos3\phi) + 4\cos\theta(\sin\chi\cos\phi + \sin3\chi\cos3\phi)$$

$$- \sin^2\theta(\cos\chi - \cos3\chi)(\sin\phi + \sin3\phi) + 4\cos^2\theta\ (\cos\chi\sin\phi + \cos3\chi\sin3\phi)]$$

$$+ (1/4)\beta_{cca}[-(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\cos\phi + \sin^2\theta(\cos\chi - \cos3\chi)\sin\phi]$$

$$\chi_{ZYZ} = -(1/2)\beta_{caa}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$- (1/2)\beta_{bca}[(\sin\theta - 2\sin^3\theta)\sin\chi\sin2\phi - \sin\theta\cos\theta\cos\chi(1 + \cos2\phi)]$$

$$- (1/4)\beta_{aaa}[(\cos\theta - \cos^3\theta)\sin\chi(3\cos\phi + \cos3\phi) + \sin^2\theta\cos\chi(\sin\phi + \sin3\phi)]$$

$$- (1/4)\beta_{bba}[(\cos\theta - \cos^3\theta)\sin\chi(\cos\phi - \cos3\phi) - \sin^2\theta\cos\chi(\sin\phi + \sin3\phi)]$$

$$+ \beta_{cca}(\cos\theta - \cos^3\theta)\sin\chi\cos\phi$$

$$\chi_{XYZ} = (1/2)\beta_{caa}[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]$$

$$+ (1/2)\beta_{bca}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi - \sin^2\theta\cos2\chi(1 + \cos2\phi)]$$

$$+ (1/8)\beta_{aaa}[\sin\theta\sin2\chi(\cos\phi - \cos3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(3\cos\phi + \cos3\phi)$$

$$- 2\sin\theta\cos\theta\cos2\chi(\sin\phi + \sin3\phi)]$$

$$+ (1/8)\beta_{bba}[\sin\theta\sin2\chi(3\cos\phi + \cos3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(\cos\phi - \cos3\phi)$$

$$+ 2\sin\theta\cos\theta\cos2\chi(\sin\phi + \sin3\phi)]$$

$$- (1/2)\beta_{cca}\sin^3\theta\sin2\chi\cos\phi$$

$$\chi_{ZYX} = (1/4)\beta_{caa}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\ \sin2\phi\}$$

$$+ (1/4)\beta_{bca}[2\cos^3\theta\sin2\chi\sin2\phi - \sin^2\theta(1 - \cos2\chi)(1 - \cos2\phi) + 2(1 + \cos2\chi\cos2\phi)]$$

$$+ (1/8)\beta_{aaa}[\sin\theta\sin2\chi(\cos\phi - \cos3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(3\cos\phi + \cos3\phi)$$

$$- 2\sin\theta\cos\theta\cos2\chi(\sin\phi + \sin3\phi)]$$

$$+ (1/8)\beta_{bba}[\sin\theta\sin2\chi(\cos\phi - \cos3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(3\cos\phi + \cos3\phi)$$

$$- 2\sin\theta\cos\theta\cos2\chi(\sin\phi + \sin3\phi)]$$

$$+ (1/2)\beta_{cca}[(\sin\theta - \sin^3\theta)\sin2\chi\cos\phi - \sin\theta\cos\theta(1 - \cos2\chi)\sin\phi]$$

(sps) $$\chi_{YXY} = -(1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)]$$

$$+ 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$$

$$+ (1/4)\beta_{bca}\{[2\sin\theta\cos\chi - (2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\sin2\phi - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi\cos2\phi)\}$$

$$+ (1/16)\beta_{aaa}[-(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)(3\cos\phi + \cos3\phi) + 4\cos\theta(\cos\chi\cos\phi - \cos3\chi\cos3\phi)$$

$$+ \sin^2\theta(\sin\chi - 3\sin3\chi)(\sin\phi + \sin3\phi) - 4(\sin\chi\sin\phi - \sin3\chi\sin3\phi)]$$

$$+ (1/16)\beta_{bba}[-(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)(\cos\phi - \cos3\phi) - 4\cos\theta(\cos\chi\cos\phi - \cos3\chi\cos3\phi)$$

$$- \sin^2\theta(\sin\chi + \sin3\chi)(\sin\phi + \sin3\phi) + 4\cos^2\theta(\sin\chi\sin\phi - \sin3\chi\sin3\phi)]$$

$$+ (1/4)\beta_{cca}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)\cos\phi + \sin^2\theta(\sin\chi + \sin3\chi)\sin\phi]$$

$$\chi_{YZY} = (1/4)\beta_{caa}\{2[\cos\theta(1 - \cos2\phi\cos2\chi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)] - (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$
$$- (1/4)\beta_{bca}\{2[(\cos\theta - \cos^3\theta) - \cos^3\theta\cos2\chi]\sin2\phi + [\sin^2\theta - (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$$
$$+ (1/8)\beta_{aaa}[\sin\theta(1 + \cos2\chi)(\cos\phi - \cos3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\chi)(3\cos\phi + \cos3\phi) + 2\sin\theta\cos\theta\sin2\chi(\sin\phi + \sin3\phi)]$$
$$+ (1/8)\beta_{bba}[-\sin\theta(1 + \cos2\chi)(\cos\phi - \cos3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\chi)(\cos\phi - \cos3\phi) + 2\sin\theta\cos\theta\sin2\chi(\sin\phi - \sin3\phi)]$$
$$- (1/2)\beta_{cca}[(\sin\theta - \sin^3\theta)(1 - \cos2\chi)\cos\phi - \sin\theta\cos\theta\sin2\chi\sin\phi]$$

(pps) $$\chi_{XXY} = (1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(1 + \cos2\phi) - \sin\theta(1 - \cos2\phi)](\sin\chi + \sin3\chi) + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$$
$$+ (1/4)\beta_{bca}[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\sin2\phi + 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\cos2\phi]$$
$$+ (1/16)\beta_{aaa}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)(3\cos\phi + \cos3\phi) - 4\cos\theta(\sin\chi\cos\phi + \sin3\chi\cos3\phi) + \sin^2\theta(\cos\chi + 3\cos3\chi)(\sin\phi + \sin3\phi) - 4(\cos\chi\sin\phi + \cos3\chi\sin3\phi)]$$
$$+ (1/16)\beta_{bba}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)(\cos\phi - \cos3\phi) - 4\cos\theta(3\sin\chi\cos\phi - \sin3\chi\cos3\phi) - \sin^2\theta(\cos\chi - \cos3\chi)(\sin\phi + \sin3\phi) - 4\cos^2\theta(3\cos\chi\sin\phi - \cos3\chi\sin3\phi)]$$
$$- (1/4)\beta_{cca}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\cos\phi + \sin^2\theta(3\cos\chi + \cos3\chi)\sin\phi]$$

$$\chi_{ZZY} = -\beta_{caa}[(\sin\theta - \sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$
$$-\beta_{bca}[(\sin\theta - \sin^3\theta)\sin\chi\sin2\phi + \sin\theta\cos\theta\cos\chi(1 - \cos2\phi)]$$
$$- (1/4)\beta_{aaa}[(\cos\theta - \cos^3\theta)\sin\chi (3\cos\phi + \cos3\phi) + \sin^2\theta\cos\chi(\sin\phi + \sin3\phi)]$$
$$- (1/4)\beta_{bba}[(\cos\theta - \cos^3\theta)\sin\chi(\cos\phi - \cos3\phi) + \sin^2\theta\cos\chi(3\sin\phi - \sin3\phi)]$$
$$- \beta_{cca}[\cos^3\theta\sin\chi\cos\phi + \cos^2\theta\cos\chi\sin\phi]$$

$$\chi_{ZXY} = (1/4)\beta_{caa}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$
$$+ (1/4)\beta_{bca}[2\cos^3\theta\sin2\chi\sin2\phi + \sin^2\theta(1 + \cos2\chi)(1 - \cos2\phi) - 2(1 - \cos2\chi\cos2\phi)]$$
$$- (1/4)\beta_{aaa}[\sin\theta\sin2\chi(\cos\phi - \cos3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(3\cos\phi + \cos3\phi) - 2\sin\theta\cos\theta\cos2\chi(\sin\phi + \sin3\phi)]$$
$$- (1/4)\beta_{bba}\{\sin\theta\sin2\chi(\cos\phi - \cos3\phi) + (\sin\theta - \sin^3\theta)\sin2\chi(\cos\phi - \cos3\phi) + 2\sin\theta\cos\theta[2\sin\phi + \cos2\chi(\sin\phi - \sin3\phi)]\}$$
$$+ (1/2)\beta_{cca}[(\sin\theta - \sin^3\theta)\sin2\chi\cos\phi + \sin\theta\cos\theta(1 + \cos2\chi)\sin\phi]$$

$$\chi_{XZY} = (1/4)\beta_{caa}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$
$$+ (1/4)\beta_{bca}[2\cos^3\theta\sin2\chi\sin2\phi + \sin^2\theta(1 + \cos2\chi)(1 - \cos2\phi) - 2(1 - \cos2\chi\cos2\phi)]$$
$$- (1/4)\beta_{aaa}[\sin\theta\sin2\chi(\cos\phi - \cos3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(3\cos\phi + \cos3\phi) - 2\sin\theta\cos\theta\cos2\chi(\sin\phi + \sin3\phi)]$$
$$- (1/4)\beta_{bba}\{\sin\theta\sin2\chi(\cos\phi - \cos3\phi) + (\sin\theta - \sin^3\theta)\sin2\chi(\cos\phi - \cos3\phi) + 2\sin\theta\cos\theta[2\sin\phi + \cos2\chi(\sin\phi - \sin3\phi)]\}$$
$$+ (1/2)\beta_{cca}[(\sin\theta - \sin^3\theta)\sin2\chi\cos\phi + \sin\theta\cos\theta(1 + \cos2\chi)\sin\phi]$$

(pss) $$\chi_{XYY} = -(1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$$

$$+ (1/4)\beta_{bca}\{[2\sin\theta\cos\chi - (2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\sin2\phi - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi\cos2\phi)\}$$
$$+ (1/16)\beta_{aaa}[-(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)(3\cos\phi + \cos3\phi) + 4\cos\theta(\cos\chi\cos\phi - \cos3\chi\cos3\phi)$$
$$+ \sin^2\theta(\sin\chi - 3\sin3\chi)(\sin\phi + \sin3\phi) - 4(\sin\chi\sin\phi - \sin3\chi\sin3\phi)]$$
$$+ (1/16)\beta_{bba}[-(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)(\cos\phi - \cos3\phi) - 4\cos\theta(\cos\chi\cos\phi - \cos3\chi\cos3\phi)$$
$$- \sin^2\theta(\sin\chi + \sin3\chi)(\sin\phi + \sin3\phi) + 4\cos^2\theta(\sin\chi\sin\phi - \sin3\chi\sin3\phi)]$$
$$+ (1/4)\beta_{cca}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)\cos\phi + \sin^2\theta(\sin\chi + \sin3\chi)\sin\phi]$$
$$\chi_{ZYY} = (1/4)\beta_{caa}\{2[\cos\theta(1 - \cos2\phi\cos2\chi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)]$$
$$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$
$$- (1/4)\beta_{bca}\{2[(\cos\theta - \cos^3\theta) - \cos^3\theta\cos2\chi]\sin2\phi + [\sin^2\theta - (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$$
$$+ (1/8)\beta_{aaa}[\sin\theta(1 + \cos2\chi)(\cos\phi - \cos3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\chi)(3\cos\phi + \cos3\phi)$$
$$+ 2\sin\theta\cos\theta\sin2\chi(\sin\phi + \sin3\phi)]$$
$$+ (1/8)\beta_{bba}[-\sin\theta(1 + \cos2\chi)(\cos\phi - \cos3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\chi)(\cos\phi - \cos3\phi)$$
$$+ 2\sin\theta\cos\theta\sin2\chi(\sin\phi - \sin3\phi)]$$
$$- (1/2)\beta_{cca}[(\sin\theta - \sin^3\theta)(1 - \cos2\chi)\cos\phi - \sin\theta\cos\theta\sin2\chi\sin\phi]$$

(sss) $$\chi_{YYY} = (1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi + \sin3\chi)(1 - \cos2\phi)]$$
$$+ 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$$
$$+ (1/4)\beta_{bca}\{[4(\sin\theta - \sin^3\theta)\sin\chi -(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\sin2\phi$$
$$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\cos2\phi\}$$
$$+ (1/16)\beta_{aaa}[(\cos\theta - \cos^3\theta)(3\sin\chi - \sin3\chi)(3\cos\phi + \cos3\phi) - 4\cos\theta(3\sin\chi\cos\phi - \sin3\chi\cos3\phi)$$
$$+ 3\sin^2\theta(\cos\chi - \cos3\chi)(\sin\phi + \sin3\phi) - 4(3\cos\chi\sin\phi - \cos3\chi\sin3\phi)]$$
$$+ (1/16)\beta_{bba}[(\cos\theta - \cos^3\theta)(3\sin\chi - \sin3\chi)(\cos\phi - \cos3\phi) - 4\cos\theta(\sin\chi\cos\phi + \sin3\chi\cos3\phi)$$
$$+ \sin^2\theta(\cos\chi - \cos3\chi)(\sin\phi - 3\sin3\phi) - 4(\cos\chi\sin\phi + \cos3\chi\sin3\phi)]$$
$$- (1/4)\beta_{cca}[(\cos\theta - \cos^3\theta)(3\sin\chi - \sin3\chi)\cos\phi + \sin^2\theta(\cos\chi - \cos3\chi)\sin\phi]$$

［面外 (b_2) 振動、b 軸に沿った振動］

(ppp) $$\chi_{XXX} = -(1/4)\beta_{cbb}\{[(\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)(1 - \cos2\phi) + \sin\theta(\cos\chi - \cos3\chi)(1 + \cos2\phi)]$$
$$+ 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi\}$$
$$+ (1/4)\beta_{cab}\{[\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\sin2\phi$$
$$- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\cos2\phi\}$$
$$+ (1/16)\beta_{aab}[-(\cos\theta - \cos^3\theta)(3\cos\chi + \cos3\chi)(\sin\phi + \sin3\phi) + 4\cos\theta(\cos\chi\sin\phi + \cos3\chi\sin3\phi)$$
$$+ 4(3\sin\chi\cos\phi + \sin3\chi\cos3\phi) - \sin^2\theta(\sin\chi + \sin3\chi)(\cos\phi + \cos3\phi)]$$
$$+ (1/16)\beta_{bbb}[-(\cos\theta - \cos^3\theta)(3\cos\chi + \cos3\chi)(3\sin\phi - \sin3\phi) + 4\cos\theta(3\cos\chi\sin\phi - \cos3\chi\sin3\phi)$$
$$+ 4(\sin\chi\cos\phi - \sin3\chi\cos3\phi) - 3\sin^2\theta(\sin\chi + \sin3\chi)(\cos\phi - \cos3\phi)]$$
$$+ (1/4)\beta_{ccb}[(\cos\theta - \cos^3\theta)(3\cos\chi + \cos3\chi)\sin\phi + \sin^2\theta(\sin\chi + \sin3\chi)\cos\phi]$$
$$+ (1/8)\beta_{abb}[-(\cos\theta - \cos^3\theta)(3\cos\chi + \cos3\chi)(\cos\phi - \cos3\phi) + 4\cos\theta(\cos\chi\cos\phi - \cos3\chi\cos3\phi)$$
$$- 4(\sin\chi\sin\phi - \sin3\chi\sin3\phi) + 3\sin^2\theta(\sin\chi + \sin3\chi)(\sin\phi - 3\sin3\phi)]$$
$$\chi_{XZZ} = (1/2)\beta_{cbb}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 - \cos2\phi) + \sin\theta\cos\theta\sin\chi\sin2\phi]$$
$$+ (1/2)\beta_{cab}[(\sin\theta - 2\sin^3\theta)\cos\chi\sin2\phi - \sin\theta\cos\theta\sin\chi(1 - \cos2\phi)]$$
$$+ (1/4)\beta_{aab}[(\cos\theta - \cos^3\theta)\cos\chi(\sin\phi + \sin3\phi) - \sin^2\theta\sin\chi(\cos\phi - \cos3\phi)]$$

$$+ (1/4)\beta_{bbb}[(\cos\theta - \cos^3\theta)\cos\chi(3\sin\phi - \sin3\phi) + \sin^2\theta\sin\chi(\cos\phi - \cos3\phi)]$$

$$+ \beta_{ccb}(\cos\theta - \cos^3\theta)\cos\chi\sin\phi$$

$$+ (1/2)\beta_{abb}[(\cos\theta - \cos^3\theta)\cos\chi(\cos\phi - \cos3\phi) - \sin^2\theta\sin\chi(\sin\phi - \sin3\phi)]$$

$$\chi_{ZXZ} = (1/2)\beta_{cbb}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 - \cos2\phi) + \sin\theta\cos\theta\sin\chi\sin2\phi]$$

$$+ (1/2)\beta_{cab}[(\sin\theta - 2\sin^3\theta)\cos\chi\sin2\phi - \sin\theta\cos\theta\sin\chi(1 - \cos2\phi)]$$

$$+ (1/4)\beta_{aab}[(\cos\theta - \cos^3\theta)\cos\chi(\sin\phi + \sin3\phi) - \sin^2\theta\sin\chi(\cos\phi - \cos3\phi)]$$

$$+ (1/4)\beta_{bbb}[(\cos\theta - \cos^3\theta)\cos\chi(3\sin\phi - \sin3\phi) + \sin^2\theta\sin\chi(\cos\phi - \cos3\phi)]$$

$$+ \beta_{ccb}(\cos\theta - \cos^3\theta)\cos\chi\sin\phi$$

$$+ (1/2)\beta_{abb}[(\cos\theta - \cos^3\theta)\cos\chi(\cos\phi - \cos3\phi) - \sin^2\theta\sin\chi(\sin\phi - \sin3\phi)]$$

$$\chi_{ZZX} = \beta_{cbb}[(\sin\theta - \sin^3\theta)\cos\chi(1 - \cos2\phi) + \sin\theta\cos\theta\sin\chi\sin2\phi]$$

$$+ \beta_{cab}[(\sin\theta - \sin^3\theta)\cos\chi\sin2\phi + \sin\theta\cos\theta\sin\chi(1 + \cos2\phi)]$$

$$+ (1/4)\beta_{aab}[(\cos\theta - \cos^3\theta)\cos\chi(\sin\phi + \sin3\phi) + \sin^2\theta\sin\chi(3\cos\phi + \cos3\phi)]$$

$$+ (1/4)\beta_{bbb}[(\cos\theta - \cos^3\theta)\cos\chi(3\sin\phi - \sin3\phi) + \sin^2\theta\sin\chi(\cos\phi - \cos3\phi)]$$

$$- \beta_{ccb}\cos^3\theta\cos\chi\sin\phi$$

$$+ (1/2)\beta_{abb}[(\cos\theta - \cos^3\theta)\cos\chi(\cos\phi - \cos3\phi) + \sin^2\theta\sin\chi(\sin\phi + \sin3\phi)]$$

$$\chi_{ZXX} = (1/4)\beta_{cbb}\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 - \cos2\phi)]$$

$$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$

$$- (1/4)\beta_{cab}\{2[(\cos\theta - \cos^3\theta) - \cos^3\theta\cos2\chi]\sin2\phi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$$

$$+ (1/8)\beta_{aab}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)(\sin\phi + \sin3\phi) + \sin\theta(1 - \cos2\chi)(\sin\phi + \sin3\phi)$$

$$+ 2\sin\theta\cos\theta\sin2\chi(\cos\phi + \cos3\phi)]$$

$$+ (1/8)\beta_{bbb}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)(3\sin\phi - \sin3\phi) - \sin\theta(1 - \cos2\chi)(\sin\phi + \sin3\phi)$$

$$+ 2\sin\theta\cos\theta\sin2\chi(\cos\phi - \cos3\phi)]$$

$$- (1/2)\beta_{ccb}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)\sin\phi + \sin\theta\cos\theta\sin2\chi\cos\phi]$$

$$+ (1/4)\beta_{abb}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)(\cos\phi - \cos3\phi) + \sin\theta(1 - \cos2\chi)(\cos\phi + \cos3\phi)$$

$$+ 2\sin\theta\cos\theta\sin2\chi\sin3\phi]$$

$$\chi_{XZX} = (1/4)\beta_{cbb}\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 - \cos2\phi)]$$

$$- (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$

$$- (1/4)\beta_{cab}\{2[(\cos\theta - \cos^3\theta) - \cos^3\theta\cos2\chi]\sin2\phi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$$

$$+ (1/8)\beta_{aab}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)(\sin\phi + \sin3\phi) - \sin\theta(1 - \cos2\chi)(\sin\phi + \sin3\phi)$$

$$+ 2\sin\theta\cos\theta\sin2\chi(\cos\phi + \cos3\phi)]$$

$$+ (1/8)\beta_{bbb}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)(3\sin\phi - \sin3\phi) + \sin\theta(1 - \cos2\chi)(\sin\phi + \sin3\phi)$$

$$+ 2\sin\theta\cos\theta\sin2\chi(\cos\phi - \cos3\phi)]$$

$$- (1/2)\beta_{ccb}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)\sin\phi + \sin\theta\cos\theta\sin2\chi\cos\phi]$$

$$+ (1/4)\beta_{abb}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)(\cos\phi - \cos3\phi) + \sin\theta(1 - \cos2\chi)(\cos\phi + \cos3\phi)$$

$$+ 2\sin\theta\cos\theta\sin2\chi\sin3\phi]$$

$$\chi_{XXZ} = -(1/2)\beta_{cbb}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)(1 - \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]$$

$$- (1/2)\beta_{cab}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)\sin2\phi - \sin^2\theta\sin2\chi(1 - \cos2\phi)]$$

$$+ (1/8)\beta_{aab}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)(\sin\phi + \sin3\phi) + \sin\theta(1 - \cos2\chi)(3\sin\phi - \sin3\phi)$$

$$- 2\sin\theta\cos\theta\sin2\chi(\cos\phi - \cos3\phi)]$$

$$+ (1/8)\beta_{bbb}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)(3\sin\phi - \sin3\phi) + \sin\theta(1 - \cos2\chi)(\sin\phi + \sin3\phi)$$

$+ \quad 2\sin\theta\cos\theta\sin 2\chi(\cos\phi - \cos 3\phi)]$

$+ (1/2)\beta_{ccb}\sin^3\theta(1 + \cos 2\chi)\sin\phi$

$+ (1/4)\beta_{abb}[[(\sin\theta - \sin^3\theta)(1 + \cos 2\chi)(\cos\phi - \cos 3\phi) - \sin\theta(1 - \cos 2\chi)(\cos\phi - \cos 3\phi)$

$- 2\sin\theta\cos\theta\sin 2\chi(\sin\phi - \sin 3\phi)]$

$\chi_{ZZZ} = \beta_{cbb}(\cos\theta - \cos^3\theta)(1 - \cos 2\phi)$

$+ \beta_{cab}(\cos\theta - \cos^3\theta)\sin 2\phi$

$+ (1/4)\beta_{aab} \sin^3\theta(\sin\phi + \sin 3\phi)$

$+ (1/4)\beta_{bbb} \sin^3\theta(3\sin\phi - \sin 3\phi)$

$+ \beta_{ccb}(\sin\theta - \sin^3\theta)\sin\phi$

$+ (1/2)\beta_{abb} \sin^3\theta(\cos\phi - \cos 3\phi)$

(spp) $\chi_{YXX} = (1/4)\beta_{cbb}\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin 3\chi)(1 - \cos 2\phi) + \sin\theta(\sin\chi - \sin 3\chi)(1 + \cos 2\phi)]$

$- 2\sin\theta\cos\theta\cos 3\chi\sin 2\phi\}$

$- (1/4)\beta_{cab}\{[\sin\theta(\sin\chi - \sin 3\chi) + (\sin\theta - \sin^3\theta)(\sin\chi + \sin 3\chi)]\sin 2\phi$

$- 2\sin\theta\cos\theta(\cos\chi - \cos 3\chi\cos 2\phi)\}$

$+ (1/16)\beta_{aab}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin 3\chi)(\sin\phi + \sin 3\phi) + 4\cos\theta(\sin\chi\sin\phi - \sin 3\chi\sin 3\phi)$

$+ \sin^2\theta(\cos\chi - \cos 3\chi)(\cos\phi - \cos 3\phi) - 4\cos^2\theta(\cos\chi\cos\phi - \cos 3\chi\cos 3\phi)]$

$+ (1/16)\beta_{bbb}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin 3\chi)(3\sin\phi - \sin 3\phi) - 4\cos\theta(\sin\chi\sin\phi - \sin 3\chi\sin 3\phi)$

$- \sin^2\theta(\cos\chi + 3\cos 3\chi)(\cos\phi - \cos 3\phi) + 4(\cos\chi\cos\phi - \cos 3\chi\cos 3\phi)]$

$- (1/4)\beta_{ccb}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin 3\chi)\sin\phi + \sin^2\theta(\cos\chi - \cos 3\chi)\cos\phi]$

$+ (1/8)\beta_{abb}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin 3\chi)(\cos\phi - \cos 3\phi) - 4\cos\theta(\sin\chi\cos\phi - \sin 3\chi\cos 3\phi)$

$- \sin^2\theta(\cos\chi - \cos 3\chi)(\sin\phi + \sin 3\phi) - 4\cos^2\theta(\cos\chi\sin\phi - \cos 3\chi\sin 3\phi)]$

$\chi_{YZZ} = -(1/2)\beta_{cbb}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 - \cos 2\phi) - \sin\theta\cos\theta\cos\chi\sin 2\phi]$

$- (1/2)\beta_{cab}[(\sin\theta - 2\sin^3\theta)\sin\chi\sin 2\phi + \sin\theta\cos\theta\cos(1 - \cos 2\phi)]$

$- (1/4)\beta_{aab}[(\cos\theta - \cos^3\theta)\sin\chi(\sin\phi + \sin 3\phi) + \sin^2\theta\cos\chi(\cos\phi - \cos 3\phi)]$

$- (1/4)\beta_{bbb}[(\cos\theta - \cos^3\theta)\sin\chi(3\sin\phi - \sin 3\phi) - \sin^2\theta\cos\chi(\cos\phi - \cos 3\phi)]$

$+ \beta_{ccb}(\cos\theta - \cos^3\theta)\sin\chi\sin\phi$

$- (1/2)\beta_{abb}[(\cos\theta - \cos^3\theta)\sin\chi(\cos\phi - \cos 3\phi) + \sin^2\theta\cos\chi(\sin\phi - \sin 3\phi)]$

$\chi_{YZX} = (1/4)\beta_{cbb}\{2[(\cos\theta - \cos^3\theta)(1 - \cos 2\phi) + \cos\theta\cos 2\phi]\sin 2\chi + [\sin^2\theta - (1 - 3\cos^2\theta)\cos 2\chi]\sin 2\phi\}$

$- (1/4)\beta_{cab}[2\cos^3\theta\sin 2\chi\sin 2\phi - \sin^2\theta(1 - \cos 2\chi)(1 + \cos 2\phi) + 2\cos^2\theta(1 - \cos 2\chi\cos 2\phi)]$

$- (1/8)\beta_{aab}\{(2\sin\theta - \sin^3\theta)\sin 2\chi(\sin\phi + \sin 3\phi) + 2\sin\theta\cos\theta[2\cos\phi - \cos 2\chi(\cos\phi - \cos 3\phi)]\}$

$+ (1/8)\beta_{bbb}[-(\sin\theta - \sin^3\theta)\sin 2\chi(3\sin\phi - \sin 3\phi) + \sin\theta\sin 2\chi(\sin\phi + \sin 3\phi)$

$+ 2\sin\theta\cos\theta\cos 2\chi(\cos\phi - \cos 3\phi)]$

$+ (1/2)\beta_{ccb}[(\sin\theta - \sin^3\theta)\sin 2\chi\sin\phi + \sin\theta\cos\theta(1 - \cos 2\chi)\cos\phi]$

$+ (1/4)\beta_{abb}[-(\sin\theta - \sin^3\theta)\sin 2\chi(\cos\phi - \cos 3\phi) + \sin\theta\sin 2\chi(\cos\phi + \cos 3\phi)$

$- 2\sin\theta\cos\theta(\sin\phi + \cos 2\chi\sin 3\phi)]$

$\chi_{YXZ} = (1/2)\beta_{cbb}[(\cos\theta - \cos^3\theta)\sin 2\chi(1 - \cos 2\phi) - \sin^2\theta\cos 2\chi\sin 2\phi]$

$+ (1/2)\beta_{cab}[(\cos\theta - \cos^3\theta)\sin 2\chi\sin 2\phi + \sin^2\theta\cos 2\chi(1 - \cos 2\phi)]$

$+ (1/8)\beta_{aab}[-(\sin\theta - \sin^3\theta)\sin 2\chi(\sin\phi + \sin 3\phi) + \sin\theta\sin 2\chi(3\sin\phi - \sin 3\phi)$

$- 2\sin\theta\cos\theta\cos 2\chi(\cos\phi - \cos 3\phi)]$

$$+ (1/8)\beta_{bbb}[-(\sin\theta - \sin^3\theta)\sin 2\chi(3\sin\phi - \sin 3\phi) + \sin\theta\sin 2\chi(\sin\phi + \sin 3\phi)$$
$$+ 2\sin\theta\cos\theta\cos 2\chi(\cos\phi - \cos 3\phi)]$$
$$- (1/2)\beta_{ccb}\sin^3\theta\sin 2\chi\sin\phi$$
$$- (1/4)\beta_{abb}[(2\sin\theta - \sin^3\theta)\sin 2\chi(\cos\phi - \cos 3\phi) + 2\sin\theta\cos\theta\cos 2\chi(\sin\phi - \sin 3\phi)]$$

(ssp) $$\chi_{YYX} = (1/4)\beta_{cbb}\{[-(\sin\theta - \sin^3\theta)(1 - \cos 2\phi) + \sin\theta(1 + \cos 2\phi)](\cos\chi - \cos 3\chi)$$
$$- 2\sin\theta\cos\theta(\sin\chi - \sin 3\chi)\sin 2\phi\}$$
$$- (1/4)\beta_{cab}\{(2\sin\theta - \sin^3\theta)(\cos\chi - \cos 3\chi)\sin 2\phi + 2\sin\theta\cos\theta[2\sin\chi - (\sin\chi - \sin 3\chi)\cos 2\phi]\}$$
$$+ (1/16)\beta_{aab}[-(\cos\theta - \cos^3\theta)(\cos\chi - \cos 3\chi)(\sin\phi + \sin 3\phi) + 4\cos\theta(3\cos\chi\sin\phi - \cos 3\chi\sin 3\phi)$$
$$+ \sin^2\theta(\sin\chi + 3\sin 3\chi)(\cos\phi + \cos 3\phi) + 4\cos^2\theta(3\sin\chi\cos\phi - \sin 3\chi\cos 3\phi)]$$
$$+ (1/16)\beta_{bbb}[-(\cos\theta - \cos^3\theta)(\cos\chi - \cos 3\chi)(3\sin\phi - \sin 3\phi) + 4\cos\theta(\cos\chi\sin\phi + \cos 3\chi\sin 3\phi)$$
$$- \sin^2\theta(\sin\chi - 3\sin 3\chi)(\cos\phi - \cos 3\phi) + 4\cos^2\theta(\sin\chi\cos\phi + \sin 3\chi\cos 3\phi)]$$
$$+ (1/4)\beta_{ccb}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos 3\chi)\sin\phi + \sin^2\theta(3\sin\chi - \sin 3\chi)\cos\phi]$$
$$+ (1/8)\beta_{abb}[-(\cos\theta - \cos^3\theta)(\cos\chi - \cos 3\chi)(\cos\phi - \cos 3\phi) - 4\cos\theta(\cos\chi\cos\phi - \cos 3\chi\cos 3\phi)$$
$$- \sin^2\theta(\sin\chi + \sin 3\chi)(\sin\phi + \sin 3\phi) + 4\cos^2\theta(\sin\chi\sin\phi - \sin 3\chi\sin 3\phi)]$$
$$\chi_{YYZ} = -(1/2)\beta_{cbb}[(\cos\theta - \cos^3\theta)(1 - \cos 2\chi)(1 - \cos 2\phi) - \sin^2\theta\sin 2\chi\sin 2\phi]$$
$$- (1/2)\beta_{cab}[(\cos\theta - \cos^3\theta)(1 - \cos 2\chi)\sin 2\phi + \sin^2\theta\sin 2\chi(1 - \cos 2\phi)]$$
$$+ (1/8)\beta_{aab}[\sin\theta(1 + \cos 2\chi)(3\sin\phi - \sin 3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos 2\chi)(\sin\phi + \sin 3\phi)$$
$$+ 2\sin\theta\cos\theta\sin 2\chi(\cos\phi - \cos 3\phi)]$$
$$+ (1/8)\beta_{bbb}[\sin\theta(1 + \cos 2\chi)(\sin\phi + \sin 3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos 2\chi)(3\sin\phi - \sin 3\phi)$$
$$- 2\sin\theta\cos\theta\sin 2\chi(\cos\phi - \cos 3\phi)]$$
$$+ (1/2)\beta_{ccb}\sin^3\theta(1 - \cos 2\chi)\sin\phi$$
$$+ (1/4)\beta_{abb}[-\sin\theta(1 + \cos 2\chi)(\cos\phi - \cos 3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos 2\chi)(\cos\phi - \cos 3\phi)$$
$$+ 2\sin\theta\cos\theta\sin 2\chi(\sin\phi - \sin 3\phi)]$$

(psp) $$\chi_{XYX} = (1/4)\beta_{cbb}\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin 3\chi)(1 - \cos 2\phi) + \sin\theta(\sin\chi - \sin 3\chi)(1 + \cos 2\phi)]$$
$$- 2\sin\theta\cos\theta\cos 3\chi\sin 2\phi\}$$
$$- (1/4)\beta_{cab}\{[2\sin\theta\sin\chi - (2\sin\theta - \sin^3\theta)(\sin\chi + \sin 3\chi)]\sin 2\phi - 2\sin\theta\cos\theta(\cos\chi - \cos 3\chi\cos 2\phi)\}$$
$$+ (1/16)\beta_{aab}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin 3\chi)(\sin\phi + \sin 3\phi) + 4\cos\theta(\sin\chi\sin\phi - \sin 3\chi\sin 3\phi)$$
$$+ \sin^2\theta(\cos\chi - \cos 3\chi)(\cos\phi - \cos 3\phi) - 4\cos^2\theta\,(\cos\chi\cos\phi - \cos 3\chi\cos 3\phi)]$$
$$+ (1/16)\beta_{bbb}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin 3\chi)(3\sin\phi - \sin 3\phi) - 4\cos\theta(\sin\chi\sin\phi - \sin 3\chi\sin 3\phi)$$
$$- \sin^2\theta(\cos\chi + 3\cos 3\chi)(\cos\phi - \cos 3\phi) + 4(\cos\chi\cos\phi - \cos 3\chi\cos 3\phi)]$$
$$- (1/4)\beta_{ccb}[-(\cos\theta - \cos^3\theta)(\sin\chi + \sin 3\chi)\sin\phi + \sin^2\theta(\cos\chi - \cos 3\chi)\mathrm{cosn}\phi]$$
$$+ (1/8)\beta_{abb}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin 3\chi)(\cos\phi - \cos 3\phi) - 4\cos\theta(\sin\chi\cos\phi - \sin 3\chi\cos 3\phi)$$
$$- \sin^2\theta(\cos\chi - \cos 3\chi)(\sin\phi + \sin 3\phi) - 4(\cos\chi\sin\phi - \cos 3\chi\sin 3\phi)]$$
$$\chi_{ZYZ} = -(1/2)\beta_{cbb}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 - \cos 2\phi) - \sin\theta\cos\theta\cos\chi\sin 2\phi]$$
$$- (1/2)\beta_{cab}[(\sin\theta - 2\sin^3\theta)\sin\chi\sin 2\phi + \sin\theta\cos\theta\cos\chi(1 - \cos 2\phi)]$$
$$- (1/4)\beta_{aab}[(\cos\theta - \cos^3\theta)\sin\chi(\sin\phi + \sin 3\phi) + \sin^2\theta\cos\chi(3\cos\phi + \cos 3\phi)]$$
$$+ (1/4)\beta_{bbb}[-(\cos\theta - \cos^3\theta)\sin\chi(3\sin\phi - \sin 3\phi) + \sin^2\theta\cos\chi(\cos\phi - \cos 3\phi)]$$
$$+ \beta_{ccb}(\cos\theta - \cos^3\theta)\sin\chi\sin\phi$$

$$- (1/2)\beta_{abb}[(\cos\theta - \cos^3\theta)\sin\chi(\cos\phi - \cos3\phi) + \sin^2\theta\cos\chi(\sin\phi - \sin3\phi)]$$

$$\chi_{XYZ} = (1/2)\beta_{cbb}[(\cos\theta - \cos^3\theta)\sin2\chi(1 - \cos2\phi) - \sin^2\theta\cos2\chi\sin2\phi]$$

$$+ (1/2)\beta_{cab}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi + \sin^2\theta\cos2\chi(1 - \cos2\phi)]$$

$$+ (1/8)\beta_{aab}[\sin\theta\sin2\chi(3\sin\phi - \sin3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(\sin\phi + \sin3\phi)$$

$$- 2\sin\theta\cos\theta\cos2\chi(\cos\phi - \cos3\phi)]$$

$$+ (1/8)\beta_{bbb}[\sin\theta\sin2\chi(\sin\phi + \sin3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(3\sin\phi - \sin3\phi)$$

$$+ 2\sin\theta\cos\theta\cos2\chi(\cos\phi - \cos3\phi)]$$

$$- (1/2)\beta_{ccb}\sin^3\theta\sin2\chi\sin\phi$$

$$- (1/4)\beta_{abb}[(2\sin\theta - \sin^3\theta)\sin2\chi(\cos\phi - \cos3\phi) + 2\sin\theta\cos\theta\cos2\chi(\sin\phi - \sin3\phi)]$$

$$\chi_{ZYX} = (1/4)\beta_{cbb}\{2[(\cos\theta - \cos^3\theta)(1 - \cos2\phi) + \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta - (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$

$$- (1/4)\beta_{cab}[2\cos^3\theta\sin2\chi\sin2\phi - \sin^2\theta(1 - \cos2\chi)(1 + \cos2\phi) + 2(1 - \cos2\chi\cos2\phi)]$$

$$- (1/8)\beta_{aab}\{(2\sin\theta - \sin^3\theta)\sin2\chi(\sin\phi + \sin3\phi) + 2\sin\theta\cos\theta[2\cos2\phi - \cos2\chi(\cos\phi + \cos3\phi)]\}$$

$$+ (1/8)\beta_{bbb}[\sin\theta\sin2\chi(\sin\phi + \sin3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(3\sin\phi - \sin3\phi)$$

$$+ 2\sin\theta\cos\theta\cos2\chi(\cos\phi - \cos3\phi)]$$

$$+ (1/2)\beta_{ccb}[(\sin\theta - \sin^3\theta)\sin2\chi\sin\phi + \sin\theta\cos\theta(1 - \cos2\chi)\cos\phi]$$

$$+ (1/4)\beta_{abb}[\sin\theta\sin2\chi(\cos\phi + \cos3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(\cos\phi - \cos3\phi)$$

$$- 2\sin\theta\cos\theta(\sin\phi + \cos2\chi\sin3\phi)]$$

(sps) $$\chi_{YXY} = -(1/4)\beta_{cbb}\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 - \cos2\phi) + \sin\theta(\cos\chi + \cos3\chi)(1 + \cos2\phi)]$$

$$- 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$$

$$+ (1/4)\beta_{cab}\{[2\sin\theta\cos\chi - (2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\sin2\phi + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi\cos2\phi)\}$$

$$+ (1/16)\beta_{aab}[-(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)(\sin\phi + \sin3\phi) - 4\cos\theta(\cos\chi\sin\phi + \cos3\chi\sin3\phi)$$

$$+ \sin^2\theta(\sin\chi + \sin3\chi)(\cos\phi - \cos3\phi) - 4\cos^2\theta(\sin\chi\cos\phi + \sin3\chi\cos3\phi)]$$

$$+ (1/16)\beta_{bbb}[-(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)(3\sin\phi - \sin3\phi) + 4\cos\theta(\cos\chi\sin\phi + \cos3\chi\sin3\phi)$$

$$- \sin^2\theta(\sin\chi - 3\sin3\chi)(\cos\phi - \cos3\phi) + 4(\sin\chi\cos\phi + \sin3\chi\cos3\phi)]$$

$$+ (1/4)\beta_{ccb}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)\sin\phi - \sin^2\theta(\sin\chi + \sin3\chi)\cos\phi]$$

$$+ (1/8)\beta_{abb}[-(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)(\cos\phi - \cos3\phi) + 4\cos\theta(\cos\chi\cos\phi + \cos3\chi\cos3\phi)$$

$$- \sin^2\theta(\sin\chi + \sin3\chi)(\sin\phi + \sin3\phi) - 4\cos^2\theta(\sin\chi\sin\phi + \sin3\chi\sin3\phi)]$$

$$\chi_{YZY} = (1/4)\beta_{cbb}\{2[\cos\theta(1 + \cos2\phi\cos2\chi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 - \cos2\phi)]$$

$$+ (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$

$$- (1/4)\beta_{cab}\{2[(\cos\theta - \cos^3\theta) + \cos^3\theta\cos2\chi]\sin2\phi - [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$$

$$- (1/8)\beta_{aab}[\sin\theta(1 + \cos2\chi)(\sin\phi + \sin3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\chi)(\sin\phi + \sin3\phi)$$

$$+ 2\sin\theta\cos\theta\sin2\chi(\cos\phi + \cos3\phi)]$$

$$+ (1/8)\beta_{bbb}[\sin\theta(1 + \cos2\chi)(\sin\phi + \sin3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\chi)(3\sin\phi - \sin3\phi)$$

$$- 2\sin\theta\cos\theta\sin2\chi(\cos\phi - \cos3\phi)]$$

$$+ (1/2)\beta_{ccb}[-(\sin\theta - \sin^3\theta)(1 - \cos2\chi)\sin\phi + \sin\theta\cos\theta\sin2\chi\cos\phi]$$

$$+ (1/4)\beta_{abb}[\sin\theta(1 + \cos2\chi)(\cos\phi + \cos3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\chi)(\cos\phi - \cos3\phi)$$

$$- 2\sin\theta\cos\theta\sin2\sin3\phi]$$

(pps) $$\chi_{XXY} = (1/4)\beta_{cbb}\{[(\sin\theta - \sin^3\theta)(1 - \cos2\phi) - \sin\theta(1 + \cos2\phi)](\sin\chi + \sin3\chi)$$

$$- 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$$

$$+ (1/4)\beta_{cab}\{(2\sin\theta - \sin^3\theta)\sin2\phi - 2\sin\theta\cos\theta[2\cos\chi - (\cos\chi + \cos3\chi)\cos2\phi]\}$$

$$+ (1/16)\beta_{aab}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)(\sin\phi + \sin3\phi) - 4\cos\theta(3\sin\chi\sin\phi + \sin3\chi\sin3\phi)$$

$$+ \sin^2\theta(\cos\chi - \cos3\chi)(\cos\phi - \cos3\phi) + 4\cos^2\theta(3\cos\chi\cos\phi + \cos3\chi\cos3\phi)]$$

$$+ (1/16)\beta_{bbb}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)(3\sin\phi - \sin3\phi) - 4\cos\theta(3\sin\chi\sin\phi + \sin3\chi\sin3\phi)$$

$$- \sin^2\theta(\cos\chi + \cos3\chi)(\cos\phi - \cos3\phi) + 4(\cos\chi\cos\phi - \cos3\chi\cos3\phi)]$$

$$+ (1/4)\beta_{ccb}[-(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\sin\phi + \sin^2\theta(3\cos\chi + \cos3\chi)\cos\phi]$$

$$+ (1/8)\beta_{abb}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)(\cos\phi - \cos3\phi) + 4\cos\theta(\sin\chi\cos\phi + \sin3\chi\cos3\phi)$$

$$- \sin^2\theta(\cos\chi - \cos3\chi)(\sin\phi + \sin3\phi) + 4\cos^2\theta(\cos\chi\sin\phi + \cos3\chi\sin3\phi)]$$

$$\chi_{ZZY} = \beta_{cbb}[-(\sin\theta - \sin^3\theta)\sin\chi(1 - \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]$$

$$- \beta_{cab}[(\sin\theta - \sin^3\theta)\sin\chi\sin2\phi - \sin\theta\cos\theta\cos\chi(1 + \cos2\phi)]$$

$$+ (1/4)\beta_{aab}[-(\cos\theta - \cos^3\theta)\sin\chi\,(\sin\phi + \sin3\phi) + \sin^2\theta\cos\chi(3\cos\phi + \cos3\phi)]$$

$$+ (1/4)\beta_{bbb}[-(\cos\theta - \cos^3\theta)\sin\chi\,(3\sin\phi - \sin3\phi) + \sin^2\theta\cos\chi(\cos\phi - \cos3\phi)]$$

$$+ \beta_{ccb}[-\cos^3\theta\sin\chi\sin\phi + \cos^2\theta\cos\chi\cos\phi]$$

$$+ (1/2)\beta_{abb}[-(\cos\theta - \cos^3\theta)\sin\chi(\cos\phi - \cos3\phi) + \sin^2\theta\cos\chi(\sin\phi + \sin3\phi)]$$

$$\chi_{ZXY} = (1/4)\beta_{cbb}\{2[(\cos\theta - \cos^3\theta)(1 - \cos2\phi) + \cos\theta\cos2\phi]\sin2\chi - [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$

$$- (1/4)\beta_{cab}[2\cos^3\theta\sin2\chi\sin2\phi + \sin^2\theta(1 + \cos2\chi)(1 + \cos2\phi) - 2\cos^2\theta(1 - \cos2\chi\cos2\phi)]$$

$$+ (1/8)\beta_{aab}\{-(2\sin\theta - \sin^3\theta)\sin2\chi(\sin\phi + \sin3\phi) + 2\sin\theta\cos\theta[2\cos\phi + \cos2\chi(\cos\phi + \cos3\phi)]\}$$

$$+ (1/8)\beta_{bbb}[\sin\theta\sin2\chi(\sin\phi + \sin3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(3\sin\phi - \sin3\phi)$$

$$+ 2\sin\theta\cos\theta\cos2\chi(\cos\phi - \cos3\phi)]$$

$$+ (1/2)\beta_{ccb}[(\sin\theta - \sin^3\theta)\sin2\chi\sin\phi - \sin\theta\cos\theta(1 + \cos2\chi)\cos\phi]$$

$$+ (1/4)\beta_{abb}\{\sin\theta\sin2\chi(\cos\phi + \cos3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(\cos\phi - \cos3\phi)$$

$$- 2\sin\theta\cos\theta\cos2\chi(\sin\phi - \sin3\phi)]\}$$

$$\chi_{XZY} = (1/4)\beta_{cbb}\{2[(\cos\theta - \cos^3\theta)(1 - \cos2\phi) + \cos\theta\cos2\phi]\sin2\chi - [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$$

$$- (1/4)\beta_{cab}[2\cos^3\theta\sin2\chi\sin2\phi + \sin^2\theta(1 + \cos2\chi)(1 + \cos2\phi) - 2\cos^2\theta(1 + \cos2\chi\cos2\phi)]$$

$$+ (1/8)\beta_{aab}\{-(2\sin\theta - \sin^3\theta)\sin2\chi(\sin\phi + \sin3\phi) + 2\sin\theta\cos\theta[2\cos\phi + \cos2\chi(\cos\phi + \cos3\phi)]\}$$

$$+ (1/8)\beta_{bbb}[\sin\theta\sin2\chi(\sin\phi + \sin3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(3\sin\phi - \sin3\phi)$$

$$+ 2\sin\theta\cos\theta\cos2\chi(\cos\phi - \cos3\phi)]$$

$$+ (1/2)\beta_{ccb}[(\sin\theta - \sin^3\theta)\sin2\chi\sin\phi - \sin\theta\cos\theta(1 + \cos2\chi)\cos\phi]$$

$$+ (1/4)\beta_{abb}\{\sin\theta\sin2\chi(\cos\phi + \cos3\phi) - (\sin\theta - \sin^3\theta)\sin2\chi(\cos\phi - \cos3\phi)$$

$$- 2\sin\theta\cos\theta\cos2\chi(\sin\phi - \sin3\phi)]\}$$

(pss)

$$\chi_{XYY} = -(1/4)\beta_{cbb}\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 - \cos2\phi) + \sin\theta(\cos\chi + \cos3\chi)(1 + \cos2\phi)]$$

$$- 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$$

$$+ (1/4)\beta_{cab}\{[2\sin\theta\cos\chi - (2\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\sin2\phi + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi\cos2\phi)\}$$

$$- (1/16)\beta_{aab}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)(\sin\phi + \sin3\phi) + 4\cos\theta(\cos\chi\sin\phi + \cos3\chi\sin3\phi)$$

$$- \sin^2\theta(\sin\chi + \sin3\chi)(\cos\phi - \cos3\phi) + 4\cos^2\theta(\sin\chi\cos\phi + \sin3\chi\cos3\phi)]$$

$$- (1/16)\beta_{bbb}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)(3\sin\phi - \sin3\phi) - 4\cos\theta(\cos\chi\sin\phi + \cos3\chi\sin3\phi)$$

$$+ \sin^2\theta(\sin\chi - 3\sin3\chi)(\cos\phi - \cos3\phi) - 4\cos^2\theta(\sin\chi\cos\phi + \sin3\chi\cos3\phi)]$$

$$+ (1/4)\beta_{ccb}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)\sin\phi - \sin^2\theta(\sin\chi + \sin3\chi)\cos\phi]$$

$$- (1/8)\beta_{abb}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)(\cos\phi - \cos3\phi) - 4\cos\theta(\cos\chi\cos\phi + \cos3\chi\cos3\phi)$$
$$+ \sin^2\theta(\sin\chi + \sin3\chi)(\sin\phi + \sin3\phi) + 4\cos^2\theta(\sin\chi\sin\phi + \sin3\chi\sin3\phi)]$$
$$\chi_{ZYY} = (1/4)\beta_{cbb}\{2[\cos\theta(1 + \cos2\phi\cos2\chi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 - \cos2\phi)]$$
$$+ (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$$
$$- (1/4)\beta_{cab}\{2[(\cos\theta - \cos^3\theta) - \cos^3\theta\cos2\chi]\sin2\phi - [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\phi]\sin2\chi\}$$
$$+ (1/8)\beta_{aab}[-\sin\theta(1 + \cos2\chi)(\sin\phi + \sin3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\chi)(\sin\phi + \sin3\phi)$$
$$- 2\sin\theta\cos\theta\sin2\chi(\cos\phi + \cos3\phi)]$$
$$+ (1/8)\beta_{bbb}[\sin\theta(1 + \cos2\chi)(\sin\phi + \sin3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\chi)(3\sin\phi - \sin3\phi)$$
$$- 2\sin\theta\cos\theta\sin2\chi(\cos\phi - \cos3\phi)]$$
$$+ (1/2)\beta_{ccb}[-(\sin\theta - \sin^3\theta)(1 - \cos2\chi)\sin\phi + \sin\theta\cos\theta\sin2\chi\cos\phi]$$
$$+ (1/4)\beta_{abb}[\sin\theta(1 + \cos2\chi)(\cos\phi + \cos3\phi) + (\sin\theta - \sin^3\theta)(1 - \cos2\chi)(\cos\phi - \cos3\phi)$$
$$- 2\sin\theta\cos\theta\sin2\chi\sin3\phi]$$

(sss)
$$\chi_{YYY} = (1/4)\beta_{cbb}\{[(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 - \cos2\phi) + \sin\theta(\sin\chi + \sin3\chi)(1 + \cos2\phi)]$$
$$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$$
$$+ (1/4)\beta_{cab}\{[4(\sin\theta - \sin^3\theta)\sin\chi -(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\sin2\phi$$
$$- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\cos2\phi\}$$
$$+ (1/16)\beta_{aab}[(\cos\theta - \cos^3\theta)(3\sin\chi - \sin3\chi)(\sin\phi + \sin3\phi) - 4\cos\theta(\sin\chi\sin\phi - \sin3\chi\sin3\phi)$$
$$- \sin^2\theta(\cos\chi - \cos3\chi)(\cos\phi + 3\cos3\phi) + 4(\cos\chi\cos\phi - \cos3\chi\cos3\phi)]$$
$$+ (1/16)\beta_{bbb}[(\cos\theta - \cos^3\theta)(3\sin\chi - \sin3\chi)(3\sin\phi - \sin3\phi) - 4\cos\theta(\sin\chi\sin\phi + \sin3\chi\sin3\phi)$$
$$- 3\sin^2\theta(\cos\chi - \cos3\chi)(\cos\phi - \cos3\phi) + 4(\cos\chi\cos\phi + \cos3\chi\cos3\phi)]$$
$$+ (1/4)\beta_{ccb}[(\cos\theta - \cos^3\theta)(3\cos\chi + \cos3\chi)\sin\phi + \sin^2\theta(\sin\chi + \sin3\chi)\cos\phi]$$
$$+ (1/8)\beta_{abb}[(\cos\theta - \cos^3\theta)(3\sin\chi - \sin3\chi)(\cos\phi - \cos3\phi) - 4\cos\theta(\sin\chi\cos\phi + \sin3\chi\cos3\phi)$$
$$+ \sin^2\theta(\cos\chi - \cos3\chi)(\sin\phi - 3\sin3\phi) - 4(\cos\chi\sin\phi + \cos3\chi\sin3\phi)]$$