# (CH<sub>3</sub>),X 基の取扱い

### 目次

1.序論	1
2.座標系とメチル基の配向	1
3.振動バンド	2
4.(CH <sub>3</sub> ) <sub>2</sub> X 基の対称性	2
5 . 分子固定 SFG テンソル	3
自由回転	3
$\phi_{A}=\phi_{B}=0,\pi$ (三角形が $2$ つとも下向き又は $2$ つとも上向き)	3
$\phi_{A}=\phi_{B}  eq 0,\pi$ (2つの三角形が反発しあうようにずれている)	4
$\phi_A=0,\phi_B=\pi$ または $\phi_A=\pi,\phi_B=0$ (1つの三角形は下向き、もう1つの三角形は下向き)	4
$\phi_{A}=-\phi_{B} eq0,\pi$ (2つの三角形が同じ側にかしいでいる。)	5
6 . 空間固定 (XYZ) 系におけるテンソル成分	5
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。)	6
$\phi_{A}=\phi_{B}=0,\pi$ ・ランダム配向(一般的な配向に対する表式は付録 ${ m C}$ に示す。)	9
$\phi_{A}=\phi_{B}  eq 0, \pi$ ・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。)	12
$\phi_{A}=0,\phi_{B}=\pi$ または $\phi_{A}=\pi,\phi_{B}=0$ (1つの三角形は下向き、もう1つの三角形は下向き)	16
付録 A:(CH3)2X 基の SFG テンソル	19
付録 B:自由回転しているときの (XYZ) 系でのテンソル成分	21(25)
付録 $C:\phi_A=\phi_B=0,\pi$ のときの (XYZ) 系でのテンソル成分	29(33)
付録 D:φ <sub>A</sub> =φ <sub>B</sub> ≠0,π のときの (XYZ) 系でのテンソル成分	38(42)
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	49(53)
付録 F:空間固定(XYZ)系でのテンソル成分 ( 一般式 )	58(62)
(括弧内は縮重振動起源のモードに対するもの)	

#### 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).  $(CH_3)_2$ X 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

- $\mathsf{U}_{\mathsf{x}}$  X 原子からメチル基の方向を正方向とする。 2 個のメ  $\mathsf{C}_{\mathsf{x}}$  軸が作る平面の上に  $\mathsf{x}$  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  $\alpha$  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  $\phi_A$ 、 $\phi_B$  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  $180^\circ$  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**;( $\chi$ ,  $\theta$ ,  $\phi$ ): 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  $2\alpha$  として、(0,  $\alpha$ ,  $\phi$ ) と ( $\pi$ ,  $\alpha$ ,  $\phi$ ) 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  $\theta$  に関しては、表で使っている  $\sin\theta$ 、 $\sin2\theta$ 、 $\sin3\theta$  の形の三角関数ではなく、下の関係式を使って変換した  $\sin\theta$ 、 $\cos\theta$  のべき乗による表式を採用した。)

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

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

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<sub>3</sub>)<sub>2</sub>X 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.振動パンド

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<sub>3</sub>)<sub>2</sub>X 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  $\pi$  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  $C_{2\nu}$  から  $D_{sh}$  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<sub>3</sub>)<sub>3</sub>X 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<sub>3</sub>)<sub>2</sub>X 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 C2v 対称

 $\phi_A = \phi_B = 0$  または  $\pi$  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<sub>2</sub> 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  $\phi_A$   $と\phi_B$  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<sub>1</sub>) 
$$\beta_{xxz} = -2(\beta_{aac} - \beta_{cac})(\cos\alpha - \cos^3\alpha) + 2\beta_{aac}\cos\alpha$$

$$\beta_{\rm vvz} = +2\beta_{\rm ax}\cos\alpha$$

$$\beta_{zz} = +2(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha) + 2\beta_{cx}\cos\alpha$$

$$(b_1) \beta_{zxx} = -2(\beta_{aac} - \beta_{cc})(\cos\alpha - \cos^3\alpha)$$

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

[縮重バンド]  $eta_{\zeta\zeta\zeta}>>eta_{\xi\xi\zeta},eta_{\eta\eta\zeta}$  のときには、  $eta_{
m caa}\sim(4/9)eta_{\zeta\zeta\zeta}$ ,  $eta_{
m aaa}\sim4\sqrt{2}$  / 9  $eta_{\zeta\zeta\zeta}$  である。

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

$$\beta_{\rm vvz} = 0$$

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

$$(b_1) \beta_{zxx} = -\beta_{cas}(\cos\alpha - 2\cos^3\alpha)$$

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

 $(b_2)$   $\beta_{zyy} = \beta_{caa} \cos \alpha$ 

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

 $\phi_A = \phi_B = 0, \pi$  (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、  $\cos\phi_A = \cos3\phi_A = \cos3\phi_$ 

[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<sub>1</sub>) 
$$\beta_{xxz} = -2(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha) + 2\beta_{ax}\cos\alpha$$
$$\beta_{yyz} = +2\beta_{ax}\cos\alpha$$
$$\beta_{zzz} = +2(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha) + 2\beta_{cx}\cos\alpha$$

(b<sub>1</sub>) 
$$\beta_{zxx} = -2(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)$$
  
 $\beta_{xzx} = -2(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)$ 

[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。。  $(\beta_{zyy} \, と \, \beta_{yzy} \,$ 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。)  $(\pm$  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<sub>1</sub>) 
$$\beta_{xxz} = 2[-2\beta_{caa}(\cos\alpha - \cos^3\alpha) \pm \beta_{aaa}(\sin\alpha - \sin^3\alpha)]$$
$$\beta_{yyz} = -(\pm 2)\beta_{aaa}\sin\alpha$$
$$\beta_{zz} = 2[2\beta_{caa}(\cos\alpha - \cos^3\alpha) \pm \beta_{aaa}\sin^3\alpha]$$

$$(b_1) \beta_{zxx} = -2[\beta_{can}(\cos\alpha - \cos^3\alpha) \pm \beta_{aan}(\sin\alpha - \sin^3\alpha)]$$
$$\beta_{xzx} = -2[\beta_{can}(\cos\alpha - \cos^3\alpha) \pm \beta_{aan}(\sin\alpha - \sin^3\alpha)]$$

(b<sub>2</sub>) 
$$\beta_{zyy} = 2[\beta_{caa}\cos\alpha - (\pm)\beta_{aaa}\sin\alpha]$$
  
 $\beta_{yzy} = 2[\beta_{caa}\cos\alpha - (\pm)\beta_{aaa}\sin\alpha]$ 

 $\phi_{A} = \phi_{B} \neq 0$ ,  $\pi$  (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。

[全対称パンド]  $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$  のときには、  $\beta_{ax} \sim (4/9)\beta_{\zeta\zeta\zeta}$ 、 $\beta_{cx} \sim (1/9)\beta_{\zeta\zeta\zeta}$  である。  $\beta_{xxz} = -2(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha) + 2\beta_{ax}\cos\alpha$ 

$$\beta_{\rm vvz} = +2\beta_{\rm aac}\cos\alpha$$

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

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

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

[縮重バンド]  $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\zeta\zeta}, \beta_{\eta\eta\zeta}$  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。) ( $\pm$  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。)

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

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

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

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

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

$$\beta_{yyz} = -\beta_{aaa} \sin\alpha(\cos 3\phi_A \pm \cos\phi_A)$$

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

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

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

$$\beta_{zxy} = -(\pm)\beta_{caa}(2\cos^2\alpha - 1)\sin 2\phi_A - \beta_{aaa}\sin \alpha\cos\alpha[\sin 3\phi_A - (\pm)\sin\phi_A]$$

$$\beta_{xzy} = -(\pm)\beta_{ca}(2\cos^2\alpha - 1)\sin 2\phi_A - \beta_{aa}\sin \alpha\cos\alpha[\sin 3\phi_A - (\pm)\sin\phi_A]$$

$$\beta_{xyz} = \pm \beta_{cap} \sin^2 \alpha \sin 2\phi_A - \beta_{aap} \sin \alpha \cos \alpha (\sin 3\phi_A \pm \sin \phi_A)$$

$$\beta_{yxz} = \pm \beta_{cas} \sin^2 \alpha \sin 2\phi_A - \beta_{aas} \sin \alpha \cos \alpha (\sin 3\phi_A \pm \sin \phi_A)$$

 $\phi_A = 0$ ,  $\phi_B = \pi$  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)

# [全対称パンド] $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \beta_{\eta\eta\zeta}$ のときには、 $\beta_{ax} \sim (4/9) \beta_{\zeta\zeta\zeta}$ 、 $\beta_{cx} \sim (1/9) \beta_{\zeta\zeta\zeta}$ である。

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

$$\beta_{\rm vvz} = +2\beta_{\rm aac}\cos\alpha$$

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

$$\beta_{\rm zxx} = -2(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)$$

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

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

 $(eta_{zyy}$  と  $eta_{yzy}$  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。)

$$(\pm$$
 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。)

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

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

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

$$\beta_{\rm vzv} = 2\beta_{\rm cas}\cos\alpha$$

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

$$\beta_{\rm vvz} = 0$$

$$\beta_{zz} = 4\beta_{ca}(\cos\alpha - \cos^3\alpha)$$

 $\phi_{\Delta} = -\phi_{R} \neq 0, \pi$  (2 つの三角形が同じ側にかしいでいる。)

# [全対称パンド] $\beta_{\text{CCC}} >> \beta_{\text{EEC}}, \beta_{\text{nnC}}$ のときには、 $\beta_{\text{aac}} \sim (4/9) \beta_{\text{CCC}}, \beta_{\text{ccc}} \sim (1/9) \beta_{\text{CCC}}$ である。

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

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

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

$$\beta_{\rm zxx} = -2(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)$$

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

#### 「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。)

$$\beta_{xxx} = -\beta_{can}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos 2\phi_A) + \beta_{aan}(\sin\alpha - \sin^3\alpha)(\cos 3\phi_A \pm \cos\phi_A)$$

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

$$\begin{split} &\beta_{zyy} = \beta_{caa} cos\alpha [1-(\pm)cos2\varphi_A] - \beta_{aaa} sin\alpha [cos3\varphi_A - (\pm)cos\varphi_A] \\ &\beta_{yzy} = \beta_{caa} cos\alpha [1-(\pm)cos2\varphi_A] - \beta_{aaa} sin\alpha [cos3\varphi_A - (\pm)cos\varphi_A] \\ &\beta_{xxz} = -2\beta_{caa} (cos\alpha - cos^3\alpha)(1\pm cos2\varphi_A) + \beta_{aaa} (sin\alpha - sin^3\alpha)(cos3\varphi_A \pm cos\varphi_A) \\ &\beta_{yyz} = -\beta_{aaa} sin\alpha (cos3\varphi_A \pm cos\varphi_A) \\ &\beta_{zzz} = 2\beta_{caa} (cos\alpha - cos^3\alpha)(1\pm cos2\varphi_A) + \beta_{aaa} sin^3\alpha (cos3\varphi_A \pm cos\varphi_A) \\ &\beta_{yxx} = \pm \beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} cos^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{xyy} = \pm \beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} cos^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{xxy} = \pm 2\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} cos^2\alpha [sin3\varphi_A - (\pm)sin\varphi_A] \\ &\beta_{yyy} = \beta_{aaa} [sin3\varphi_A - (\pm)sin\varphi_A] \\ &\beta_{zzy} = -(\pm)2\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha [sin3\varphi_A - (\pm)sin\varphi_A] \\ &\beta_{yzz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zyz} = -\beta_{caa} sin\alpha cos\alpha sin2\varphi_A - \beta_{aaa} sin^2\alpha (sin3\varphi_A \pm sin\varphi_A) \\ &\beta_{zy$$

#### 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  $(\chi, \theta, \phi)$  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<sub>3</sub>)<sub>2</sub>X 基の配向の関係は、次のようになる。

- (1) 内部回転角  $\phi$ : 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 ( $<90^\circ$ ) 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  $\pi$ 、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  $\phi$  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  $\phi$  は  $0\sim2\pi$  の任意の値を同じウェイトで取る。(c) 傾き角・c1 は c2 前の定義に合わせて、c3 軸 (c3 なのときの法線の間の角と定義し、c3 軸 を外向きの法線に重ねる方向をプラス回転とする。c3 軸 は下向きの法線であるから、オイラー角 c4 は c5 である。また、(c6 c7 を真空側に向けているときには c6 の c7 である。
- (3) **面内配向角**  $\chi_{\text{in-plane}}$  ( $\chi_{\text{ip}}$  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  $\chi$  は  $\pi/2 + \chi_{\text{ip}}$  である。(a) 射影した CXC の Z 等分線が X 軸から角  $\alpha$  だけずれているときには、Y 軸と Y 軸がなす角も  $\alpha$  である。射影した CXC の Z 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  $\chi_{\text{ip}}$  は X と X で表される。(b) 面内配向がランダムなときには、X は X 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  $\pi$  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、 $\beta_{zxx} = \beta_{xzx}$ 、 $\beta_{zvy} = \beta_{vzv}$ 、(最後のケースでは次も) $\beta_{vzx} = \beta_{zvx}$ 、 $\beta_{zxy} = \beta_{xzv}$ 、 $\beta_{xvz} = \beta_{vxz}$ 

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  $(\phi)$  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  $\beta_{ax} \sim (4/9)\beta_{\zeta\zeta\zeta}, \beta_{ccc} \sim (1/9)\beta_{\zeta\zeta\zeta}$  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。

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

$$\begin{split} \text{(ppp)} \qquad & \chi_{XZX} = (1/2)(\beta_{a\alpha} - \beta_{c\alpha})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) \\ & \chi_{ZXX} = (1/2)(\beta_{a\alpha} - \beta_{c\alpha})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) \\ & \chi_{XXZ} = (1/2)(\beta_{a\alpha} - \beta_{c\alpha})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) \\ & - 2(\cos\alpha - \cos^3\alpha)\cos\theta\} \end{split}$$

$$+ 2\beta_{aa}\cos\alpha\cos\theta$$

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

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

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

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

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

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

(sss) (none)

### [逆対称 (b<sub>1</sub>) 振動]

$$\begin{split} (ppp) \qquad & \chi_{XX} = -(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)] \\ \chi_{XZX} = -(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)] \\ \chi_{XXZ} = & (\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \\ \chi_{ZZZ} = & -2(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \end{split}$$

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

(pps) (none)

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

(sss) (none)

[縮重パンド]  $\beta_{\zeta\zeta\zeta}>>\beta_{\xi\xi\zeta},\ \beta_{\eta\eta\zeta}$  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。

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

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

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

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

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

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

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

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

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

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

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

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

### [逆対称 (b<sub>1</sub>) 振動]

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

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

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

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

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

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

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

#### [面外 (b<sub>2</sub>) 振動]

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

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

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

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

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

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

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

(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** $\mathbb C$ に示す。)

[全対称バンド]  $\beta_{\text{CCC}} >> \beta_{\text{EEC}}$ ,  $\beta_{\text{nnC}}$  のときには  $\beta_{\text{ax}} \sim (4/9)$   $\beta_{\text{CCC}}$ 、 $\beta_{\text{coc}} \sim (1/9)$   $\beta_{\text{CCC}}$  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。

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

### [対称 (a<sub>1</sub>) 振動]

(ppp) 
$$\begin{split} \chi_{XZX} &= (1/2)(\beta_{a\alpha} - \beta_{c\omega})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) \\ \chi_{ZXX} &= (1/2)(\beta_{a\alpha} - \beta_{c\omega})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) \\ \chi_{XXZ} &= (1/2)(\beta_{a\alpha} - \beta_{c\omega})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) - 2(\cos\alpha - \cos^3\alpha)\cos\theta\} \\ &+ 2\beta_{a\alpha}\cos\alpha\cos\theta \end{split}$$

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

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

$$\begin{split} (ssp) \qquad \chi_{YYZ} &= (1/2)(\beta_{a\alpha} - \beta_{c\alpha})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) - 2(\cos\alpha - \cos^3\alpha)\cos\theta\} \\ &+ 2\beta_{a\alpha}\cos\alpha\cos\theta \end{split}$$

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

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

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

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

(sss) (none)

### [逆対称 (b<sub>1</sub>) 振動]

$$\begin{split} (\text{ppp}) \qquad & \chi_{ZXX} = -(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)] \\ \chi_{XZX} = -(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)] \\ \chi_{XXZ} = & (\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \\ \chi_{ZZZ} = & -2(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \end{split}$$

(spp) (none)

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

(psp) (none)

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

(pps) (none)

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

(sss) (none)

[縮重パンド]  $\beta_{\zeta\zeta\zeta}>>\beta_{\xi\xi\zeta},\ \beta_{\eta\eta\zeta}$  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。

$$eta_{xxz}+eta_{yyz}=-4eta_{caa}(\coslpha-\cos^3lpha)\pm2eta_{aaa}\sin^3lpha$$
  $eta_{xxz}-eta_{yyz}=-4eta_{caa}(\coslpha-\cos^3lpha)\pm2eta_{aaa}(2\sinlpha+\sin^3lpha)$   $eta_{xxz}+eta_{yyz}-2eta_{zz}=-12eta_{caa}(\coslpha-\cos^3lpha)-(\pm)2eta_{aaa}\sin^3lpha$   $eta_{zxx}=-2eta_{caa}(\coslpha-2\cos^3lpha)-(\pm)2eta_{aaa}(\sinlpha-\sin^3lpha)$   $eta_{zyy}=2eta_{caa}\coslpha-(\pm)2eta_{aaa}\sinlpha$  であるから、

### [対称 (a<sub>1</sub>) 振動]

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

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

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

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

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

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

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

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

$$\pm (1/2)\beta_{aaa}(2\sin\alpha + \sin^3\alpha)]\sin^2\theta\sin2\phi$$

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

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

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

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

$$\pm (1/2)\beta_{aaa}(2\sin\alpha + \sin^{3}\alpha)]\sin^{2}\theta\sin 2\phi$$

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

$$\pm (1/2)\beta_{aaa}(2\sin\alpha + \sin^{3}\alpha)]\sin^{2}\theta\sin 2\phi$$

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

(sss) (none)

### [逆対称 (b<sub>1</sub>) 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)、 $3/8$   $\beta_{\zeta\zeta\zeta}$  (sp²)である。)

$$\begin{split} (\text{ppp}) \qquad & \chi_{ZXX} = \left[ -\beta_{\text{can}} (\cos\alpha - 2\cos^3\alpha) - (\pm)\beta_{\text{aan}} (\sin\alpha - \sin^3\alpha) \right] [\cos\theta - (\cos\theta - \cos^3\theta) (1 + \cos2\phi)] \\ \chi_{XZX} = \left[ -\beta_{\text{can}} (\cos\alpha - 2\cos^3\alpha) - (\pm)\beta_{\text{aan}} (\sin\alpha - \sin^3\alpha) \right] [\cos\theta - (\cos\theta - \cos^3\theta) (1 + \cos2\phi)] \\ \chi_{XXZ} = -\left[ -\beta_{\text{can}} (\cos\alpha - 2\cos^3\alpha) - (\pm)\beta_{\text{aan}} (\sin\alpha - \sin^3\alpha) \right] (\cos\theta - \cos^3\theta) (1 + \cos2\phi) \\ \chi_{ZZZ} = 2\left[ -\beta_{\text{can}} (\cos\alpha - 2\cos^3\alpha) - (\pm)\beta_{\text{aan}} (\sin\alpha - \sin^3\alpha) \right] (\cos\theta - \cos^3\theta) (1 + \cos2\phi) \end{split}$$

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

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

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

(sss) (none)

### [面外 (b<sub>2</sub>) 振動]

$$\begin{split} (ppp) \qquad & \chi_{ZXX} = [\beta_{caa} cos\alpha - (\pm)\beta_{aaa} sin\alpha][cos\theta - (cos\theta - cos^3\theta)(1 - cos2\phi)] \\ \chi_{XZX} = [\beta_{caa} cos\alpha - (\pm)\beta_{aaa} sin\alpha][cos\theta - (cos\theta - cos^3\theta)(1 - cos2\phi)] \\ \chi_{XXZ} = -[\beta_{caa} cos\alpha - (\pm)\beta_{aaa} sin\alpha](cos\theta - cos^3\theta)(1 - cos2\phi) \\ \chi_{ZZZ} = 2[\beta_{caa} cos\alpha - (\pm)\beta_{aaa} sin\alpha](cos\theta - cos^3\theta)(1 - cos2\phi) \end{split}$$

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

(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  $\beta_{aac} \sim (4/9) \beta_{\zeta\zeta\zeta}$ 、 $\beta_{cac} \sim (1/9) \beta_{\zeta\zeta\zeta}$  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。

$$eta_{xxz} + eta_{yyz} = -2(eta_{ax} - eta_{cx})(\cos\alpha - \cos^3\alpha) + 4eta_{ax}\cos\alpha$$
 $eta_{xxz} - eta_{yyz} = -2(eta_{ax} - eta_{cx})(\cos\alpha - \cos^3\alpha)$ 
 $eta_{xxz} + eta_{yyz} - 2eta_{zz} = -2(eta_{ax} - eta_{cx})[3(\cos\alpha - \cos^3\alpha) - 2\cos\alpha]$ 
 $eta_{zxx} = -2(eta_{ax} - eta_{cx})(\cos\alpha - \cos^3\alpha)$  であるから、

### [対称(a<sub>1</sub>)振動]

$$\begin{split} (\text{ppp}) \qquad & \chi_{\text{XZX}} = (1/2)(\beta_{\text{a}\alpha} - \beta_{\text{c}\alpha})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) \\ \chi_{\text{ZXX}} = & (1/2)(\beta_{\text{a}\alpha} - \beta_{\text{c}\alpha})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) \\ \chi_{\text{XXZ}} = & (1/2)(\beta_{\text{a}\alpha} - \beta_{\text{c}\alpha})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) - 2(\cos\alpha - \cos^3\alpha)\cos\theta\} \\ & + 2\beta_{\text{a}\alpha}\cos\alpha\cos\theta \\ \chi_{\text{ZZZ}} = & -(\beta_{\text{a}\alpha} - \beta_{\text{c}\alpha})[(\cos\alpha - \cos^3\alpha)(1 + \cos2\varphi)(\cos\theta - \cos^3\theta) + 2\cos^3\alpha\cos^3\theta] \end{split}$$

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

$$\begin{split} (ssp) \qquad \chi_{YYZ} &= (1/2)(\beta_{a\alpha} - \beta_{c\alpha})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) - 2(\cos\alpha - \cos^3\alpha)\cos\theta\} \\ &+ 2\beta_{a\alpha}\cos\alpha\cos\theta \end{split}$$

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

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

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

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

(sss) (none)

#### [逆対称 (b<sub>1</sub>) 振動]

$$\begin{split} (ppp) \qquad & \chi_{ZXX} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)] \\ \chi_{XZX} = -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)] \\ \chi_{XXZ} = & (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \\ \chi_{ZZZ} = & -2(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \end{split}$$

(spp) (none)

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

(psp) (none)

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

(pps) (none)

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

(sss) (none)

**[縮重バンド]**  $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\zeta\zeta}$ ,  $\beta_{\eta\eta\zeta}$  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)
\tau あるから、
```

### [対称 (a<sub>1</sub>) 振動]

$$\begin{aligned} (\text{ppp}) \quad & \chi_{\text{XZX}} = (3/4)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) - \beta_{\text{am}}\sin^3\alpha(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})](\cos\theta - \cos^3\theta) \\ & + (1/4)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) - \beta_{\text{am}}(2\sin\alpha - \sin^3\alpha)(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})]\cos2\varphi(\cos\theta - \cos^3\theta) \\ & - (1/2)[\pm\beta_{\text{cm}}\sin^2\alpha\sin2\varphi_{\text{A}} - \beta_{\text{am}}\sin\alpha\cos\alpha(\sin3\varphi_{\text{A}} \pm \sin\varphi_{\text{A}})](\cos\theta - \cos^3\theta)\sin2\varphi \\ & \chi_{\text{ZXX}} = (3/4)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) - \beta_{\text{am}}\sin^3\alpha(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})](\cos\theta - \cos^3\theta) \\ & + (1/4)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) - \beta_{\text{am}}\sin^3\alpha(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})]\cos\theta - \cos^3\theta) \\ & + (1/4)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) - \beta_{\text{am}}(2\sin\alpha - \sin^3\alpha)(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})]\cos2\varphi(\cos\theta - \cos^3\theta) \\ & - (1/2)[\pm\beta_{\text{cm}}\sin^2\alpha\sin2\varphi_{\text{A}} - \beta_{\text{am}}\sin\alpha\cos\alpha(\sin3\varphi_{\text{A}} \pm \sin\varphi_{\text{A}})](\cos\theta - \cos^3\theta)\sin2\varphi \\ & \chi_{\text{XXZ}} = -(1/2)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) + \beta_{\text{am}}\sin^3\alpha(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})]\cos\theta \\ & + (3/4)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) + \beta_{\text{am}}\sin^3\alpha(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})]\cos\theta - \cos^3\theta) \\ & + (1/4)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) - \beta_{\text{am}}(2\sin\alpha - \sin^3\alpha)(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})]\cos2\varphi(\cos\theta - \cos^3\theta) \\ & - (1/2)[\pm\beta_{\text{cm}}\sin^2\alpha\sin2\varphi_{\text{A}} - \beta_{\text{am}}\sin\alpha\cos\alpha(\sin3\varphi_{\text{A}} \pm \sin\varphi_{\text{A}})](\cos\theta - \cos^3\theta)\sin2\varphi \\ & \chi_{\text{ZZZ}} = -(1/2)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) + \beta_{\text{am}}\sin^3\alpha(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})]\cos\theta \\ & + (3/2)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) + \beta_{\text{am}}\sin^3\alpha(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})]\cos\theta \\ & - (1/2)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) + \beta_{\text{am}}\sin^3\alpha(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})]\cos\theta \\ & + (3/2)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) + \beta_{\text{am}}\sin^3\alpha(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})]\cos\theta \\ & + (1/2)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) + \beta_{\text{am}}\sin^3\alpha(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})]\cos2\varphi(\cos\theta - \cos^3\theta) \\ & + [\pm\beta_{\text{cm}}\sin^2\alpha\sin2\varphi_{\text{A}} - \beta_{\text{am}}\sin\alpha\cos\alpha(\sin3\varphi_{\text{A}} \pm \sin\varphi_{\text{A}})](\cos\theta - \cos^3\theta)\sin2\varphi \\ & \chi_{\text{ZZZ}} = -(1/4)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) - \beta_{\text{am}}(2\sin\alpha - \sin^3\alpha)(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})]\sin2\varphi\sin2\varphi \\ & \chi_{\text{ZZZ}} = -(1/4)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) - \beta_{\text{am}}(2\sin\alpha - \sin^3\alpha)(\cos3\varphi_{\text{A}} \pm \cos\varphi_{\text{A}})]\sin2\varphi\sin2\varphi \\ & \chi_{\text{ZZZ}} = -(1/2)[2\beta_{\text{cm}}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_{\text{A}}) - \beta_{\text{am}}$$

$$\begin{split} (ssp) \qquad & \chi_{YYZ} = -(1/2)[2\beta_{cas}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_A) + \beta_{aas}\sin^3\alpha(\cos3\varphi_A \pm \cos\varphi_A)]\cos\theta \\ & + (3/4)[2\beta_{cas}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_A) + \beta_{aas}\sin^3\alpha(\cos3\varphi_A \pm \cos\varphi_A)](\cos\theta - \cos^3\theta) \\ & + (1/4)[2\beta_{cas}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_A) - \beta_{aas}(2\sin\alpha - \sin^3\alpha)(\cos3\varphi_A \pm \cos\varphi_A)]\cos2\varphi(\cos\theta - \cos^3\theta) \\ & - (1/2)[\pm\beta_{cas}\sin^2\alpha\sin2\varphi_A - \beta_{aas}\sin\alpha\cos\alpha(\sin3\varphi_A \pm \sin\varphi_A)](\cos\theta - \cos^3\theta)\sin2\varphi \\ (psp) \qquad & \chi_{ZYX} = -(1/4)[2\beta_{cas}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_A) - \beta_{aas}(2\sin\alpha - \sin^3\alpha)(\cos3\varphi_A \pm \cos\varphi_A)]\sin2\varphi\sin^2\theta \end{split}$$

 $-(1/2)[\pm\beta_{\rm can}\sin^2\alpha\sin^2\phi_{\rm A}-\beta_{\rm aaa}\sin\alpha\cos\alpha(\sin3\phi_{\rm A}\pm\sin\phi_{\rm A})]\sin^2\theta\cos2\phi$ 

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

(pps) 
$$\chi_{ZYY} = -(1/4)[2\beta_{cm} \cos \alpha - \cos^3 \alpha)(1 \pm \cos 2\phi_A) - \beta_{am} \sin \alpha \cos \alpha(\sin 3\phi_A \pm \sin \phi_A)](\cos 3\phi_A \pm \cos \phi_A)]\sin 2\phi \sin 2\phi$$
 (pps)  $\chi_{ZYY} = -(1/4)[2\beta_{cm} (\cos \alpha - \cos^3 \alpha)(1 \pm \cos 2\phi_A) - \beta_{am} (2\sin \alpha - \sin^3 \alpha)(\cos 3\phi_A \pm \cos \phi_A)]\sin 2\phi \sin^2 \theta$   $+ (1/2)[\pm \beta_{cm} \sin^2 \alpha \sin 2\phi_A - \beta_{am} \sin \alpha \cos \alpha \cos(\sin 3\phi_A \pm \sin \phi_A)]\sin^2 \theta \cos 2\phi$   $\chi_{ZXY} = -(1/4)[2\beta_{cm} (\cos \alpha - \cos^3 \alpha)(1 \pm \cos 2\phi_A) - \beta_{am} (2\sin \alpha - \sin^3 \alpha)(\cos 3\phi_A \pm \cos \phi_A)]\sin 2\phi \sin^2 \theta$   $+ (1/2)[\pm \beta_{cm} \sin^2 \alpha \sin 2\phi_A - \beta_{am} \sin \alpha \cos \alpha (\sin 3\phi_A \pm \sin \phi_A)]\sin^3 \theta \cos 2\phi$  (pss)  $\chi_{ZYY} = (3/4)[2\beta_{cm} (\cos \alpha - \cos^3 \alpha)(1 \pm \cos 2\phi_A) + \beta_{am} \sin^3 \alpha (\cos 3\phi_A \pm \cos \phi_A)](\cos \theta - \cos^3 \theta)$   $+ (1/4)[2\beta_{cm} (\cos \alpha - \cos^3 \alpha)(1 \pm \cos 2\phi_A) - \beta_{am} (2\sin \alpha - \sin^3 \alpha)(\cos 3\phi_A \pm \cos \phi_A)]\cos 2\phi (\cos \theta - \cos^3 \theta)$   $+ (1/2)[\pm \beta_{cm} \sin^2 \alpha \sin 2\phi_A - \beta_{am} \sin \alpha \cos \alpha (\sin 3\phi_A \pm \sin \phi_A)](\cos \theta - \cos^3 \theta)\sin 2\phi$  (sss) (none)

[**逆対称 (b.) 振動 ]** ( $\beta_{\xi\xi\xi} > \beta_{\eta\eta\xi} \succeq \sigma \delta \succeq \beta_{\eta\eta} = \beta_{\xi\xi\xi} (\cos \alpha - \cos^3 \alpha) - 2\sqrt{3/9} \beta_{\xi\xi\xi} (Td), 3/8 \beta_{\xi\xi\xi} (sp^2)$ である。) (ppp)  $\chi_{ZXX} = -(1/2)[\beta_{cm} (\cos \alpha - 2\cos^3 \alpha)(1 \pm \cos 2\phi_A) - \beta_{am} (\sin \alpha - \sin^3 \alpha)(\cos 3\phi_A \pm \cos \phi_A)] \times [\cos \theta - (1 + \cos 2\phi)(\cos \theta - \cos^3 \theta)]$   $+ (1/2)[(\pm)\beta_{cm} \sin^2 \alpha \sin 2\phi_A + \beta_{am} \sin \alpha \cos \alpha (\sin 3\phi_A \pm \sin \phi_A)](\cos \theta - \cos^3 \theta)\sin 2\phi$   $\chi_{ZXX} = -(1/2)[\beta_{cm} (\cos \alpha - 2\cos^3 \alpha)(1 \pm \cos 2\phi_A) - \beta_{am} (\sin \alpha - \sin^3 \alpha)(\cos 3\phi_A \pm \cos \phi_A)] \times [\cos \theta - (1 + \cos 2\phi)(\cos \theta - \cos^3 \theta)]$   $+ (1/2)[(\pm)\beta_{cm} \cos \alpha - 2\cos^3 \alpha)(1 \pm \cos 2\phi_A) - \beta_{am} (\sin \alpha - \sin^3 \alpha)(\cos 3\phi_A \pm \cos \phi_A)] \times [\cos \theta - (1 + \cos 2\phi)(\cos \theta - \cos^3 \theta)]$   $+ (1/2)\beta_{cm} (\cos \alpha - 2\cos^3 \alpha)(1 \pm \cos 2\phi_A) - \beta_{am} (\sin \alpha - \sin^3 \alpha)(\cos 3\phi_A \pm \cos \phi_A)]$   $\times [\cos \theta - (1 + \cos 2\phi)(\cos \theta - \cos^3 \theta)]$   $+ \beta_{am} \sin \alpha \cos \alpha (\sin 3\phi_A \pm \sin \phi_A)](\cos \theta - \cos^3 \theta)\sin 2\phi$   $\chi_{ZZZ} = -[\beta_{cm} (\cos \alpha - 2\cos^3 \alpha)(1 \pm \cos 2\phi_A) - \beta_{am} (\sin \alpha - \sin^3 \alpha)(\cos 3\phi_A \pm \cos \phi_A)]$   $\times (1 + \cos 2\phi)(\cos \theta - \cos^3 \theta)$   $+ \beta_{am} \sin \alpha \cos \alpha (\sin 3\phi_A \pm \sin \phi_A)](\cos \theta - \cos^3 \theta)\sin 2\phi$   $\chi_{ZZZ} = -[\beta_{cm} (\cos \alpha - 2\cos^3 \alpha)(1 \pm \cos 2\phi_A) - \beta_{am} (\sin \alpha - \sin^3 \alpha)(\cos 3\phi_A \pm \cos \phi_A)]$   $\times (1 + \cos 2\phi)(\cos \theta - \cos^3 \theta)$   $- [(\pm)\beta_{cm} \sin^2 \alpha \sin 2\phi_A + \beta_{am} \sin \alpha \cos \alpha (\sin 3\phi_A \pm \sin \phi_A)](\cos \theta - \cos^3 \theta)\sin 2\phi$   $\times (1 + \cos 2\phi)(\cos \theta - \cos^3 \theta)$   $- [(\pm)\beta_{cm} \sin^2 \alpha \sin 2\phi_A + \beta_{am} \sin \alpha \cos \alpha (\sin 3\phi_A \pm \sin \phi_A)](\cos \theta - \cos^3 \theta)\sin 2\phi$   $- [(\pm)\beta_{cm}$ 

$$\begin{split} (ssp) \qquad \chi_{YYZ} &= (1/2) [\beta_{caa} (cos\alpha - 2cos^3\alpha) (1 \pm cos2\varphi_A) - \beta_{aaa} (sin\alpha - sin^3\alpha) (cos3\varphi_A \pm cos\varphi_A)] \\ &\times (1 + cos2\varphi) (cos\theta - cos^3\theta) \end{split}$$

$$+ (1/2)[(\pm)\beta_{cas}\sin^{2}\alpha\sin^{2}\phi_{A} + \beta_{aas}\sin\alpha\cos\alpha(\sin3\phi_{A} \pm \sin\phi_{A})](\cos\theta - \cos^{3}\theta)\sin2\phi$$
(psp) 
$$\chi_{ZYX} = (1/4)[(\pm)\beta_{cas}\sin^{2}\alpha\sin2\phi_{A} + \beta_{aas}\sin\alpha\cos\alpha(\sin3\phi_{A} \pm \sin\phi_{A})](1 - 3\cos^{2}\theta - \sin^{2}\theta\cos2\phi)$$

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

(pps) 
$$\chi_{ZXY} = -(1/4)[(\pm)\beta_{cas}\sin^2\alpha\sin^2\phi_A + \beta_{aas}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](1 - 3\cos^2\theta - \sin^2\theta\cos2\phi)$$
$$\chi_{XZY} = -(1/4)[(\pm)\beta_{cas}\sin^2\alpha\sin^2\phi_A + \beta_{aas}\sin\alpha\cos\alpha(\sin3\phi_A \pm \sin\phi_A)](1 - 3\cos^2\theta - \sin^2\theta\cos2\phi)$$

$$\begin{split} (pss) \qquad & \chi_{ZYY} = -(1/2) [\beta_{caa} (cos\alpha - 2cos^3\alpha) (1 \pm cos2\varphi_A) - \beta_{aaa} (sin\alpha - sin^3\alpha) (cos3\varphi_A \pm cos\varphi_A)] \\ & \times [cos\theta - (1 + cos2\varphi) (cos\theta - cos^3\theta)] \\ & \qquad \qquad + (1/2) [(\pm)\beta_{caa} sin^2\alpha sin2\varphi_A + \beta_{aaa} sin\alpha cos\alpha (sin3\varphi_A \pm sin\varphi_A)] (cos\theta - cos^3\theta) sin2\varphi \\ (sss) \qquad & (none) \end{split}$$

### [面外 (b<sub>2</sub>) 振動]

$$(pss) \qquad \chi_{ZYY} = (1/2)[\beta_{cas} cos\alpha(1 - (\pm)cos2\phi_A) - \beta_{aas} sin\alpha(cos3\phi_A - (\pm)cos\phi_A)][cos\theta - (1 - cos2\phi)(cos\theta - cos^3\theta)]$$

+  $(1/2)[(\pm)\beta_{ca}(2\cos^2\alpha - 1)\sin 2\phi_A + \beta_{aaa}\sin \alpha\cos\alpha(\sin 3\phi_A - (\pm)\sin\phi_A)](\cos\theta - \cos^3\theta)\sin 2\phi$ 

(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。

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

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

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

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

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

$$\beta_{xzz} = -2(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)$$

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

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

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

$$\beta_{zxx} = -2(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)$$
 ౌవర్స్

### [対称 (a<sub>1</sub>) 振動]

$$\begin{split} (\text{ppp}) \qquad & \chi_{\text{XZX}} = (1/2)(\beta_{\text{aac}} - \beta_{\text{cw}})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) \\ & \chi_{\text{ZXX}} = (1/2)(\beta_{\text{aac}} - \beta_{\text{cw}})[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) \\ & \chi_{\text{XXZ}} = (1/2)(\beta_{\text{aac}} - \beta_{\text{cw}})\{[(\cos\alpha - \cos^3\alpha)(3 + \cos2\varphi) - 2\cos\alpha](\cos\theta - \cos^3\theta) \\ & - 2(\cos\alpha - \cos^3\alpha)\cos\theta\} + 2\beta_{\text{aac}}\cos\alpha\cos\theta \\ & \chi_{\text{ZZZ}} = -(\beta_{\text{aac}} - \beta_{\text{cw}})[(\cos\alpha - \cos^3\alpha)(1 + \cos2\varphi)(\cos\theta - \cos^3\theta) + 2\cos^3\alpha\cos^3\theta] \end{split}$$

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

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

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

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

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

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

(sss) (none)

### [逆対称 (b<sub>1</sub>) 振動]

$$\begin{split} (\text{ppp}) \qquad & \chi_{ZXX} = -(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)] \\ & \chi_{XZX} = -(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)[\cos\theta - (\cos\theta - \cos^3\theta)(1 + \cos2\phi)] \\ & \chi_{XXZ} = (\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \\ & \chi_{ZZZ} = -2(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \end{split}$$

(spp) (none)

(ssp) 
$$\chi_{yyz} = (\beta_{axc} - \beta_{cxc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos 2\phi)$$

(psp) (none)

$$(sps) \hspace{1cm} \chi_{YZY} = -(\beta_{a\alpha} - \beta_{c\alpha})(cos\alpha - cos^3\alpha)[cos\theta - (cos\theta - cos^3\theta)(1 + cos2\phi)]$$

(pps) (none)

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

(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。

 $(\beta_{zyy}$ と $\beta_{yzy}$ 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。)

 $(\pm$  記号の上側は $\varphi_A=0,\,\varphi_B=\pi$  に、下側は  $\varphi_A=\pi,\,\varphi_B=0$  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。

$$\beta_{\rm xxx} = -2\beta_{\rm cas}(\cos\alpha - 2\cos^3\alpha)$$

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

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

$$\beta_{\rm vzv} = 2\beta_{\rm caa}\cos\alpha$$

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

$$\beta_{\rm vvz} = 0$$

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

# [対称 (a<sub>1</sub>) 振動]

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

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

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

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

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

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

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

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

$$(pps) \hspace{1cm} \chi_{XZY} = -\beta_{caa}(cos\alpha - cos^{3}\alpha)sin2\phi sin^{2}\theta$$

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

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

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

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

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

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

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

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

(pps) (none)

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

(sss) (none)

### [面外 (b<sub>2</sub>) 振動]

$$\begin{split} (\text{ppp}) \qquad & \chi_{\text{ZXX}} = \beta_{\text{cas}} \text{cos} \alpha [\text{cos}\theta - (\text{cos}\theta - \text{cos}^3\theta)(1 - \text{cos}2\phi)] \\ & \chi_{\text{XZX}} = \beta_{\text{cas}} \text{cos} \alpha [\text{cos}\theta - (\text{cos}\theta - \text{cos}^3\theta)(1 - \text{cos}2\phi)] \\ & \chi_{\text{XXZ}} = -\beta_{\text{cas}} \text{cos}(\text{cos}\theta - \text{cos}^3\theta)(1 - \text{cos}2\phi) \\ & \chi_{\text{ZZZ}} = 2\beta_{\text{cas}} \text{cos}(\text{cos}\theta - \text{cos}^3\theta)(1 - \text{cos}2\phi) \end{split}$$

(none) (spp)

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

(none) (psp)

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

(pps) (none)

(pss) 
$$\gamma_{ZYY} = \beta_{cm} \cos\alpha [\cos\theta - (\cos\theta - \cos^3\theta)(1 - \cos2\phi)]$$

(none) (sss)

### 付録 A: (CH<sub>3</sub>)<sub>2</sub>X 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<sub>3</sub>)<sub>2</sub>X 基に固定した座標系; (x, y, z) 系: 2個のメチル基の C<sub>3</sub>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  $\alpha$  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  $\phi_A,\phi_B$  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  $180^\circ$  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;** $(\chi,\theta,\phi)$ : 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  $2\alpha$  として、 $(0, \alpha, \phi)$ と  $(\pi, \alpha, \phi)$ 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、

$$\beta_{ik} = \sum U_{ik:abc} \beta_{abc}$$
 (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  $U_{ij:cabc}$  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  $\theta$  に関しては表で使っている  $\sin\theta$ 、 $\sin2\theta$ 、 $\sin3\theta$  の形の三角関数ではなく、下の関係式で変換した  $\sin\theta$ 、 $\cos\theta$  のべき乗による表式を採用する。)

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

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

$$\begin{split} \beta_{xxz} &= -2(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha) + 2\beta_{aac}\!\!\cos\!\alpha \\ \beta_{yyz} &= +2\beta_{a\alpha}\!\!\cos\!\alpha \\ \beta_{zzz} &= +2(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha) + 2\beta_{c\alpha}\!\!\cos\!\alpha \\ \beta_{zxx} &= -2(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha) \\ \beta_{xzx} &= -2(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha) \end{split}$$

[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。) ( $\pm$  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

$$\begin{split} \beta_{zxx} &= -(1/2)\beta_{caa}(cos\alpha - 2cos^3\alpha)[2 \pm (cos2\varphi_A + cos2\varphi_B)] \\ &+ (1/2)\beta_{aaa}(sin\alpha - sin^3\alpha)[(cos3\varphi_A + cos3\varphi_B) \pm (cos\varphi_A + cos\varphi_B)] \\ \beta_{xzx} &= -(1/2)\beta_{caa}(cos\alpha - 2cos^3\alpha)[2 \pm (cos2\varphi_A + cos2\varphi_B)] \\ &+ (1/2)\beta_{aaa}(sin\alpha - sin^3\alpha)[(cos3\varphi_A + cos3\varphi_B) \pm (cos\varphi_A + cos\varphi_B)] \\ \beta_{zyy} &= (1/2)\beta_{caa}cos\alpha[2 - (\pm)(cos2\varphi_A + cos2\varphi_B)] \\ &- (1/2)\beta_{aaa}sin\alpha[(cos3\varphi_A + cos3\varphi_B) - (\pm)(cos\varphi_A + cos\varphi_B)] \\ \beta_{yzy} &= (1/2)\beta_{caa}cos\alpha[2 - (\pm)(cos2\varphi_A + cos2\varphi_B)] \\ &- (1/2)\beta_{aaa}sin\alpha[(cos3\varphi_A + cos3\varphi_B) - (\pm)(cos\varphi_A + cos\varphi_B)] \\ \beta_{xxz} &= -\beta_{caa}(cos\alpha - cos^3\alpha)[2 \pm (cos2\varphi_A + cos2\varphi_B)] \\ &+ (1/2)\beta_{aaa}(sin\alpha - sin^3\alpha)[(cos3\varphi_A + cos3\varphi_B) \pm (cos\varphi_A + cos\varphi_B)] \\ \beta_{yyz} &= -(1/2)\beta_{aaa}sin\alpha[(cos3\varphi_A + cos3\varphi_B) \pm (cos\varphi_A + cos\varphi_B)] \\ \beta_{zzz} &= \beta_{caa}(cos\alpha - cos^3\alpha)[2 \pm (cos2\varphi_A + cos2\varphi_B)] \\ &+ (1/2)\beta_{aaa}sin\alpha[(cos3\varphi_A + cos3\varphi_B) \pm (cos\varphi_A + cos\varphi_B)] \\ \end{pmatrix} \\ &+ (1/2)\beta_{aaa}sin^3\alpha[(cos3\varphi_A + cos3\varphi_B) \pm (cos\varphi_A + cos\varphi_B)] \\ \end{pmatrix}$$

### グループ 2

$$\begin{split} \beta_{yzx} &= -(\pm)(1/2)\beta_{caa}\cos^2\alpha(\sin 2\varphi_A + \sin 2\varphi_B) \\ &- (1/2)\beta_{aaa}\sin\alpha\cos\alpha[(\sin 3\varphi_A + \sin 3\varphi_B) \pm (\sin \varphi_A + \sin \varphi_B)] \\ \beta_{zyx} &= -(\pm)(1/2)\beta_{caa}\cos^2\alpha(\sin 2\varphi_A + \sin 2\varphi_B) \\ &- (1/2)\beta_{aaa}\sin\alpha\cos\alpha[(\sin 3\varphi_A + \sin 3\varphi_B) \pm (\sin \varphi_A + \sin \varphi_B)] \\ \beta_{zxy} &= -(\pm)(1/2)\beta_{caa}(2\cos^2\alpha - 1)(\sin 2\varphi_A + \sin 2\varphi_B) \\ &- (1/2)\beta_{aaa}\sin\alpha\cos\alpha[(\sin 3\varphi_A + \sin 3\varphi_B) - (\pm)(\sin \varphi_A + \sin \varphi_B)] \\ \beta_{xzy} &= -(\pm)(1/2)\beta_{caa}(2\cos^2\alpha - 1)(\sin 2\varphi_A + \sin 2\varphi_B) \\ &- (1/2)\beta_{aaa}\sin\alpha\cos\alpha[(\sin 3\varphi_A + \sin 3\varphi_B) - (\pm)(\sin \varphi_A + \sin \varphi_B)] \\ \beta_{xyz} &= \pm (1/2)\beta_{caa}\sin^2\alpha(\sin 2\varphi_A + \sin 2\varphi_B) \\ &- (1/2)\beta_{aaa}\sin\alpha\cos\alpha[(\sin 3\varphi_A + \sin 3\varphi_B) \pm (\sin \varphi_A + \sin \varphi_B)] \\ \beta_{yxz} &= \pm (1/2)\beta_{caa}\sin^2\alpha(\sin 2\varphi_A + \sin 2\varphi_B) \\ &- (1/2)\beta_{aaa}\sin\alpha\cos\alpha[(\sin 3\varphi_A + \sin 3\varphi_B) \pm (\sin \varphi_A + \sin \varphi_B)] \\ - (1/2)\beta_{aaa}\sin\alpha\cos\alpha[(\sin 3\varphi_A + \sin 3\varphi_B) \pm (\sin \varphi_A + \sin \varphi_B)] \\ \end{pmatrix} \end{split}$$

### グループ 3

$$\begin{split} \beta_{xxx} &= -(\pm)\beta_{cas}(\sin\alpha - \sin^3\alpha)(\cos2\varphi_A - \cos2\varphi_B) \\ &- (1/2)\beta_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\varphi_A - \cos3\varphi_B) \pm (\cos\varphi_A - \cos\varphi_B)] \\ \beta_{yyx} &= -(1/2)\beta_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\varphi_A - \cos3\varphi_B) \pm (\cos\varphi_A - \cos\varphi_B)] \\ \beta_{zzx} &= \pm\beta_{cas}(\sin\alpha - \sin^3\alpha)(\cos2\varphi_A - \cos2\varphi_B) \\ &+ (1/2)\beta_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\varphi_A - \cos3\varphi_B) \pm (\cos\varphi_A - \cos\varphi_B)] \\ \beta_{xyy} &= \pm (1/2)\beta_{cas}\sin\alpha (\cos2\varphi_A - \cos2\varphi_B) \\ &- (1/2)\beta_{aaa}\cos\alpha [(\cos3\varphi_A - \cos2\varphi_B) \\ &- (1/2)\beta_{aaa}\cos\alpha [(\cos3\varphi_A - \cos2\varphi_B) \\ &- (1/2)\beta_{cas}\sin\alpha (\cos2\varphi_A - \cos2\varphi_B) \\ &- (1/2)\beta_{aaa}\cos\alpha [(\cos3\varphi_A - \cos2\varphi_B) \\ &- (1/2)\beta_{aaa}\cos\alpha [(\cos3\varphi_A - \cos2\varphi_B) \\ &+ (1/2)\beta_{aaa}(\cos\alpha - 2\sin^3\alpha)(\cos2\varphi_A - \cos2\varphi_B) \\ &+ (1/2)\beta_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\varphi_A - \cos3\varphi_B) \pm (\cos\varphi_A - \cos\varphi_B)] \\ \beta_{zxz} &= \pm (1/2)\beta_{caa}(\sin\alpha - 2\sin^3\alpha)(\cos2\varphi_A - \cos2\varphi_B) \\ &+ (1/2)\beta_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\varphi_A - \cos3\varphi_B) \pm (\cos\varphi_A - \cos\varphi_B)] \\ \end{pmatrix} \\ + (1/2)\beta_{aaa}(\cos\alpha - \cos^3\alpha)[(\cos3\varphi_A - \cos3\varphi_B) \pm (\cos\varphi_A - \cos\varphi_B)] \\ \end{split}$$

# グループ 4

$$\begin{split} \beta_{yxx} &= \pm (1/2)\beta_{caa} sin\alpha cos\alpha \ (sin2\varphi_A - sin2\varphi_B) \\ &- (1/2)\beta_{aaa} cos^2\alpha \ [(sin3\varphi_A - sin3\varphi_B) \pm (sin\varphi_A - sin\varphi_B)] \\ \beta_{xyx} &= \pm (1/2)\beta_{caa} sin\alpha cos\alpha \ (sin2\varphi_A - sin2\varphi_B) \\ &- (1/2)\beta_{aaa} cos^2\alpha \ [(sin3\varphi_A - sin3\varphi_B) \pm (sin\varphi_A - sin\varphi_B)] \\ \beta_{xxy} &= \pm \beta_{caa} sin\alpha cos\alpha \ (sin2\varphi_A - sin2\varphi_B) \\ &- (1/2)\beta_{aaa} \ cos^2\alpha \ [(sin3\varphi_A - sin3\varphi_B) - (\pm)(sin\varphi_A - sin\varphi_B)] \\ \beta_{yyy} &= (1/2)\beta_{aaa} [(sin3\varphi_A - sin3\varphi_B) - (\pm)(sin\varphi_A - sin\varphi_B)] \\ \beta_{zzy} &= -(\pm)\beta_{caa} sin\alpha cos\alpha \ (sin2\varphi_A - sin2\varphi_B) \\ &- (1/2)\beta_{aaa} sin^2\alpha \ [(sin3\varphi_A - sin3\varphi_B) - (\pm)(sin\varphi_A - sin\varphi_B)] \\ \beta_{yzz} &= -(\pm 1/2)\beta_{caa} sin\alpha cos\alpha \ (sin2\varphi_A - sin2\varphi_B) \end{split}$$

$$\begin{split} &-(1/2)\!\beta_{aaa}sin^2\alpha\;[(sin3\varphi_A-sin3\varphi_B)\pm(sin\varphi_A-sin\varphi_B)]\\ \beta_{zyz} &= -(\pm1/2)\!\beta_{caa}sin\alpha\!cos\alpha\;(sin2\varphi_A-sin2\varphi_B)\\ &-(1/2)\!\beta_{aaa}sin^2\alpha\;[(sin3\varphi_A-sin3\varphi_B)\pm(sin\varphi_A-sin\varphi_B)] \end{split}$$

### 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。

$$eta_{xxz} + eta_{yyz} = -2(eta_{ax} - eta_{cx})(\cos\alpha - \cos^3\alpha) + 4eta_{ax}\cos\alpha$$
 $eta_{xxz} - eta_{yyz} = -2(eta_{ax} - eta_{cx})(\cos\alpha - \cos^3\alpha)$ 
 $eta_{xxz} + eta_{yyz} - 2eta_{zzz} = -2(eta_{ax} - eta_{cx})[3(\cos\alpha - \cos^3\alpha) - 2\cos\alpha]$ 
 $eta_{zxx} = -2(eta_{ax} - eta_{cx})(\cos\alpha - \cos^3\alpha)$  であるから、

$$\begin{aligned} & (\text{ppp}) \quad \chi_{\text{XXX}} = -2\beta_{\text{asc}}\cos\alpha\sin\theta\cos\chi \\ & + (1/4)(\beta_{\text{asc}} - \beta_{\text{cec}})(\cos\alpha - \cos^3\alpha) \{ 4\sin\theta\cos\chi - 3\sin^3\theta(3\cos\chi + \cos3\chi) \\ & - [\sin\theta(\cos\chi - \cos^3\alpha) - (\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_{\text{asc}} - \beta_{\text{cec}})\cos\alpha\sin^3\theta(3\cos\chi + \cos3\chi) \\ & \chi_{\text{XZZ}} = -(\beta_{\text{asc}} - \beta_{\text{cec}})(\cos\alpha - \cos^2\alpha) [(\sin\theta - \sin^3\theta)\cos\chi(3 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi] \\ & + 2(\beta_{\text{asc}} - \beta_{\text{cec}})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi \\ & \chi_{\text{ZXZ}} = -(\beta_{\text{asc}} - \beta_{\text{cec}})(\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_{\text{asc}} - \beta_{\text{cec}})(\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_{\text{asc}} - \beta_{\text{cec}})(\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_{\text{asc}} - \beta_{\text{cec}})(\cos\alpha - \cos^3\alpha) [\cos\theta - \sin^3\theta)\cos\chi \\ & \chi_{\text{ZZX}} = -2\beta_{\text{asc}}\cos\alpha\sin\theta\cos\chi \\ & \chi_{\text{ZZX}} = (1/2)(\beta_{\text{asc}} - \beta_{\text{cec}})(\cos\alpha - \cos^3\alpha) [(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi] \\ & - (\beta_{\text{asc}} - \beta_{\text{cec}})(\cos\alpha - \cos^3\alpha) [(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi] \\ & - (\beta_{\text{asc}} - \beta_{\text{cec}})(\cos\alpha - \cos^3\alpha) [(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi] \\ & - (\beta_{\text{asc}} - \beta_{\text{cec}})(\cos\alpha - \cos^3\alpha) [-\cos\theta + \cos^3\theta)(1 + \cos2\chi) \\ & \chi_{\text{XXZ}} = (1/2)(\beta_{\text{aac}} - \beta_{\text{cec}})(\cos\alpha - \cos^3\alpha) [-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 + \cos2\chi) \\ & \chi_{\text{XXZ}} = 2\beta_{\text{asc}}\cos\alpha\cos\theta \\ & + (1/2)(\beta_{\text{aac}} - \beta_{\text{cec}})(\cos\alpha - \cos^3\alpha) [-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 + \cos2\chi) \\ & \chi_{\text{ZZZ}} = -2\beta_{\text{asc}}\cos\cos\cos\theta \\ & + (\beta_{\text{asc}} - \beta_{\text{cec}})(\cos\alpha - \cos^3\alpha) [-\cos\theta + \cos^3\theta)\cos2\chi]\cos2\phi + 2\cos^3\theta\sin2\chi\sin2\phi \} \\ & - (\beta_{\text{asc}} - \beta_{\text{cec}})\cos\alpha\cos\theta \\ & + (\beta_{\text{asc}} - \beta_{\text{cec}})(\cos\alpha - \cos^3\alpha) [-\cos\theta + 3\cos^3\theta - (\cos\theta - \cos^3\theta)\cos2\phi] \\ & - 2(\beta_{\text{asc}} - \beta_{\text{cec}})(\cos\alpha - \cos^3\alpha) [-\cos\theta + 3\cos^3\theta - (\cos\theta - \cos^3\theta)\cos2\phi] \\ & - 2(\beta_{\text{asc}} - \beta_{\text{cec}})\cos\alpha\cos^3\theta \end{aligned}$$

```
+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_{\text{YZZ}} = (\beta_{\text{ax}} - \beta_{\text{cx}})(\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_{ax} - \beta_{cx})\cos\alpha(\sin\theta - \sin^3\theta)\sin\alpha
                 \chi_{YZX} = -(1/2)(\beta_{ax} - \beta_{cx})(\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_{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\alpha\}
                                       -2\cos^2\theta\cos 2\chi\sin 2\phi
                        + (\beta_{aac} - \beta_{coc})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                \chi_{yyx} = -2\beta_{ax}\cos\alpha\sin\theta\cos\chi
(ssp)
                        + (1/4)(\beta_{aac} - \beta_{coc})(\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)\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 - \cos2\chi)
                \chi_{XYX} = (1/4)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)\}
(psp)
                                       + 2\sin\theta\cos\theta (\cos\chi + \cos3\chi)\sin2\phi
                       -(1/2)(\beta_{\rm aac} - \beta_{\rm cc})\cos\alpha\sin^3\theta (\sin\chi + \sin3\chi)
                \chi_{\rm ZYZ} = (\beta_{\rm ax} - \beta_{\rm cx})(\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_{ax} - \beta_{cx})\cos\alpha (\sin\theta - \sin^3\theta)\sin\alpha
                 \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\alpha\}
                                       -2\cos^2\theta\cos 2\chi\sin 2\phi
                          + (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                \chi_{\rm ZYX} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\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_{cc})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                \chi_{\rm YXY} = (1/4)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)\}
(sps)
                                          -2\sin\theta\cos\theta (\sin\chi - \sin3\chi)\sin2\phi
                          + (1/2)(\beta_{aac} - \beta_{coc})\cos\alpha\sin^3\theta (cos\chi - cos3\chi)
                 \chi_{\rm YZY} = (1/2)(\beta_{\rm asc} - \beta_{\rm cc})(\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})cosα(cosθ - cos<sup>3</sup>θ)(1 - cos2χ)
                \chi_{XXY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\gamma
(pps)
                        + (1/4)(\beta_{ax} - \beta_{cx})(\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 sinΦcosθ (cosχ - cos3χ)sin2φ}
- (1/2)
$$\beta_{ax}$$
 -  $\beta_{ccx}$  (cosαsin θ(sinχ + sin3χ)

 $\chi_{ZZY} = 2\beta_{ax}$  cosαsinθsinχ
+  $(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\alpha$ )[-sinθ + 3(sinθ - sin  $^3\theta$ ) - sin  $^3\theta$ cos2φ]sinχ
-  $2(\beta_{ax} - \beta_{ccx})$  cosα(sinθ - sin  $^3\theta$ ) sinχ

 $\chi_{ZZY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

 $\chi_{ZXY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

 $\chi_{ZXY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

 $\chi_{ZXY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(pss)  $\chi_{XYY} = (1/4)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(pss)  $\chi_{XYY} = (1/4)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(pss)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(pss)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(pss)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(pss)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(pss)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(pss)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(pss)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(pss)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(psc)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(psc)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(psc)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(psc)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(psc)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(psc)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(psc)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(psc)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(psc)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(psc)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(psc)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(psc)  $\chi_{XYY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )sin2χ

(psc)  $\chi_{XY} = (1/2)(\beta_{ax} - \beta_{ccx})$  (cosα - cos  $^3\theta$ )

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

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

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

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

```
+\sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}
                \chi_{YZZ} = (\beta_{axc} - \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_{cc})(\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
                \chi_{YXZ} = -(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]
               \chi_{YYX} = -(1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[-(\sin\theta - \sin^3\theta)(1 + \cos2\phi) + \sin\theta(1 - \cos2\phi)](\cos\chi - \cos3\chi)\}
(ssp)
                               + 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi}
                \chi_{\rm YYZ} = (\beta_{\rm aac} - \beta_{\rm cc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]
               \chi_{\rm XYX} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi)\}
(psp)
                                      +\sin\theta(\sin\chi-\sin3\chi)(1-\cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi
                \chi_{ZYZ} = (\beta_{ax} - \beta_{cx})(\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_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]
                \chi_{\rm ZYX} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\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}
               \chi_{\text{YXY}} = (1/2)(\beta_{\text{ac}} - \beta_{\text{cm}})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi)\}
(sps)
                                        +\sin\theta(\cos\chi+\cos3\chi)(1-\cos2\phi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}
                \chi_{yzy} = -(1/2)(\beta_{ax} - \beta_{cx})(\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)\sin 2\chi \sin 2\phi
               \chi_{\rm XXY} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(1 + \cos2\phi) - \sin\theta(1 - \cos2\phi)](\sin\chi + \sin3\chi)\}
(pps)
                               + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi
                \chi_{ZZY} = 2(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]
                \chi_{\rm ZXY} = -(1/2)(\beta_{\rm acc} - \beta_{\rm 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_{\rm XZY} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\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_{XYY} = (1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi)\}
(pss)
                                    + (1 - \cos 2\phi)\sin\theta(\cos\chi + \cos 3\chi)] + 2\sin\theta\cos\theta\sin 3\chi\sin 2\phi}
                \chi_{\rm ZYY} = -(1/2)(\beta_{\rm aac} - \beta_{\rm cc})(\cos\alpha - \cos^3\alpha)\{2[\cos\theta \ (1 - \cos2\chi\cos2\varphi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\varphi)]\}
                               -(1 - 3\cos^2\theta)\sin 2\chi \sin 2\phi
               \chi_{\text{YYY}} = -(1/2)(\beta_{\text{asc}} - \beta_{\text{coc}})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 + \cos2\phi)\}
(sss)
                                      +\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
```

# [縮重パンド] $\beta_{\text{CCC}} >> \beta_{\text{EEC}}, \beta_{\text{nnc}}$ のときには $\beta_{\text{caa}} \sim (4/9) \beta_{\text{CCC}}, \beta_{\text{aaa}} \sim (4\sqrt{2}/9) \beta_{\text{CCC}}$ 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。

$$eta_{xxz} + eta_{yyz} = -2eta_{caa}(\cos\alpha - \cos^3\alpha)$$
 $eta_{xxz} - eta_{yyz} = -2eta_{caa}(\cos\alpha - \cos^3\alpha)$ 
 $eta_{xxz} + eta_{yyz} - 2eta_{zzz} = -6eta_{caa}(\cos\alpha - \cos^3\alpha)$ 
 $eta_{zxx} = -eta_{caa}(\cos\alpha - \cos^3\alpha)$ 
 $eta_{zxy} = eta_{caa}\cos\alpha$  であるから、

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

$$\begin{split} (\text{spp}) \qquad & \chi_{\text{YXX}} = (1/4)\beta_{\text{cas}}(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi) \\ & - 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\} \\ \chi_{\text{YZZ}} = & \beta_{\text{cas}}(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi] \\ \chi_{\text{YZX}} = & -(1/2)\beta_{\text{cas}}(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi] \\ \chi_{\text{YXZ}} = & -(1/2)\beta_{\text{cas}}(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 - \cos2\phi) - 2\cos^2\theta\cos2\chi\sin2\phi] \end{split}$$

$$\begin{split} (ssp) \qquad \chi_{YYX} &= (1/4)\beta_{caa}(\cos\alpha - \cos^3\alpha)\{4\sin\theta\cos\chi - 3\sin^3\theta\ (\cos\chi - \cos3\chi) \\ &\quad - [\sin\theta(3\cos\chi + \cos3\chi) - (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\cos2\varphi + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\varphi\} \\ \chi_{YYZ} &= (1/2)\beta_{caa}(\cos\alpha - \cos^3\alpha)\{-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 - \cos2\chi) \\ &\quad + [(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos2\chi]\cos2\varphi - 2\cos^2\theta\sin2\chi\sin2\varphi\} \end{split}$$

$$\begin{split} (psp) \qquad & \chi_{XYX} = (1/4)\beta_{cas}(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi) \\ & - 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\} \\ \chi_{ZYZ} = & \beta_{cas}(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(3 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi] \\ \chi_{XYZ} = & (1/2)\beta_{cas}(\cos\alpha - \cos^3\alpha)[-3(\cos\theta - \cos^3\theta)\sin2\chi + (\cos\theta + \cos^3\theta)\sin2\chi\cos2\phi + 2\cos^2\theta\cos2\chi\sin2\phi] \\ \chi_{ZYX} = & -(1/2)\beta_{cas}(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi] \end{split}$$

$$\begin{split} (\mathrm{sps}) \qquad \chi_{\mathrm{YXY}} &= (1/4)\beta_{\mathrm{cas}}(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi) \\ &\quad - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\} \\ \chi_{\mathrm{YZY}} &= (1/2)\beta_{\mathrm{cas}}(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi] \end{split}$$
 
$$(\mathrm{pps}) \qquad \chi_{\mathrm{XXY}} &= (1/4)\beta_{\mathrm{cas}}(\cos\alpha - \cos^3\alpha)\{-4\sin\theta\sin\chi + 3\sin^3\theta(\sin\chi + \sin3\chi) \\ &\quad + [\sin\theta(3\sin\chi - \sin3\chi) - (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)]\cos2\phi + 2\sin\theta\cos\theta (\cos\chi - \cos3\chi)\sin2\phi\} \end{split}$$

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

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

$$\begin{split} \chi_{\rm YYY} &= (1/4)\beta_{\rm caa}(\cos\alpha - \cos^3\alpha)\{-\sin\theta\sin\chi + 3\sin^3\theta(3\sin\chi - \sin3\chi) \\ &+ [\sin\theta(\sin\chi + \sin3\chi) - (\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)]\cos2\varphi \\ &- 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\varphi\} \end{split}$$

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

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

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

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

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

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

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

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

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

```
\chi_{\text{ZXX}} = (1/4)\beta_{\text{cas}}\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)\sin 2\chi \sin 2\phi
                \chi_{xzx} = (1/4)\beta_{\text{cas}} 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)\sin 2\chi \sin 2\phi
                \chi_{XXZ} = -(1/2)\beta_{cos}\cos\alpha[(\cos\theta - \cos^3\theta)(1 + \cos2\gamma)(1 - \cos2\phi) + \sin^2\theta\sin2\gamma\sin2\phi]
                \chi_{ZZZ} = \beta_{caa} \cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\phi)
              \chi_{\rm YXX} = (1/4)\beta_{\rm cm}\cos\alpha\{[\sin\theta(\sin\chi - \sin3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 - \cos2\phi)]
(spp)
                              -2\sin\theta\cos\theta\cos3\gamma\sin2\phi
                \chi_{YZZ} = -(1/2)\beta_{ca}\cos\alpha[(\sin\theta - 2\sin^3\theta)\sin\chi(1 - \cos2\phi) - \sin\theta\cos\theta\cos\chi\sin2\phi]
                \chi_{\text{YZX}} = (1/4)\beta_{\text{CM}}\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)\cos 2\chi]\sin 2\phi}
                \chi_{\text{YXZ}} = (1/2)\beta_{\text{cso}}\cos\alpha[(\cos\theta - \cos^3\theta)\sin2\chi(1 - \cos2\phi) - \sin^2\theta\cos2\chi\sin2\phi]
               \chi_{\text{YYX}} = (1/4)\beta_{\text{cas}}\cos\alpha\{[\sin\theta(1+\cos2\phi) - (\sin\theta - \sin^3\theta)(1-\cos2\phi)](\cos\chi - \cos3\chi)
(ssp)
                              -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]
               \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)]
(psp)
                              -2\sin\theta\cos\theta\cos3\chi\sin2\phi
                \chi_{ZYZ} = -(1/2)\beta_{cas}\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_{\text{ZYX}} = (1/4)\beta_{\text{cas}}\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)\cos 2\chi]\sin 2\phi}
               \chi_{\text{YXY}} = -(1/4)\beta_{\text{cas}}\cos\alpha\{[\sin\theta(\cos\chi + \cos3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 - \cos2\phi)]
(sps)
                              - 2\sin\theta\cos\theta\sin3\chi\sin2\phi}
                \chi_{yzy} = (1/4)\beta_{\text{cas}} 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)\sin 2\chi \sin 2\phi
               \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)
(pps)
                              -\sin\theta\cos\theta(\cos\chi+\cos3\chi)\sin2\phi
               \chi_{ZZY} = \beta_{con} \cos\alpha[-(\sin\theta - \sin^3\theta)\sin\chi(1 - \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]
                \chi_{\rm ZXY} = (1/4)\beta_{\rm cm}\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)\cos 2\chi]\sin 2\phi
                \chi_{XZY} = (1/4)\beta_{ca}\cos\alpha\{2[(\cos\theta - \cos^3\theta)(1 - \cos2\phi) + \cos\theta\cos2\phi]\sin2\chi
                           -\left[\sin^2\theta + (1 - 3\cos^2\theta)\cos 2\chi\right]\sin 2\phi
               \chi_{\rm XYY} = -(1/4)\beta_{\rm cas}\cos\alpha\{[\sin\theta(\cos\chi + \cos3\chi)(1 + \cos2\varphi) + (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 - \cos2\varphi)]
(pss)
                              -2\sin\theta\cos\theta\sin3\chi\sin2\phi
```

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

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

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

### 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。

$$\begin{split} \beta_{xxz} + \beta_{yyz} &= -2(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha) + 4\beta_{ax}\cos\alpha \\ \beta_{xxz} - \beta_{yyz} &= -2(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha) \\ \beta_{xxz} + \beta_{yyzv} - 2\beta_{zzz} &= -2(\beta_{ax} - \beta_{cx})[3(\cos\alpha - \cos^3\alpha) - 2\cos\alpha] \\ \beta_{zxx} &= -2(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha) \end{split}$$
 であるから、

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

```
-(\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos2\chi)
                 \chi_{ZZZ} = -2\beta_{aac}\cos\alpha\cos\theta
                          + (\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)[-\cos\theta + 3\cos^3\theta - (\cos\theta - \cos^3\theta)\cos2\phi]
                          -2(\beta_{\rm ax} - \beta_{\rm cx})\cos\alpha\cos^3\theta
                \chi_{\rm YXX} = (1/4)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)\}
(spp)
                                       +2\sin\theta\cos\theta(\cos\chi+\cos3\chi)\sin2\phi
                          -(1/2)(\beta_{ax} - \beta_{cx})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)
                 \chi_{YZZ} = (\beta_{ax} - \beta_{cx})(\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_{ax} - \beta_{cx})\cos\alpha(\sin\theta - \sin^3\theta)\sin\alpha
                 \chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{cc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta (1 + \cos2\chi)\sin2\phi]
                          + (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                 \chi_{YXZ} = -(1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\chi\}
                                         -2\cos^2\theta\cos 2\chi\sin 2\phi
                          + (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                \chi_{YYX} = -2\beta_{aac}\cos\alpha\sin\theta\cos\chi
(ssp)
                          + (1/4)(\beta_{ax} - \beta_{cx})(\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_{cc})\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_{cc})(\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)\cos 2\chi]\cos 2\phi - 2\cos^2\theta\sin 2\chi\sin 2\phi
                          -(\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)
                \chi_{XYX} = (1/4)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)\}
(psp)
                                          +2\sin\theta\cos\theta(\cos\chi+\cos3\chi)\sin2\phi
                          -(1/2)(\beta_{\rm ac} - \beta_{\rm cc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)
                 \chi_{\rm ZYZ} = (\beta_{\rm ax} - \beta_{\rm cx})(\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_{\rm acc} - \beta_{\rm ccc})cosα(sinθ - sin<sup>3</sup>θ)sinχ
                 \chi_{XYZ} = -(1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\chi\}
                                          -2\cos^2\theta\cos 2\chi\sin 2\phi
                          + (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                 \chi_{\rm ZYX} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi]
                          + (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                \chi_{\rm YXY} = (1/4)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)\}
(sps)
                                          -2\sin\theta\cos\theta(\sin\chi-\sin3\chi)\sin2\phi
                          + (1/2)(\beta_{ax} - \beta_{cx})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)
```

$$\begin{split} \chi_{YZY} &= (1/2)(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi] \\ &- (\beta_{a\alpha} - \beta_{c\alpha})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi) \end{split}$$

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

$$\begin{split} (pss) \qquad & \chi_{XYY} = (1/4)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi) \\ & - 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\} \\ & + (1/2)(\beta_{ax} - \beta_{cx})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi) \\ & \chi_{ZYY} = (1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi] \\ & - (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi) \end{split}$$

$$\begin{split} \chi_{\rm YYY} &= 2\beta_{\rm ax} {\rm cos}\alpha{\rm sin}\theta{\rm sin}\chi \\ &+ (1/4)(\beta_{\rm ax} - \beta_{\rm cx})({\rm cos}\alpha - {\rm cos}^3\alpha)\{-4{\rm sin}\theta{\rm sin}\chi + 3{\rm sin}^3\theta(3{\rm sin}\chi - {\rm sin}3\chi) \\ &+ [{\rm sin}\theta({\rm sin}\chi + {\rm sin}3\chi) - ({\rm sin}\theta - {\rm sin}^3\theta)(3{\rm sin}\chi - {\rm sin}3\chi)]{\rm cos}2\varphi \\ &- 2{\rm sin}\theta{\rm cos}\theta({\rm cos}\chi - {\rm cos}3\chi){\rm sin}2\varphi\} \\ &- (1/2)(\beta_{\rm ax} - \beta_{\rm cx}){\rm cos}\alpha{\rm sin}^3\theta(3{\rm sin}\chi - {\rm sin}3\chi) \end{split}$$

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

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

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

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

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

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

```
\chi_{XZX} = -(1/2)(\beta_{ax} - \beta_{cx})(\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_{ax} - \beta_{cx})(\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)
               \chi_{\rm YXX} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi)\}
(spp)
                                      +\sin\theta(\sin\chi-\sin3\chi)(1-\cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi
                \chi_{YZZ} = (\beta_{ax} - \beta_{cx})(\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_{\rm YZX} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\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
                \chi_{YXZ} = -(\beta_{ax} - \beta_{cx})(cos\alpha - cos^3\alpha)[(cos\theta - cos^3\theta)sin2\chi (1 + cos2\phi) + sin^2\theta cos2\chi sin2\phi]
               \chi_{\rm YYX} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)\{[-(\sin\theta - \sin^3\theta)(1 + \cos2\phi) + \sin\theta(1 - \cos2\phi)](\cos\chi - \cos3\chi)\}
(ssp)
                                      + 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi}
                \chi_{YYZ} = (\beta_{aac} - \beta_{coc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]
               \chi_{XYX} = -(1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi)\}
(psp)
                                      +\sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi\}
                \chi_{\rm ZYZ} = (\beta_{\rm acc} - \beta_{\rm 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_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi]
                \chi_{\text{ZYX}} = -(1/2)(\beta_{\text{ax}} - \beta_{\text{cx}})(\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)\cos 2\chi]\sin 2\phi}
               \chi_{\rm YXY} = (1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi)\}
(sps)
                                      +\sin\theta(\cos\chi+\cos3\chi)(1-\cos2\phi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}
                \chi_{yzy} = -(1/2)(\beta_{ax} - \beta_{cx})(\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)\sin 2\chi \sin 2\phi
(pps)
               \chi_{\rm XXY} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\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_{\rm ZXY} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\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)\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 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\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\alpha - \cos3\alpha)(1 + \cos2\phi)\}
                                      + (1 - \cos 2\phi)\sin\theta(\cos\chi + \cos 3\chi)] + 2\sin\theta\cos\theta\sin 3\chi\sin 2\phi}
                \chi_{\rm ZYY} = -(1/2)(\beta_{\rm aac} - \beta_{\rm cc})(\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)\sin 2\chi \sin 2\phi
```

$$\begin{split} \chi_{YYY} &= -(1/2)(\beta_{a\alpha} - \beta_{c\alpha})(\cos\alpha - \cos^3\alpha) \{ [(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 + \cos2\varphi) \\ &+ \sin\theta(\sin\chi + \sin3\chi)(1 - \cos2\varphi)] + 2\sin\theta\cos\theta \; (\cos\chi - \cos3\chi)\sin2\varphi \} \end{split}$$

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

[縮重パンド]  $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}$ ,  $\beta_{\eta\eta\zeta}$  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。

$$eta_{xxz}+eta_{yyz}=-4eta_{caa}(\coslpha-\cos^3lpha)\pm2eta_{aaa}\sin^3lpha$$
  $eta_{xxz}-eta_{yyz}=-4eta_{caa}(\coslpha-\cos^3lpha)\pm2eta_{aaa}(2\sinlpha+\sin^3lpha)$   $eta_{xxz}+eta_{yyz}-2eta_{zz}=-12eta_{caa}(\coslpha-\cos^3lpha)-(\pm)2eta_{aaa}\sin^3lpha$   $eta_{zxx}=-2eta_{caa}(\coslpha-2\cos^3lpha)-(\pm)2eta_{aaa}(\sinlpha-\sin^3lpha)$   $eta_{zyy}=2eta_{caa}\coslpha-(\pm)2eta_{aaa}\sinlpha$  であるから、

$$\begin{array}{ll} (ppp) & \chi_{XXX} = -(1/2)(\beta_{aac} + \beta_{bbc}) sin\theta cos\chi \\ & + (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{cac}) sin^3\theta (3cos\chi + cos3\chi) \\ & + (1/8)(\beta_{aac} + \beta_{bbc}) \{ [sin\theta (cos\chi - cos3\chi) - (sin\theta - sin^3\theta) (3cos\chi + cos3\chi) ] cos2\varphi \\ & + 2sin\theta cos\theta (sin\chi + sin3\chi) sin2\varphi \} \\ \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 - sin2\varphi sin\theta cos\theta sin\chi ] cos2\varphi \\ \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 - sin2\varphi sin\theta cos\theta sin\chi ] cos2\varphi \\ \chi_{ZZX} = -(1/2)(\beta_{aac} + \beta_{bbc}) [ (sin\theta - sin^3\theta) cos\chi - sin2\varphi sin\theta cos\theta sin\chi ] cos2\varphi \\ \chi_{ZZX} = -(1/2)(\beta_{aac} + \beta_{bbc}) sin^3\theta cos\chi \\ & + (1/2)(\beta_{aac} + \beta_{bbc}) sin^3\theta cos\chi cos2\varphi \\ \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) - sin2\varphi sin^2\theta sin2\chi ] cos2\varphi \\ \chi_{ZXX} = -(1/4)(\beta_{aac} + \beta_{bbc}) [ (cos\theta - cos^3\theta) (1 + cos2\chi) - sin2\varphi sin^2\theta sin2\chi ] cos2\varphi \\ \chi_{XXZ} = (1/2)(\beta_{aac} + \beta_{bbc}) [ (cos\theta - cos^3\theta) (1 + cos2\chi) - sin2\varphi sin^2\theta sin2\chi ] cos2\varphi \\ \chi_{XXZ} = (1/2)(\beta_{aac} + \beta_{bbc}) cos\theta \\ & - (1/4)(\beta_{aac} + \beta_{bbc}) cos\theta \\ & - (1/4)(\beta_{aac} + \beta_{bbc}) cos\theta - cos^3\theta) - (cos\theta + cos^3\theta) cos2\chi ] + 2sin2\varphi cos^2\theta sin2\chi \} cos2\varphi \\ \chi_{ZZZ} = (1/2)(\beta_{aac} + \beta_{bbc}) cos\theta \\ & - (1/2)(\beta_{aac} + \beta_{bbc}) cos2\varphi (cos\theta - cos^3\theta) \\ & - (1/2)(\beta_{aac} + \beta_{bbc}) cos2\varphi (cos\theta - cos^3\theta) \\ & - (1/2)(\beta_{aac} + \beta_{bbc}) cos2\varphi (cos\theta - cos^3\theta) \\ & - (1/2)(\beta_{aac} + \beta_{bbc}) cos2\varphi (cos\theta - cos^3\theta) \\ & - (1/2)(\beta_{aac} + \beta_{bbc}) cos2\varphi (cos\theta - cos^3\theta) \\ & - (1/2)(\beta_{aac} + \beta_{bbc}) cos2\varphi (cos\theta - cos^3\theta) \\ & - (1/2)(\beta_{aac} + \beta_{bbc}) cos2\varphi (cos\theta - cos^3\theta) \\ & - (1/2)(\beta_{aac} + \beta_{bbc}) cos2\varphi (cos\theta - cos^3\theta) \\ & - (1/2)(\beta_{aac} + \beta_{bbc}) cos2\varphi (cos\theta - cos^3\theta) \\ & - (1/$$

```
\chi_{\rm YXX} = -(1/8)(\beta_{\rm ac} + \beta_{\rm bbc} - 2\beta_{\rm cc})\sin^3\!\theta(\sin\!\chi + \sin\!3\chi)
(spp)
                         +(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_{ax} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi + \sin2\phi\sin\theta\cos\theta\cos\chi]\cos2\phi
                \chi_{YZX} = (1/4)(\beta_{ax} + \beta_{bbc} - 2\beta_{cx})(\cos\theta - \cos^3\theta)\sin 2\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_{\rm YXZ} = (1/4)(\beta_{\rm ac} + \beta_{\rm bbc} - 2\beta_{\rm cc})(\cos\theta - \cos^3\theta)\sin 2\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_{coc})\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_{ax} + \beta_{bbc} - 2\beta_{cx})(\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_{cc})\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_{\rm ZYZ} = -(1/2)(\beta_{\rm ac} + \beta_{\rm bbc} - 2\beta_{\rm cc})(\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_{cc})(\cos\theta - \cos^3\theta)\sin 2\chi
                         -(1/4)(\beta_{aac}-\beta_{bbc})[(cos\theta+cos^3\theta)sin2\chi cos2\varphi+2cos^2\theta cos2\chi sin2\varphi]
                \chi_{\rm ZYX} = (1/4)(\beta_{\rm ax} + \beta_{\rm bbc} - 2\beta_{\rm cx})(\cos\theta - \cos^3\theta)\sin 2\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_{\rm YXY} = (1/8)(\beta_{\rm ac} + \beta_{\rm bbc} - 2\beta_{\rm cc})\sin^3\!\theta(\cos\!\chi - \cos\!3\chi)
(sps)
                          -(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_{ax} + \beta_{bbc} - 2\beta_{cx})(\cos\theta - \cos^3\theta)(1 - \cos2\chi)
                         -(1/4)(\beta_{ax} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\cos2\phi + \sin^2\theta\sin2\chi\sin2\phi]
                \chi_{XXY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi
(pps)
                          -(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)\sin 2\chi
                         + (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi - \sin^2\theta(1 - \cos2\chi)\sin2\phi]
```

$$\begin{split} \chi_{ZXY} &= (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{cc})(\cos\theta - \cos^3\theta)sin2\chi \\ &+ (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)sin2\chi cos2\varphi - sin^2\theta(1 - \cos2\chi)sin2\varphi] \end{split}$$

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

$$\begin{split} \chi_{YYY} &= (1/2)(\beta_{aac} + \beta_{bbc}) sin\theta sin\chi \\ &- (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{cc}) sin^3\theta (3sin\chi - sin3\chi) \\ &- (1/8)(\beta_{aac} - \beta_{bbc}) \{ [sin\theta (sin\chi + sin3\chi) - (sin\theta - sin^3\theta) (3sin\chi - sin3\chi)] cos2\varphi \\ &- 2sin\theta cos\theta (cos\chi - cos3\chi) sin2\varphi \} \end{split}$$

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

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

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

(psp) 
$$\chi_{NYX} = (1/4)\beta_{nm} \{[(1 + \cos 2\phi)(\sin \theta - \sin^2 \theta)(\sin \chi + \sin 3\chi) + (1 - \cos 2\phi)\sin \theta(\sin \chi - \sin 3\chi)] + 2\sin 2\phi\sin \theta\cos \theta\cos 3\chi]$$
  $\chi_{ZYZ} = (1/2)\beta_{nm} [(1 + \cos 2\phi)(\cos \theta - \cos^3 \theta)\sin 2\chi + \sin 2\phi\sin \theta\cos \theta\cos \chi]$   $\chi_{XYZ} = (1/2)\beta_{nm} [(1 + \cos 2\phi)(\cos \theta - \cos^3 \theta)\sin 2\chi + \sin 2\phi\sin^2 \theta\cos 2\chi]$   $\chi_{XYX} = (1/4)\beta_{nm} \{2[(1 + \cos 2\phi)(\cos \theta - \cos^3 \theta) - \cos 2\phi\cos \theta]\sin 2\chi + \sin 2\phi[-\sin^2 \theta + (1 - 3\cos^2 \theta)\cos 2\chi]]$  (sps)  $\chi_{XXY} = (1/4)\beta_{nm} \{[(1 + \cos 2\phi)(\sin \theta - \sin^3 \theta)(\cos \chi - \cos 3\chi) + (1 - \cos 2\phi)\sin \theta(\cos \chi + \cos 3\chi)] + 2\sin 2\phi\sin \theta\cos \theta\sin 3\chi\}$   $\chi_{YZY} = (1/4)\beta_{nm} \{[(1 + \cos 2\phi)(\sin \theta - \sin^3 \theta)(\cos \chi - \cos 3\psi) + (1 - \cos 2\phi)\sin \theta(\cos \chi + \cos 3\chi)] + \sin 2\phi[(1 - 3\cos^2 \theta)\sin 2\chi]$  (pps)  $\chi_{XXY} = (1/4)\beta_{nm} \{[(1 + \cos 2\phi)(\sin \theta - \sin^2 \theta) - (1 - \cos 2\phi)\sin \theta](\sin \chi + \sin 3\chi) + 2\sin 2\phi\sin \theta\cos \theta(\cos \chi + \cos 3\chi)\}$   $\chi_{ZXY} = (1/4)\beta_{nm} \{[(1 + \cos 2\phi)(\sin \theta - \sin^2 \theta) - (1 - \cos 2\phi)\sin \theta](\sin \chi + \sin 3\chi) + 2\sin 2\phi\sin \theta\cos \theta\cos \chi + \cos 3\chi)\}$   $\chi_{ZXY} = (1/4)\beta_{nm} \{2[(1 + \cos 2\phi)(\cos \theta - \cos^3 \theta) - \cos 2\phi\cos \theta]\sin 2\chi + \sin 2\phi[\sin^2 \theta + (1 - 3\cos^2 \theta)\cos 2\chi]\}$   $\chi_{ZXY} = (1/4)\beta_{nm} \{2[(1 + \cos 2\phi)(\cos \theta - \cos^3 \theta) - \cos 2\phi\cos \theta]\sin 2\chi + \sin 2\phi[\sin^2 \theta + (1 - 3\cos^2 \theta)\cos 2\chi]\}$  (pss)  $\chi_{ZYY} = (1/4)\beta_{nm} \{[(1 + \cos 2\phi)(\sin \theta - \sin^3 \theta)(\cos \chi - \cos 3\chi) + (1 - \cos 2\phi)\sin \theta(\cos \chi + \cos 3\chi)] + 2\sin 2\phi\sin \theta\cos \theta\sin 3\chi]$   $\chi_{ZYY} = (1/4)\beta_{nm} \{[(1 + \cos 2\phi)(\sin \theta - \sin^3 \theta)(\cos \chi - \cos 3\chi) + (1 - \cos 2\phi)\sin \theta(\sin \chi + \sin 3\chi)] + 2\sin 2\phi\sin \theta\cos \theta\sin 3\chi]$  (sss)  $\chi_{YYY} = (1/4)\beta_{nm} \{[(1 + \cos 2\phi)(\sin \theta - \sin^2 \theta)(3\sin \chi - \sin 3\chi) + (1 - \cos 2\phi)\sin \theta(\sin \chi + \sin 3\chi)] + 2\sin 2\phi\sin \theta\cos \theta(\cos \chi - \cos 3\chi)\}$   $\chi_{ZYY} = (1/4)\beta_{nm} \{[(1 + \cos 2\phi)(\sin \theta - \sin^2 \theta)(3\sin \chi - \sin 3\chi) + (1 - \cos 2\phi)\sin \theta(\sin \chi + \sin 3\chi)] + 2\sin 2\phi\sin \theta\cos \theta(\cos \chi - \cos 3\chi)\}$   $\chi_{ZXY} = (1/4)\beta_{nm} \{[(1 + \cos 2\phi)(\sin \theta - \sin^2 \theta)(3\sin \chi - \sin 3\chi) + (1 - \cos 2\phi)\sin \theta(\sin \chi + \sin 3\chi)] + 2\sin 2\phi\sin \theta\cos \theta(\sin \chi + \sin 3\chi)\}$   $\chi_{ZZY} = (1/2)\beta_{nm} \{[(1 + \cos 2\phi)(\sin \theta - \sin^2 \theta)\cos \chi + \sin 2\phi\sin \theta\cos \theta\sin \chi] \}$   $\chi_{ZZZ} = (1/2)\beta_{nm} \{(1 - \cos 2\phi)(\sin \theta - \sin^2 \theta)\cos \chi + \sin 2\phi\sin \theta\cos \theta\sin \chi] \}$   $\chi_{ZZZ} = (1/2)\beta_{nm} \{(1 - \cos 2\phi)(\sin \theta - \sin^2 \theta)\cos \chi + \sin 2\phi\sin \theta\cos \theta\sin \chi] \}$   $\chi_{ZZZ} = (1/2)\beta_{nm} \{(1 - \cos 2\phi)(\sin \theta - \sin^2 \theta)\cos \chi + \sin 2\phi\sin \theta\cos \theta\sin \chi] \}$   $\chi_{ZZZ} = (1/2)\beta_{nm} \{(1 - \cos 2\phi)(\sin \theta - \sin^2 \theta)\cos \chi + \sin 2\phi\sin \theta\cos \theta\sin \chi] \}$   $\chi_{ZZZ} = (1/2)\beta_{nm} \{(1 - \cos 2\phi)(\sin \theta - \sin^2 \theta)\cos \chi + \sin 2\phi\sin \theta\cos \theta\sin \chi] \}$ 

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

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

 $-\sin 2\phi(1 - 3\cos^2\theta)\sin 2\gamma$ 

 $-\sin 2\phi(1 - 3\cos^2\theta)\sin 2\chi$ 

 $\chi_{ZZZ} = \beta_{cbb}(1 - \cos 2\phi)(\cos \theta - \cos^3 \theta)$ 

```
\chi_{\rm YXX} = (1/4)\beta_{\rm cbb} \{ [(1+\cos 2\phi)\sin \theta (\sin \chi - \sin 3\chi) + (1-\cos 2\phi)(\sin \theta - \sin^3 \theta)(\sin \chi + \sin 3\chi) \}
(spp)
                                -2\sin 2\phi \sin \theta \cos \theta \cos 3\chi
                \chi_{YZZ} = -(1/2)\beta_{cbb}[(1-\cos 2\phi)(\sin \theta - 2\sin^3 \theta)\sin \chi - \sin 2\phi \sin \theta \cos \theta \cos \chi]
                \chi_{yzx} = (1/4)\beta_{cbb}\{2[(1 - \cos 2\phi)(\cos \theta - \cos^3 \theta) + \cos 2\phi \cos \theta]\sin 2\chi + \sin 2\phi[\sin^2 \theta - (1 - 3\cos^2 \theta)\cos 2\chi]\}
                \chi_{\rm YXZ} = (1/2)\beta_{\rm cbb}[(1-\cos 2\phi)(\cos \theta - \cos^3 \theta)\sin 2\chi - \sin 2\phi \sin^2 \theta \cos 2\chi]
                \chi_{\text{YYX}} = (1/4)\beta_{\text{cbb}} \{ [(1 + \cos 2\phi)\sin\theta - (1 - \cos 2\phi)(\sin\theta - \sin^3\theta)](\cos\chi - \cos 3\chi) \}
(ssp)
                                -2\sin 2\underline{\phi}\sin\theta\cos\theta(\sin\chi-\sin 3\chi)
                \chi_{\text{YYZ}} = -(1/2)\beta_{\text{cbb}}[(1 - \cos 2\phi)(\cos \theta - \cos^3 \theta)(1 - \cos 2\chi) - \sin 2\phi \sin^2 \theta \sin 2\chi]
                \chi_{XYX} = (1/4)\beta_{cbb}\{[(1 + \cos 2\phi)\sin \theta(\sin \chi - \sin 3\chi) + (1 - \cos 2\phi)(\sin \theta - \sin^3 \theta)(\sin \chi + \sin 3\chi)]\}
(psp)
                                - 2\sin 2\phi \sin \theta \cos \theta \cos 3\chi}
                \chi_{\rm ZYZ} = -(1/2)\beta_{\rm cbb}[(1-\cos 2\phi)(\sin \theta - 2\sin^3 \theta)\sin \chi - \sin 2\phi\sin \theta\cos \theta\cos \chi]
                \chi_{XYZ} = (1/2)\beta_{cbb}[(1 - \cos 2\phi)(\cos \theta - \cos^3 \theta)\sin 2\chi - \sin 2\phi \sin^2 \theta \cos 2\chi]
                \chi_{\rm ZYX} = (1/4)\beta_{\rm obb} \{2[(1-\cos 2\phi)(\cos \theta - \cos^3 \theta) + \cos 2\phi \cos \theta]\sin 2\chi + \sin 2\phi[\sin^2 \theta - (1-3\cos^2 \theta)\cos 2\chi]\}
                \chi_{\rm YXY} = -(1/4)\beta_{\rm cbb}\{[(1+\cos2\phi)\sin\theta(\cos\chi+\cos3\chi)+(1-\cos2\phi)(\sin\theta-\sin^3\theta)(\cos\chi-\cos3\chi)]
(sps)
                                       -2\sin 2\phi \sin \theta \cos \theta \sin 3\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) \}
                                      +\sin 2\phi(1-3\cos^2\theta)\sin 2\chi
               \chi_{XXY} = (1/4)\beta_{cbb} \left[ \left[ -(1 + \cos 2\phi)\sin\theta + (1 - \cos 2\phi)(\sin\theta - \sin^3\theta) \right] (\sin \chi + \sin 3\chi) \right]
(pps)
                                       -\sin 2\phi \sin \theta \cos \theta (\cos \chi + \cos 3\chi)
                \chi_{ZZY} = \beta_{cbb}[-(1 - \cos 2\phi)(\sin \theta - \sin^3 \theta)\sin \chi + \sin 2\phi \sin \theta \cos \theta \cos \chi]
                \chi_{ZXY} = (1/4)\beta_{cbb} \{ 2[(1 - \cos 2\phi)(\cos \theta - \cos^3 \theta) + \cos 2\phi \cos \theta] \sin 2\chi - \sin 2\phi [\sin^2 \theta + (1 - 3\cos^2 \theta)\cos 2\chi] \}
                \chi_{XZY} = (1/4)\beta_{cbb} \{ 2[(1 - \cos 2\phi)(\cos \theta - \cos^3 \theta) + \cos 2\phi \cos \theta] \sin 2\chi - \sin 2\phi [\sin^2 \theta + (1 - 3\cos^2 \theta)\cos 2\chi] \}
                \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)]\}
(pss)
                                      -2\sin 2\phi \sin \theta \cos \theta \sin 3\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) \}
                                       +\sin 2\phi(1 - 3\cos^2\theta)\sin 2\chi
                \chi_{\text{YYY}} = (1/4)\beta_{\text{cbb}} \{ [(1 + \cos 2\phi)\sin\theta(\sin\chi + \sin 3\chi) + (1 - \cos 2\phi)(\sin\theta - \sin^3\theta)(3\sin\chi - \sin 3\chi) \}
(sss)
                                       -2\sin 2\phi \sin \theta \cos \theta (\cos \chi - \cos 3\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]  $\beta_{\text{CCC}} >> \beta_{\text{EEC}}, \beta_{nnC}$  のときには  $\beta_{aac} \sim (4/9)\beta_{\text{CCC}}, \beta_{cac} \sim (1/9)\beta_{\text{CCC}}$  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。

$$eta_{xxz} + eta_{yyz} = -2(eta_{ax} - eta_{cx})(\cos\alpha - \cos^3\alpha) + 4eta_{ax}\cos\alpha$$
 $eta_{xxz} - eta_{yyz} = -2(eta_{ax} - eta_{cx})(\cos\alpha - \cos^3\alpha)$ 
 $eta_{xxz} + eta_{yyz} - 2eta_{zzz} = -2(eta_{ax} - eta_{cx})[3(\cos\alpha - \cos^3\alpha) - 2\cos\alpha]$ 
 $eta_{zxx} = -2(eta_{ax} - eta_{cx})(\cos\alpha - \cos^3\alpha)$  であるから、

$$(ppp) \quad \chi_{XXX} = -2\beta_{nac}\cos\alpha\sin\theta\cos\chi \\ + (1/4)(\beta_{nac} - \beta_{coc})(\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_{nac} - \beta_{coc})\cos\alpha\sin^3\theta(3\cos\chi + \cos3\chi) \\ \chi_{ZZZ} = -(\beta_{nac} - \beta_{coc})\cos\alpha\sin^3\theta(3\cos\chi + \cos3\chi) \\ \chi_{ZZZ} = -(\beta_{nac} - \beta_{coc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi(3 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi] \\ + 2(\beta_{nac} - \beta_{coc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi \\ \chi_{ZXZ} = -(\beta_{nac} - \beta_{coc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi \\ \chi_{ZXZ} = -(\beta_{nac} - \beta_{coc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi \\ \chi_{ZZZ} = -(\beta_{nac} - \beta_{coc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi \\ \chi_{ZZZ} = -2\beta_{nac}\cos\alpha\sin\theta\cos\chi \\ + (\beta_{nac} - \beta_{coc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi \\ \chi_{ZZZ} = -2\beta_{nac}\cos\alpha\sin\theta\cos\chi \\ + (\beta_{nac} - \beta_{coc})\cos\alpha(\sin\theta - \sin^3\theta)\cos\chi \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})\cos\alpha(\cos\theta - \cos^3\theta)\{(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi] \\ - (\beta_{nac} - \beta_{coc})\cos\alpha(\cos\theta - \cos^3\theta)\{(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi] \\ - (\beta_{nac} - \beta_{coc})\cos\alpha(\cos\theta - \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{XXZ} = (1/2)(\beta_{nac} - \beta_{coc})(\cos\alpha - \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{XXZ} = 2\beta_{nac}\cos\alpha\cos\theta \\ + (1/2)(\beta_{nac} - \beta_{coc})(\cos\alpha - \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = 2\beta_{nac}\cos\alpha\cos\theta \\ + (1/2)(\beta_{nac} - \beta_{coc})(\cos\alpha - \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = 2\beta_{nac}\cos\alpha\cos\theta \\ + (\beta_{nac} - \beta_{coc})(\cos\alpha - \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = 2\beta_{nac}\cos\alpha\cos\theta \\ + (\beta_{nac} - \beta_{coc})(\cos\alpha - \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = 2\beta_{nac}\cos\alpha\cos\theta \\ + (\beta_{nac} - \beta_{coc})(\cos\alpha - \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = (1/4)(\beta_{nac} - \beta_{coc})(\cos\alpha + \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})(\cos\alpha + \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})(\cos\alpha + \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})(\cos\alpha + \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})(\cos\alpha + \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})(\cos\alpha + \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})(\cos\alpha + \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})(\cos\alpha - \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})(\cos\alpha - \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})(\cos\alpha - \cos^3\theta)\{(1 + \cos2\chi) \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})\cos\alpha\sin^3\theta \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})\cos\alpha\sin^3\theta \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})\cos\alpha\sin^3\theta \\ \chi_{ZZZ} = (1/2)(\beta_{nac} - \beta_{coc})\cos\alpha\sin^$$

```
\chi_{\rm YXZ} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\chi\}
                                       -2\cos^2\theta\cos 2\chi\sin 2\phi
                          + (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                \chi_{YYX} = -2\beta_{ax}\cos\alpha\sin\theta\cos\chi
(ssp)
                          +(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_{ax} - \beta_{cx})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)
                 \chi_{YYZ} = 2\beta_{aac}\cos\alpha\sin\theta\cos\chi
                          +(1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{-2\cos\theta + 3(\cos\theta - \cos^3\theta)(1 - \cos2\alpha)\}
                                       + [(\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_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)
                \chi_{XYX} = (1/4)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)\}
(psp)
                                          + 2\sin\theta\cos\theta (\cos\chi + \cos3\chi)\sin2\phi
                          -(1/2)(\beta_{ax} - \beta_{cx})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)
                \chi_{\rm ZYZ} = (\beta_{\rm acc} - \beta_{\rm 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_{ax} - \beta_{cx})\cos\alpha(\sin\theta - \sin^3\theta)\sin\alpha
                 \chi_{XYZ} = -(1/2)(\beta_{ax} - \beta_{cor})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\chi\}
                                       -2\cos^2\theta\cos 2\chi\sin 2\phi
                          + (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                \chi_{\rm ZYX} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi]
                          + (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                \chi_{\rm YXY} = (1/4)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)\}
(sps)
                                            -2\sin\theta\cos\theta(\sin\chi-\sin3\chi)\sin2\phi
                          + (1/2)(\beta_{ax} - \beta_{cx})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)
                 \chi_{YZY} = (1/2)(\beta_{aac} - \beta_{cac})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]
                          - (\beta_{\rm aac} - \beta_{\rm cc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)
                \chi_{XXY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\gamma
(pps)
                          +(1/4)(\beta_{aac} - \beta_{coc})(\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 in^3\theta(\sin\chi + \sin3\chi)
                 \chi_{ZZY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\gamma
                          +(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)[-\sin\theta + 3(\sin\theta - \sin^3\theta) - \sin^3\theta\cos2\phi]\sin\alpha
                          - 2(\beta_{ax} - \beta_{cx})\cos\alpha(\sin\theta - \sin^3\theta)\sin\alpha
                 \chi_{xzy} = -(1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]
```

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

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

$$\begin{split} \chi_{\Upsilon\Upsilon\Upsilon} &= 2\beta_{\rm ax} {\rm cos}\alpha {\rm sin}\theta {\rm sin}\chi \\ &+ (1/4)(\beta_{\rm ax} - \beta_{\rm cx})({\rm cos}\alpha - {\rm cos}^3\alpha) \{-4{\rm sin}\theta {\rm sin}\chi + 3{\rm sin}^3\theta (3{\rm sin}\chi - {\rm sin}3\chi) \\ &+ [{\rm sin}\theta ({\rm sin}\chi + {\rm sin}3\chi) - ({\rm sin}\theta - {\rm sin}^3\theta)(3{\rm sin}\chi - {\rm sin}3\chi)]{\rm cos}2\varphi \\ &- 2{\rm sin}\theta {\rm cos}\theta ({\rm cos}\chi - {\rm cos}3\chi){\rm sin}2\varphi \} \\ &- (1/2)(\beta_{\rm ax} - \beta_{\rm cx}){\rm cos}\alpha {\rm sin}^3\theta (3{\rm sin}\chi - {\rm sin}3\chi) \end{split}$$

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

$$\begin{array}{ll} (ppp) & \chi_{\rm XXX} = (1/2)(\beta_{\rm aac} - \beta_{\rm ccc})(\cos\alpha - \cos^3\alpha) \{ [(\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)(1 + \cos2\phi) \\ & + \sin\theta(\cos\chi - \cos3\chi)(1 - \cos2\phi) ] - 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi \} \\ \chi_{\rm XZZ} = -(\beta_{\rm aac} - \beta_{\rm ccc})(\cos\alpha - \cos^3\alpha) [(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi] \\ \chi_{\rm ZXZ} = -(\beta_{\rm aac} - \beta_{\rm ccc})(\cos\alpha - \cos^3\alpha) [(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi] \\ \chi_{\rm ZZX} = -2(\beta_{\rm aac} - \beta_{\rm ccc})(\cos\alpha - \cos^3\alpha) [(\sin\theta - \sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi] \\ \chi_{\rm ZXX} = -(1/2)(\beta_{\rm aac} - \beta_{\rm ccc})(\cos\alpha - \cos^3\alpha) \{ 2[\cos\theta(1 + \cos2\chi\cos2\phi) \\ & - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi) ] + (1 - 3\cos^2\theta)\sin2\chi\sin2\phi \} \\ \chi_{\rm XZX} = -(1/2)(\beta_{\rm aac} - \beta_{\rm ccc})(\cos\alpha - \cos^3\alpha) \{ 2[\cos\theta(1 + \cos2\chi\cos2\phi) \\ & - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi) ] + (1 - 3\cos^2\theta)\sin2\chi\sin2\phi \} \\ \chi_{\rm XXZ} = -(\beta_{\rm aac} - \beta_{\rm ccc})(\cos\alpha - \cos^3\alpha) [-(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi ] \\ \chi_{\rm ZZZ} = -2(\beta_{\rm aac} - \beta_{\rm ccc})(\cos\alpha - \cos^3\alpha) [-(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi ] \\ \chi_{\rm ZZZ} = -2(\beta_{\rm aac} - \beta_{\rm ccc})(\cos\alpha - \cos^3\alpha)(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \end{array}$$

$$\begin{split} (\text{spp}) \qquad \chi_{\text{YXX}} &= -(1/2)(\beta_{\text{aac}} - \beta_{\text{ccc}})(\cos\alpha - \cos^3\alpha) \{ [(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) \\ &\quad + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi \} \\ \chi_{\text{YZZ}} &= (\beta_{\text{aac}} - \beta_{\text{ccc}})(\cos\alpha - \cos^3\alpha) [(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi] \\ \chi_{\text{YZX}} &= -(1/2)(\beta_{\text{aac}} - \beta_{\text{ccc}})(\cos\alpha - \cos^3\alpha) \{ 2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \\ &\quad - \cos\theta\cos2\phi ]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi \} \\ \chi_{\text{YXZ}} &= -(\beta_{\text{aac}} - \beta_{\text{ccc}})(\cos\alpha - \cos^3\alpha) [(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi] \end{split}$$

$$\begin{split} (ssp) \qquad \chi_{YYX} &= -(1/2)(\beta_{axc} - \beta_{cxc})(\cos\alpha - \cos^3\alpha)\{[-(\sin\theta - \sin^3\theta)(1 + \cos2\phi) + \sin\theta(1 - \cos2\phi)](\cos\chi - \cos3\chi) \\ &\qquad + 2\sin\theta\cos\theta(\sin\chi - \sin3\chi)\sin2\phi\} \\ \chi_{YYZ} &= (\beta_{axc} - \beta_{cxc})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi] \end{split}$$

$$\begin{split} (\text{psp}) \qquad \chi_{\text{XYX}} &= -(1/2)(\beta_{\text{ax}} - \beta_{\text{cx}})(\cos\alpha - \cos^3\alpha) \{ [(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) \\ &+ \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi \} \\ \chi_{\text{ZYZ}} &= (\beta_{\text{ax}} - \beta_{\text{cx}})(\cos\alpha - \cos^3\alpha) [(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi] \\ \chi_{\text{XYZ}} &= -(\beta_{\text{ax}} - \beta_{\text{cx}})(\cos\alpha - \cos^3\alpha) [(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi] \\ \chi_{\text{ZYX}} &= -(1/2)(\beta_{\text{ax}} - \beta_{\text{cx}})(\cos\alpha - \cos^3\alpha) \{ 2 [(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \\ &- \cos\theta\cos2\phi ]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi \} \end{split}$$

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

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

$$\begin{split} (pss) \qquad & \chi_{XYY} = (1/2)(\beta_{aac} - \beta_{cc})(\cos\alpha - \cos^3\alpha) \{ [(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\varphi) \\ & + \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\varphi) ] + 2\sin\theta\cos\theta\sin3\chi\sin2\varphi \} \\ \chi_{ZYY} = -(1/2)(\beta_{aac} - \beta_{cc})(\cos\alpha - \cos^3\alpha) \{ 2[\cos\theta(1 - \cos2\chi\cos2\varphi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\varphi) ] \\ & - (1 - 3\cos^2\theta)\sin2\chi\sin2\varphi \} \end{split}$$

$$\begin{split} \chi_{\rm YYY} &= -(1/2)(\beta_{\rm aac} - \beta_{\rm cc})(\cos\alpha - \cos^3\alpha) \{ [(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 + \cos2\varphi) \\ &+ \sin\theta(\sin\chi + \sin3\chi)(1 - \cos2\varphi)] + 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\varphi \} \end{split}$$

$$\chi_{xxx} + \chi_{yyx} + \chi_{zzx} = \chi_{xxy} + \chi_{yyy} + \chi_{zzy} = \chi_{xxz} + \chi_{yyz} + \chi_{zzz} = 0$$

**[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。

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

$$\begin{split} &\beta_{xxz} + \beta_{yyz} - 2\beta_{zzz} = -6\beta_{cac}(\cos\alpha - \cos^3\alpha)(1 \pm \cos2\varphi_A) - 3\beta_{aaa}\sin^3\alpha(\cos3\varphi_A \pm \cos\varphi_A) \\ &\beta_{zxx} = -\beta_{cac}(\cos\alpha - 2\cos^3\alpha)(1 \pm \cos2\varphi_A) + \beta_{aac}(\sin\alpha - \sin^3\alpha)(\cos3\varphi_A \pm \cos\varphi_A) \\ &\beta_{zyy} = \beta_{cac}\cos\alpha(1 - (\pm)\cos2\varphi_A) - \beta_{aac}\sin\alpha(\cos3\varphi_A - (\pm)\cos\varphi_A) \\ &\beta_{xyz} = \beta_{yxz} = \pm\beta_{cac}\sin^2\alpha\sin2\varphi_A - \beta_{aac}\sin\alpha\cos\alpha(\sin3\varphi_A \pm \sin\varphi_A) \\ &\beta_{yzx} = \beta_{zyx} = -(\pm)\beta_{cac}\sin^2\alpha\sin2\varphi_A - \beta_{aac}\sin\alpha\cos\alpha(\sin3\varphi_A \pm \sin\varphi_A) \\ &\beta_{zxy} = \beta_{xzy} = -(\pm)\beta_{cac}(2\cos^2\alpha - 1)\sin2\varphi_A - \beta_{aac}\sin\alpha\cos\alpha(\sin3\varphi_A - (\pm)\sin\varphi_A) \end{split}$$

$$\begin{array}{ll} (\text{ppp}) & \chi_{\text{XXX}} = -(1/2)(\beta_{\text{lax}} + \beta_{\text{blc}}) \sin \theta \cos x \chi \\ & + (1/8)(\beta_{\text{lax}} + \beta_{\text{blc}} - 2\beta_{\text{ccc}}) \sin^3 \theta (3\cos \chi + \cos 3 \chi) \\ & + (1/8)(\beta_{\text{lax}} + \beta_{\text{blc}} - 2\beta_{\text{ccc}}) \sin^3 \theta (3\cos \chi + \cos 3 \chi) \\ & + (1/8)(\beta_{\text{lac}} + \beta_{\text{blc}}) (\sin \theta (\cos \chi - \cos 3 \chi) - (\sin \theta - \sin^3 \theta) (3\cos \chi + \cos 3 \chi)] \cos 2 \varphi \\ & + 2\sin \theta \cos \theta (\sin \chi + \sin 3 \chi) \sin 2 \varphi \\ & + (1/4)\beta_{\text{abc}} [ [\sin \theta (\cos \chi - \cos 3 \chi) - (\sin \theta - \sin^3 \theta) (3\cos \chi + \cos 3 \chi)] \sin 2 \varphi \\ & - 2\sin \theta \cos \theta (\sin \chi + \sin 3 \chi) \cos 2 \varphi ) \\ \chi_{\text{XZZ}} = (1/2)(\beta_{\text{lax}} + \beta_{\text{blc}} - 2\beta_{\text{ccc}}) (\sin \theta - \sin^3 \theta) \cos \chi \\ & + (1/2)(\beta_{\text{lax}} - \beta_{\text{blc}}) [ (\sin \theta - \sin^3 \theta) \cos \chi \cos 2 \varphi - \sin \theta \cos \theta \sin \chi \sin 2 \varphi ] \\ & + \beta_{\text{abc}} [ (\sin \theta - \sin^3 \theta) \cos \chi \sin 2 \varphi + \sin \theta \cos \theta \sin \chi \cos 2 \varphi ] \\ \chi_{\text{ZXZ}} = (1/2)(\beta_{\text{lax}} + \beta_{\text{blc}} - 2\beta_{\text{ccc}}) (\sin \theta - \sin^3 \theta) \cos \chi \\ & + (1/2)(\beta_{\text{lax}} - \beta_{\text{blc}}) [ (\sin \theta - \sin^3 \theta) \cos \chi \cos 2 \varphi - \sin \theta \cos \theta \sin \chi \sin 2 \varphi ] \\ & + \beta_{\text{abc}} [ (\sin \theta - \sin^3 \theta) \cos \chi \sin 2 \varphi + \sin \theta \cos \theta \sin \chi \cos 2 \varphi ] \\ \chi_{\text{ZZX}} = -(1/2)(\beta_{\text{lax}} + \beta_{\text{blc}} - 2\beta_{\text{ccc}}) (\sin \theta - \sin^3 \theta) \cos \chi \\ & - (1/2)(\beta_{\text{lax}} + \beta_{\text{blc}} - 2\beta_{\text{ccc}}) (\sin \theta - \sin^3 \theta) \cos \chi \\ & - (1/2)(\beta_{\text{lax}} + \beta_{\text{blc}} - 2\beta_{\text{ccc}}) (\cos \theta - \sin^3 \theta) (\cos \chi \\ & - (1/2)(\beta_{\text{lax}} + \beta_{\text{blc}} - 2\beta_{\text{ccc}}) (\cos \theta - \cos^3 \theta) (1 + \cos 2 \chi) \\ & - (1/4)(\beta_{\text{lax}} + \beta_{\text{blc}} - 2\beta_{\text{ccc}}) (\cos \theta - \cos^3 \theta) (1 + \cos 2 \chi) \cos 2 \varphi - \sin^2 \theta \sin 2 \chi \sin 2 \varphi ] \\ & - (1/2)\beta_{\text{abc}} [ (\cos \theta - \cos^3 \theta) (1 + \cos 2 \chi) \cos 2 \varphi - \sin^2 \theta \sin 2 \chi \sin 2 \varphi ] \\ & - (1/2)\beta_{\text{abc}} [ (\cos \theta - \cos^3 \theta) (1 + \cos 2 \chi) \cos 2 \varphi - \sin^2 \theta \sin 2 \chi \sin 2 \varphi ] \\ & - (1/2)\beta_{\text{abc}} [ (\cos \theta - \cos^3 \theta) (1 + \cos 2 \chi) \cos 2 \varphi - \sin^2 \theta \sin 2 \chi \sin 2 \varphi ] \\ & - (1/2)\beta_{\text{abc}} [ (\cos \theta - \cos^3 \theta) (1 + \cos 2 \chi) \cos 2 \varphi - \sin^2 \theta \sin 2 \chi \sin 2 \varphi ] \\ & - (1/2)\beta_{\text{abc}} [ (\cos \theta - \cos^3 \theta) (1 + \cos 2 \chi) \sin 2 \varphi + \sin^2 \theta \sin 2 \chi \sin 2 \varphi ] \\ & - (1/2)\beta_{\text{abc}} [ (\cos \theta - \cos^3 \theta) (1 + \cos 2 \chi) \sin 2 \varphi + \sin^2 \theta \sin 2 \chi \sin 2 \varphi ] \\ & - (1/2)\beta_{\text{abc}} [ (\cos \theta - \cos^3 \theta) (1 + \cos 2 \chi) \sin 2 \varphi + \sin^2 \theta \sin 2 \chi \sin 2 \varphi ] \\ & - (1/2)(\beta_{\text{ac}} + \beta_{\text{bbc}} - 2\beta_{\text{ccc}}) (\cos \theta - \cos^3 \theta) (1 + \cos 2 \chi) \\ & - (1/2)(\beta_{\text{ac}} + \beta_{\text{bbc}} - 2\beta_{\text{ccc}}) (\cos \theta - \cos^3 \theta) \cos 2 \chi ] \sin 2 \varphi - 2\cos^2 \theta \sin 2 \chi \sin 2 \varphi ) \\$$

(spp) 
$$\chi_{YXX} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{cac})\sin^3\theta(\sin\chi + \sin3\chi)$$

```
+(1/8)(\beta_{ax} - \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\cos 2\phi + \sin\theta\cos\theta\cos\chi\sin 2\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_{ax} + \beta_{bbc} - 2\beta_{cx})(\cos\theta - \cos^3\theta)\sin 2\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_{\rm YXZ} = (1/4)(\beta_{\rm ac} + \beta_{\rm bbc} - 2\beta_{\rm cc})(\cos\theta - \cos^3\theta)\sin 2\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_{YYX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi
(ssp)
                           +(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi)
                           +(1/8)(\beta_{ax} - \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_{ax} - \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)\cos 2\chi]\sin 2\phi + \cos^2\theta\sin 2\chi\cos 2\phi\}
               \chi_{XYX} = -(1/8)(\beta_{ax} + \beta_{bbc} - 2\beta_{cx})\sin^3\theta(\sin\chi + \sin3\chi)
(psp)
                           + (1/8)(\beta_{aac} - \beta_{bbc})[(2sin\theta - sin^3\theta)(sin\chi + sin3\chi)cos2\phi + 2sin\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_{\rm ZYZ} = -(1/2)(\beta_{\rm aac} + \beta_{\rm bbc} - 2\beta_{\rm ccc})(\sin\theta - \sin^3\theta)\sin\chi
                           -(1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi\cos 2\phi + \sin\theta\cos\theta\cos\chi\sin 2\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)\sin 2\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_{\rm ZYX} = (1/4)(\beta_{\rm aac} + \beta_{\rm bbc} - 2\beta_{\rm ccc})(\cos\theta - \cos^3\theta)\sin 2\chi
                           +(1/4)(\beta_{ac} - \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]
```

```
\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_{cm}[(\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_{cap} [(\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_{cas} \{ 2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\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 \}
               \chi_{XZX} = (1/4)\beta_{cas} \{ 2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi) \}
                                           + (1 - 3\cos^2\theta)\sin 2\gamma \sin 2\phi
                        -(1/4)\beta_{bca}\left\{2\left[(\cos\theta-\cos^3\theta)-\cos^3\theta\cos2\chi\right]\sin2\phi-\left[\sin^2\theta-(1-3\cos^2\theta)\cos2\phi\right]\sin2\chi\right\}
               \chi_{XXZ} = -(1/2)\beta_{cm}[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]
                          -(1/2)\beta_{\text{bcal}}[(\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 + \cos 2\phi)
                        + \beta_{bca}(\cos\theta - \cos^3\theta)\sin 2\phi
               \chi_{\text{YXX}} = (1/4)\beta_{\text{CM}} \left\{ \left[ (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi) \right] \right\}
(spp)
                                           + 2\sin\theta\cos\theta\cos3\gamma\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_{cm}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]
                          -(1/2)\beta_{hca}[(\sin\theta - 2\sin^3\theta)\sin2\gamma\sin2\phi - \sin\theta\cos\theta\cos\gamma(1 + \cos2\phi)]
               \chi_{YZX} = (1/4)\beta_{cas} \{ 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)]
               \chi_{YYX} = (1/4)\beta_{cm} \{ [-(\sin\theta - \sin^3\theta)(1 + \cos 2\phi) + \sin\theta(1 - \cos 2\phi)](\cos\chi - \cos 3\chi) \}
(ssp)
                                           + 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)]
               \chi_{XYX} = (1/4)\beta_{cm} \{ [(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] 
(psp)
                                           + 2\sin\theta\cos\theta\cos3\gamma\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_{can}[(\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_{cm}[(\cos\theta - \cos^3\theta)\sin 2\chi(1 + \cos 2\phi) + \sin^2\theta\cos 2\chi\sin 2\phi]
                        +(1/2)\beta_{bca}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi - \sin^2\theta\cos2\chi(1 + \cos2\phi)]
```

```
\chi_{\rm ZYX} = (1/4)\beta_{\rm cm} \{ 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_{\text{YXY}} = -(1/4)\beta_{\text{cm}} \{ [(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi) ]
           (sps)
                                                     + 2\sin\theta\cos\theta\sin3\gamma\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\}
                          \chi_{yzy} = (1/4)\beta_{cso} \{2[\cos\theta(1 - \cos2\phi\cos2\chi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\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\}
                         \chi_{XXY} = (1/4)\beta_{cm} \{ [(\sin\theta - \sin^3\theta)(1 + \cos2\phi) - \sin\theta(1 - \cos2\phi)](\sin\chi + \sin3\chi) 
           (pps)
                                                     + 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]
                          \chi_{ZZY} = -\beta_{can}[(\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)]
                          \chi_{ZXY} = (1/4)\beta_{cm} \{ 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)]
                          \chi_{XZY} = (1/4)\beta_{cas}\{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)]
                         \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)]
           (pss)
                                                     + 2\sin\theta\cos\theta\sin3\gamma\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\}
                          \chi_{ZYY} = (1/4)\beta_{cm} \{2[\cos\theta(1 - \cos2\phi\cos2\chi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)]
                                                     -(1 - 3\cos^2\theta)\sin 2\chi \sin 2\phi
                                   -(1/4)\beta_{bca}\left\{2\left[(\cos\theta-\cos^3\theta)-\cos^3\theta\cos2\chi\right]\sin2\phi+\left[\sin^2\theta-(1-3\cos^2\theta)\cos2\phi\right]\sin2\chi\right\}
                          \chi_{\text{YYY}} = (1/4)\beta_{\text{cm}} \{ [(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi + \sin3\chi)(1 - \cos2\phi)] \}
           (sss)
                                                     + 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
           \chi_{XXX} + \chi_{YYX} + \chi_{ZZX} = \chi_{XXY} + \chi_{YYY} + \chi_{ZZY} = \chi_{XXZ} + \chi_{YYZ} + \chi_{ZZZ} = 0
[面外 (b<sub>2</sub>) 振動]
                          \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) \}
           (ppp)
                                                     + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi
                                     +(1/4)\beta_{csh}\{[\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_{cbb}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 - \cos2\phi) + \sin\theta\cos\theta\sin\chi\sin2\phi]
                                   +(1/2)\beta_{csh}[(\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)\sin 2\chi \sin 2\phi
                        -(1/4)\beta_{csh}\{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\}
                \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)\sin 2\gamma \sin 2\phi
                        -(1/4)\beta_{csb}\left\{2\left[(\cos\theta-\cos^3\theta)-\cos^3\theta\cos2\chi\right]\sin2\phi+\left[\sin^2\theta+(1-3\cos^2\theta)\cos2\phi\right]\sin2\chi\right\}
                \chi_{XXZ} = -(1/2)\beta_{chb}[(\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 - \cos 2\phi)
                        + \beta_{cab}(\cos\theta - \cos^3\theta)\sin 2\phi
               \chi_{\rm YXX} = (1/4)\beta_{\rm cbb} \{ [\sin\theta(\sin\chi - \sin3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 - \cos2\phi) \}
(spp)
                                           -2\sin\theta\cos\theta\cos3\gamma\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_{csb}[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_{\rm YXZ} = (1/2)\beta_{\rm cbb}[(\cos\theta - \cos^3\theta)\sin2\chi(1 - \cos2\phi) - \sin^2\theta\cos2\chi\sin2\phi]
                        +(1/2)\beta_{csh}[(\cos\theta - \cos^3\theta)\sin2\chi\sin2\phi + \sin^2\theta\cos2\chi(1 - \cos2\phi)]
               \chi_{\text{YYX}} = (1/4)\beta_{\text{cbb}} \{ [\sin\theta(1 + \cos2\phi) - (\sin\theta - \sin^3\theta)(1 - \cos2\phi)](\cos\chi - \cos3\chi) 
(ssp)
                                           -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_{\text{YYZ}} = -(1/2)\beta_{\text{cbb}}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 - \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]
                          -(1/2)\beta_{csh}[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)\sin2\phi + \sin^2\theta\sin2\chi(1 - \cos2\phi)]
               \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) \}
(psp)
                                           -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\varphi\}
                                            -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)\sin 2\chi(1 - \cos 2\phi) - \sin^2\theta\cos 2\chi\sin 2\phi]
                        +(1/2)\beta_{csb}[(\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_{csh}[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_{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)]
(sps)
                                          -2\sin\theta\cos\theta\sin3\gamma\sin2\phi
                          +(1/4)\beta_{csh}\{[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_{chh} \{ 2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 - \cos2\phi) \}
                                          + (1 - 3\cos^2\theta)\sin 2\chi \sin 2\phi
                        -(1/4)\beta_{csh}\left\{2\left[(\cos\theta-\cos^3\theta)+\cos^3\theta\cos2\chi\right]\sin2\phi-\left[\sin^2\theta+(1-3\cos^2\theta)\cos2\phi\right]\sin2\chi\right\}
              \chi_{XXY} = (1/4)\beta_{cbb} \{ [-\sin\theta(1+\cos2\phi) + (\sin\theta - \sin^3\theta)(1-\cos2\phi)](\sin\chi + \sin3\chi) \}
(pps)
                                          -\sin\theta\cos\theta(\cos\chi+\cos3\chi)\sin2\phi
                        +(1/4)\beta_{csh}\{(2\sin\theta - \sin^3\theta)\sin 2\phi - 2\sin\theta\cos\theta [2\cos\chi - (\cos\chi + \cos3\chi)\cos 2\phi]\}
               \chi_{ZZY} = \beta_{cbb} [-(\sin\theta - \sin^3\theta)\sin\chi(1 - \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]
                        -\beta_{coh}[(\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_{csb}[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_{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) \}
(pss)
                                          -2\sin\theta\cos\theta\sin3\gamma\sin2\phi
                          +(1/4)\beta_{csh}\{[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)\sin 2\chi \sin 2\phi
                        -(1/4)\beta_{csb}\left\{2\left[(\cos\theta-\cos^3\theta)+\cos^3\theta\cos2\chi\right]\sin2\phi-\left[\sin^2\theta+(1-3\cos^2\theta)\cos2\phi\right]\sin2\chi\right\}
               \chi_{\text{YYY}} = (1/4)\beta_{\text{cbb}} \left\{ \left[ \sin\theta (\sin\chi + \sin3\chi)(1 + \cos2\phi) + (\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 - \cos2\phi) \right] \right\}
(sss)
                                          -2\sin\theta\cos\theta(\cos\chi-\cos3\chi)\sin2\phi
                        +(1/4)\beta_{csh}\{[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** ]  $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\zeta\zeta}$ ,  $\beta_{\eta\eta\zeta}$  のときには  $\beta_{aac} \sim (4/9) \beta_{\zeta\zeta\zeta}$ 、 $\beta_{cac} \sim (1/9) \beta_{\zeta\zeta\zeta}$  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。

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

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

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

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

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

(ppp) 
$$\chi_{XXX} = -2\beta_{abc}\cos \sin \theta \cos \chi$$
 +  $(1/4)/\beta_{abc} - \beta_{cac}/(\cos \alpha - \cos^2 \alpha) \{4\sin \theta \cos \chi - 3\sin^2 \theta (3\cos \chi + \cos 3\chi) - (\sin \theta (\cos \chi - \cos 3\chi) + (\sin \theta (\cos \chi - \cos 3\chi)) \cos 2\phi$  -  $2\sin \theta (\cos \theta (\sin \chi + \sin 3\chi) \sin 2\phi) \}$  +  $(1/2)/\beta_{abc} - \beta_{cac}/\cos \cos \sin^3 \theta (3\cos \chi + \cos 3\chi) \}$   $\chi_{XZZ} = -(\beta_{abc} - \beta_{cac})(\cos \alpha - \cos^2 \alpha) [(\sin \theta - \sin^3 \theta) \cos \chi (3 + \cos 2\phi) - \sin \theta \cos \theta \sin \chi \sin 2\phi] \}$  +  $2(\beta_{abc} - \beta_{cac})(\cos \alpha (\sin \theta - \sin^3 \theta) \cos \chi (3 + \cos 2\phi) - \sin \theta \cos \theta \sin \chi \sin 2\phi] \}$  +  $2(\beta_{abc} - \beta_{cac})(\cos \alpha (\sin \theta - \sin^3 \theta) \cos \chi (3 + \cos 2\phi) - \sin \theta \cos \theta \sin \chi \sin 2\phi] \}$  +  $2(\beta_{abc} - \beta_{cac})(\cos \alpha (\sin \theta - \sin^3 \theta) \cos \chi) \}$  +  $2(\beta_{abc} - \beta_{cac})(\cos \alpha (\sin \theta - \sin^3 \theta) \cos \chi) \}$  +  $2(\beta_{abc} - \beta_{cac})(\cos \alpha (\sin \theta - \sin^3 \theta) \cos \chi) \}$  +  $2(\beta_{abc} - \beta_{cac})(\cos \alpha (\sin \theta - \sin^3 \theta) \cos \chi) \}$  +  $2(\beta_{abc} - \beta_{cac})(\cos \alpha (\sin \theta - \sin^3 \theta) \cos \chi) \}$  +  $2(\beta_{abc} - \beta_{cac})(\cos \alpha (\sin \theta - \sin^3 \theta) \cos \chi) \}$  +  $2(\beta_{abc} - \beta_{cac})(\cos \alpha (\sin \theta - \sin^3 \theta) \cos \chi) \}$  +  $2(\beta_{abc} - \beta_{cac})(\cos \alpha (\cos \theta - \cos^3 \theta) (\cos \theta - \cos^3 \theta) (1 + \cos 2\chi) (3 + \cos 2\phi) - \sin^2 \theta \sin 2\chi \sin 2\phi) \}$  +  $2(\beta_{abc} - \beta_{cac})(\cos \alpha (\cos \theta - \cos^3 \theta) (\cos \theta - \cos^3 \theta) (1 + \cos 2\chi) (3 + \cos 2\phi) - \sin^2 \theta \sin 2\chi \sin 2\phi) \}$  +  $2(\beta_{abc} - \beta_{cac})(\cos \alpha (\cos \theta - \cos^3 \theta) (1 + \cos 2\chi) )$  \(\lambda\_{abc} - \beta\_{abc} \end{acc} - \beta\_{cac})(\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) \} +  $2(\beta_{abc} - \beta_{cac})(\cos \alpha - \cos^3 \alpha) [(\cos \theta - \cos^3 \theta) (1 + \cos 2\chi) (3 + \cos 2\phi) - \sin^2 \theta \sin 2\chi \sin 2\phi) \}$  +  $2(\cos \theta - \cos^3 \alpha) (\cos \theta - \cos^3 \alpha) (\cos \theta - \cos^3 \theta) (1 + \cos 2\chi) \}$  \(\lambda\_{abc} - \beta\_{cac} \co \sigma(\co \alpha - \co \alpha^2)(\co \alpha - \c

```
(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_{ax} - \beta_{cx})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)
                \chi_{YYZ} = 2\beta_{aac}\cos\alpha\sin\theta\cos\chi
                          +(1/2)(\beta_{ax} - \beta_{cx})(\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)\cos 2\chi]\cos 2\phi - 2\cos^2\theta\sin 2\chi\sin 2\phi
                          -(\beta_{ax} - \beta_{coc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)
                \chi_{XYX} = (1/4)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)\}
(psp)
                                         +2\sin\theta\cos\theta(\cos\chi+\cos3\chi)\sin2\phi
                          -(1/2)(\beta_{ax} - \beta_{cx})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)
                \chi_{\rm ZYZ} = (\beta_{\rm ax} - \beta_{\rm cx})(\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_{ax} - \beta_{cx})\cos\alpha(\sin\theta - \sin^3\theta)\sin\alpha
                 \chi_{XYZ} = -(1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\alpha\}
                                         -2\cos^2\theta\cos 2\gamma\sin 2\phi
                          + (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                 \chi_{\text{ZYX}} = -(1/2)(\beta_{\text{ax}} - \beta_{\text{cx}})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) + \sin^2\theta(1 + \cos2\chi)\sin2\phi]
                          + (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                \chi_{\rm YXY} = (1/4)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)\}
(sps)
                                            -2\sin\theta\cos\theta(\sin\chi-\sin3\chi)\sin2\phi
                            + (1/2)(\beta_{ax} - \beta_{cx})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)
                 \chi_{\rm YZY} = (1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]
                                - (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)
                \chi_{XXY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\gamma
(pps)
                          +(1/4)(\beta_{aa} - \beta_{ca})(\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_{ax} - \beta_{cx})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)
                 \chi_{ZZY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\chi
                          +(\beta_{a\alpha}-\beta_{c\alpha})(\cos\alpha-\cos^3\alpha)[-\sin\theta+3(\sin\theta-\sin^3\theta)-\sin^3\theta\cos2\phi]\sin\chi
                          -2(\beta_{ax} - \beta_{cx})\cos\alpha(\sin\theta - \sin^3\theta)\sin\chi
                 \chi_{XZY} = -(1/2)(\beta_{ax} - \beta_{cx})(\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_{coc})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                 \chi_{\rm ZXY} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]
```

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

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

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

$$\begin{split} \chi_{\Upsilon\Upsilon\Upsilon} &= 2\beta_{\rm aac} {\rm cos}\alpha {\rm sin}\theta {\rm sin}\chi \\ &+ (1/4)(\beta_{\rm aac} - \beta_{\rm coc})({\rm cos}\alpha - {\rm cos}^3\alpha)\{-4{\rm sin}\theta {\rm sin}\chi + 3{\rm sin}^3\theta(3{\rm sin}\chi - {\rm sin}3\chi) \\ &+ [{\rm sin}\theta({\rm sin}\chi + {\rm sin}3\chi) - ({\rm sin}\theta - {\rm sin}^3\theta)(3{\rm sin}\chi - {\rm sin}3\chi)]{\rm cos}2\varphi \\ &- 2{\rm sin}\theta {\rm cos}\theta({\rm cos}\chi - {\rm cos}3\chi){\rm sin}2\varphi\} \\ &- (1/2)(\beta_{\rm aac} - \beta_{\rm coc}){\rm cos}\alpha {\rm sin}^3\theta(3{\rm sin}\chi - {\rm sin}3\chi) \end{split}$$

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

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

$$\begin{split} (\mathrm{spp}) \qquad \chi_{\mathrm{YXX}} &= -(1/2)(\beta_{\mathrm{axc}} - \beta_{\mathrm{cxc}})(\cos\alpha - \cos^3\alpha) \{ [(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) \\ &+ \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi \} \\ \chi_{\mathrm{YZZ}} &= (\beta_{\mathrm{axc}} - \beta_{\mathrm{cxc}})(\cos\alpha - \cos^3\alpha) [(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi] \\ \chi_{\mathrm{YZX}} &= -(1/2)(\beta_{\mathrm{axc}} - \beta_{\mathrm{cxc}})(\cos\alpha - \cos^3\alpha) \{ 2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \\ &- \cos2\phi\cos\theta]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi \} \\ \chi_{\mathrm{YXZ}} &= -(\beta_{\mathrm{axc}} - \beta_{\mathrm{cxc}})(\cos\alpha - \cos^3\alpha) [(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi] \end{split}$$

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

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

$$\begin{split} (\text{psp}) \qquad & \chi_{\text{XYX}} = -(1/2)(\beta_{\text{aac}} - \beta_{\text{coc}})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) \\ & + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi\} \\ \chi_{\text{ZYZ}} = & (\beta_{\text{aac}} - \beta_{\text{coc}})(\cos\alpha - \cos^3\alpha)[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi] \\ \chi_{\text{XYZ}} = & -(\beta_{\text{aac}} - \beta_{\text{coc}})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi] \\ \chi_{\text{ZYX}} = & -(1/2)(\beta_{\text{aac}} - \beta_{\text{coc}})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \\ & - \cos2\phi\cos\theta]\sin2\chi + [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\} \end{split}$$

$$\begin{split} (\mathrm{sps}) \qquad \chi_{\mathrm{YXY}} &= (1/2)(\beta_{\mathrm{axc}} - \beta_{\mathrm{cxc}})(\cos\alpha - \cos^3\alpha) \{ [(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) \\ &\quad + \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi \} \\ \chi_{\mathrm{YZY}} &= -(1/2)(\beta_{\mathrm{axc}} - \beta_{\mathrm{cxc}})(\cos\alpha - \cos^3\alpha) \{ 2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\phi)] \\ &\quad - (1 - 3\cos^2\theta)\sin2\chi\sin2\phi \} \end{split}$$

$$\begin{split} (\text{pps}) \qquad & \chi_{\text{XXY}} = -(1/2)(\beta_{\text{a}\alpha} - \beta_{\text{c}\omega})(\cos\alpha - \cos^3\alpha)\{[(\sin\theta - \sin^3\theta)(1 + \cos2\phi) - \sin\theta(1 - \cos2\phi)](\sin\chi + \sin3\chi) \\ & + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\} \\ \chi_{\text{ZZY}} = & 2(\beta_{\text{a}\alpha} - \beta_{\text{c}\omega})(\cos\alpha - \cos^3\alpha)[(\sin\theta - \sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi] \\ \chi_{\text{ZXY}} = & -(1/2)(\beta_{\text{a}\alpha} - \beta_{\text{c}\omega})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \\ & - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\} \\ \chi_{\text{XZY}} = & -(1/2)(\beta_{\text{a}\alpha} - \beta_{\text{c}\omega})(\cos\alpha - \cos^3\alpha)\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) \\ & - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\} \end{split}$$

$$\begin{split} \chi_{XYY} &= (1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha) \{ [(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\varphi) \\ &+ \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\varphi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\varphi \} \\ \chi_{ZYY} &= -(1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha) \{ 2[\cos\theta(1 - \cos2\chi\cos2\varphi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\varphi)] \\ &- (1 - 3\cos^2\theta)\sin2\chi\sin2\varphi \} \end{split}$$

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

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

[縮重パンド]  $\beta_{\zeta\zeta\zeta} >> \beta_{\xi\xi\zeta}, \, \beta_{\eta\eta\zeta}$  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。

 $(eta_{zyy}$  と  $eta_{yzy}$  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。) ( $\pm$  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。)  $eta_{zxx}=-2eta_{caa}(\cos\alpha-2\cos^3\alpha)$   $eta_{xzx}=-2eta_{caa}(\cos\alpha-2\cos^3\alpha)$ 

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

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

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

$$\beta_{yyz} = 0$$

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

(ppp) 
$$\chi_{\text{XXX}} = -(1/2)(\beta_{\text{asc}} + \beta_{\text{bbc}}) \sin \theta \cos y$$
 $+ (1/8)(\beta_{\text{asc}} + \beta_{\text{bbc}} - 2\beta_{\text{cac}}) \sin^3 \theta (3\cos y + \cos 3y)$ 
 $+ (1/8)(\beta_{\text{asc}} + \beta_{\text{bbc}} - 2\beta_{\text{cac}}) \sin^3 \theta (3\cos y + \cos 3y)$ 
 $+ (1/8)(\beta_{\text{asc}} + \beta_{\text{bbc}} - 2\beta_{\text{cac}}) \sin^3 \theta (3\cos y + \cos 3y)$ 
 $+ (1/8)(\beta_{\text{asc}} + \beta_{\text{bbc}} - 2\beta_{\text{cac}}) (\sin \theta - \sin^3 \theta) \cos y$ 
 $+ (1/2)(\beta_{\text{asc}} + \beta_{\text{bbc}} - 2\beta_{\text{cac}}) (\sin \theta - \sin^3 \theta) \cos y$ 
 $+ (1/2)(\beta_{\text{asc}} + \beta_{\text{bbc}} - 2\beta_{\text{cac}}) (\sin \theta - \sin^3 \theta) \cos y$ 
 $+ (1/2)(\beta_{\text{asc}} + \beta_{\text{bbc}} - 2\beta_{\text{cac}}) (\sin \theta - \sin^3 \theta) \cos y$ 
 $+ (1/2)(\beta_{\text{asc}} + \beta_{\text{bbc}}) [(\sin \theta - \sin^3 \theta) \cos y \cos 2\phi - \sin \theta \cos \theta \sin y \sin 2\phi]$ 
 $\chi_{\text{ZXZ}} = (1/2)(\beta_{\text{bac}} + \beta_{\text{bbc}}) \sin^3 \theta \cos y$ 
 $+ (1/2)(\beta_{\text{asc}} + \beta_{\text{bbc}}) [(\sin \theta - \sin^3 \theta) \cos y \cos 2\phi - \sin \theta \cos \theta \sin y \sin 2\phi]$ 
 $\chi_{\text{ZXZ}} = (1/2)(\beta_{\text{bac}} + \beta_{\text{bbc}}) \sin^3 \theta \cos y \cos 2\phi$ 
 $\chi_{\text{ZZZ}} = (1/2)(\beta_{\text{asc}} + \beta_{\text{bbc}}) \sin^3 \theta \cos y \cos 2\phi$ 
 $\chi_{\text{ZZZ}} = (1/4)(\beta_{\text{bac}} + \beta_{\text{bbc}}) \sin^3 \theta \cos y \cos 2\phi$ 
 $\chi_{\text{ZZZ}} = (1/4)(\beta_{\text{bac}} + \beta_{\text{bbc}}) (\cos \theta - \cos^3 \theta) (1 + \cos 2y)$ 
 $- (1/4)(\beta_{\text{bac}} + \beta_{\text{bbc}}) (\cos \theta - \cos^3 \theta) (1 + \cos 2y) \cos 2\phi - \sin^2 \theta \sin 2y \sin 2\phi]$ 
 $\chi_{\text{ZXZ}} = (1/2)(\beta_{\text{asc}} + \beta_{\text{bbc}}) (\cos \theta - \cos^3 \theta) (1 + \cos 2y)$ 
 $- (1/4)(\beta_{\text{bac}} + \beta_{\text{bbc}}) (\cos \theta - \cos^3 \theta) (1 + \cos 2y)$ 
 $- (1/4)(\beta_{\text{bac}} + \beta_{\text{bbc}}) (\cos \theta - \cos^3 \theta) (1 + \cos 2y)$ 
 $- (1/4)(\beta_{\text{bac}} + \beta_{\text{bbc}}) (\cos \theta - \cos^3 \theta) (1 + \cos 2y)$ 
 $- (1/4)(\beta_{\text{bac}} + \beta_{\text{bbc}}) (\cos \theta - \cos^3 \theta) (1 + \cos 2y)$ 
 $- (1/4)(\beta_{\text{bac}} + \beta_{\text{bbc}}) (\cos \theta - \cos^3 \theta) (1 + \cos 2y)$ 
 $- (1/4)(\beta_{\text{bac}} + \beta_{\text{bbc}}) (\cos \theta - \cos^3 \theta) (1 + \cos 2y)$ 
 $- (1/4)(\beta_{\text{bac}} + \beta_{\text{bbc}}) (\cos \theta - \cos^3 \theta) (\cos \theta + \cos^3 \theta) (\cos \theta + \cos^3 \theta) \cos 2\phi + 2\cos^3 \theta \sin 2y \sin 2\phi)$ 
 $\chi_{\text{ZZZ}} = (1/2)(\beta_{\text{bac}} + \beta_{\text{bbc}} - 2\beta_{\text{cac}}) (\cos \theta - \cos^3 \theta) (\sin y + \sin 3y)$ 
 $+ (1/8)(\beta_{\text{acc}} + \beta_{\text{bbc}} - 2\beta_{\text{cac}}) (\sin \theta - \sin^3 \theta) \sin y$ 
 $- (1/2)(\beta_{\text{bac}} + \beta_{\text{bbc}} - 2\beta_{\text{cac}}) (\sin \theta - \sin^3 \theta) \sin y$ 
 $- (1/2)(\beta_{\text{bac}} + \beta_{\text{bbc}} - 2\beta_{\text{cac}}) (\cos \theta - \cos^3 \theta) \sin 2y$ 
 $- (1/4)(\beta_{\text{bac}} + \beta_{\text{bbc}} - 2\beta_{\text{cac}}) (\cos \theta - \cos^3 \theta) \sin 2y$ 
 $- (1/4)(\beta_{\text{bac}} + \beta_{\text{bbc}} - 2\beta_{\text{cac}}) (\cos \theta - \cos^3 \theta) \sin 2y$ 

```
+ (1/8)(\beta_{aac} - \beta_{bbc})\{cos2\phi[sin\theta(3cos\chi + cos3\chi) - (sin\theta - sin^3\theta)(cos\chi - cos3\chi)]
                                -2\sin 2\phi \sin \theta \cos \theta (\sin \chi + \sin 3\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})[\cos 2\phi[(\cos \theta - \cos^3 \theta) + (\cos \theta + \cos^3 \theta)\cos 2\chi] - 2\sin 2\phi\cos^2 \theta\sin 2\chi)]
               \chi_{XYX} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{cc})\sin^3\theta(\sin\chi + \sin3\chi)
(psp)
                          +(1/8)(\beta_{ax}-\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_{\rm ZYZ} = -(1/2)(\beta_{\rm acc} + \beta_{\rm bbc} - 2\beta_{\rm 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_{cm})(\cos\theta - \cos^3\theta)\sin 2\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_{\text{ZYX}} = (1/4)(\beta_{\text{ac}} + \beta_{\text{bbc}} - 2\beta_{\text{cm}})(\cos\theta - \cos^3\theta)\sin 2\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_{\rm YXY} = (1/8)(\beta_{\rm ac} + \beta_{\rm bbc} - 2\beta_{\rm cc})\sin^3\theta(\cos\chi - \cos3\chi)
(sps)
                          -(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_{axc} + \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_{XXY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi
(pps)
                          -(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)\sin 2\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_{\rm ZXY} = (1/4)(\beta_{\rm aac} + \beta_{\rm bbc} - 2\beta_{\rm cc})(\cos\theta - \cos^3\theta)\sin 2\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_{XYY} = (1/8)(\beta_{ax} + \beta_{bbc} - 2\beta_{cx})\sin^3\theta(\cos\chi - \cos3\chi)
(pss)
                          -(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]
                \chi_{YYY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi
(sss)
                          -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{cac})\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)]\}
```

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

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

### [逆対称 (b<sub>1</sub>) 振動]

$$(ppp) \quad \chi_{XXX} = -(1/4)\beta_{cm} \{ \{ (\sin\theta - \sin^3\theta) (3\cos\chi + \cos3\chi) (1 + \cos2\phi) + \sin\theta(\cos\chi - \cos3\chi) (1 - \cos2\phi) \}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\chi_{YYZ} = (1/2)\beta_{cm} [(\cos\theta - \cos^3\theta) (1 + \cos2\phi) + \sin\theta(1 - \cos2\phi)] (\cos\chi - \cos3\chi)$$

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

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

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

$$\chi_{YYZ} = (1/2)\beta_{cm} [(\sin\theta - \sin^3\theta) (\sin\chi + \sin3\chi) (1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi) (1 - \cos2\phi) ]$$

$$\chi_{YYZ} = (1/2)\beta_{cm} [(\sin\theta - \sin^3\theta) (\sin\chi + \sin3\chi) (1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi) (1 - \cos2\phi) ]$$

$$\chi_{YYZ} = (1/2)\beta_{cm} [(\sin\theta - \sin^3\theta) (\sin\chi + \sin3\chi) (1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi) (1 - \cos2\phi) ]$$

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

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

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

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

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

$$\chi_{YYZ} = (1/2)\beta_{cm} [\{ (\sin\theta - \sin^3\theta) (\cos\chi -$$

 $-(1 - 3\cos^2\theta)\sin 2\gamma \sin 2\phi$ 

(pps) 
$$\chi_{XXY} = (1/4)\beta_{cm}\{[(\sin\theta - \sin^3\theta)(1 + \cos2\phi) - \sin\theta(1 - \cos2\phi)](\sin\chi + \sin3\chi) + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi\}$$
 $\chi_{ZZY} = -\beta_{cm}[(\sin\theta - \sin^3\theta)\sin\chi (1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi \sin2\phi]$ 
 $\chi_{ZXY} = (1/4)\beta_{cm}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$ 
 $\chi_{XZY} = (1/4)\beta_{cm}\{2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos\theta\cos2\phi]\sin2\chi + [\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi\}$ 
(pss)  $\chi_{XYY} = -(1/4)\beta_{cm}\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + (1 - \cos2\phi)\sin\theta(\cos\chi + \cos3\chi)] + 2\sin\theta\cos\theta\sin3\chi\sin2\phi\}$ 
 $\chi_{ZYY} = (1/4)\beta_{cm}\{2[\cos\theta(1 - \cos2\chi\cos2\phi) - (\cos\theta - \cos^2\theta)(1 - \cos2\chi)(1 + \cos2\phi)] - (1 - 3\cos^2\theta)\sin2\chi\sin2\phi\}$ 
(sss)  $\chi_{YYY} = (1/4)\beta_{cm}\{[(\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi + \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta(\cos\chi - \cos3\chi)\sin2\phi\}$ 

### [面外 (b<sub>2</sub>) 振動]

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

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

$$\begin{split} \chi_{YYX} &= (1/4)\beta_{cbb}\{[\sin\theta(1-\cos2\varphi)-(\sin\theta-\sin^3\!\theta)(1-\cos2\varphi)](\cos\chi-\cos3\chi)\\ &-2\sin\theta\cos\theta(\sin\chi-\sin3\chi)\sin2\varphi\}\\ \chi_{YYZ} &= -(1/2)\beta_{cbb}[(\cos\theta-\cos^3\!\theta)(1-\cos2\chi)(1-\cos2\varphi)-\sin^2\!\theta\sin2\chi\sin2\varphi] \end{split}$$

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

 $-2\sin\theta\cos\theta\cos3\chi\sin2\phi$ 

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

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

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

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

$$\begin{split} \chi_{YZY} &= (1/4)\beta_{cbb} \{ 2[cos\theta(1 + cos2\chi cos2\varphi) - (cos\theta - cos^3\theta)(1 - cos2\chi)(1 - cos2\varphi) ] \\ &+ (1 - 3cos^2\theta) sin2\gamma sin2\varphi \} \end{split}$$

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

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

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

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

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

$$\begin{split} \chi_{\rm ZYY} &= (1/4)\beta_{\rm cbb}\{2[\cos\!\theta(1+\cos\!2\chi\!\cos\!2\varphi) - (\cos\!\theta - \cos^3\!\theta)(1-\cos\!2\chi)(1-\cos\!2\varphi)] \\ &\quad + (1-3\cos^2\!\theta)\!\sin\!2\chi\!\sin\!2\varphi\} \end{split}$$

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

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

#### 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]  $\beta_{\text{CCC}} >> \beta_{\text{EEC}}, \beta_{nnC}$  のときには  $\beta_{aac} \sim (4/9)\beta_{\text{CCC}}, \beta_{cac} \sim (1/9)\beta_{\text{CCC}}$  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。

$$eta_{xxz} + eta_{yyz} = -2(eta_{ax} - eta_{cx})(\cos\alpha - \cos^3\alpha) + 4eta_{ax}\cos\alpha$$
 $eta_{xxz} - eta_{yyz} = -2(eta_{ax} - eta_{cx})(\cos\alpha - \cos^3\alpha)$ 
 $eta_{xxz} + eta_{yyz} - 2eta_{zzz} = -2(eta_{ax} - eta_{cx})[3(\cos\alpha - \cos^3\alpha) - 2\cos\alpha]$ 
 $eta_{zxx} = -2(eta_{ax} - eta_{cx})(\cos\alpha - \cos^3\alpha)$  であるから、

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

```
-[\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+\sin3\chi)\sin2\phi
                     +(1/2)(\beta_{ac} - \beta_{cc})\cos\alpha\sin^3\theta(3\cos\chi + \cos3\chi)
                 \chi_{XZZ} = -(\beta_{a\alpha} - \beta_{c\alpha})(\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_{\rm ac}-\beta_{\rm cc})\cos\alpha(\sin\theta-\sin^3\theta)\cos\chi
                 \chi_{ZXZ} = -(\beta_{aac} - \beta_{cac})(\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_{ax}-\beta_{cx})\cos\alpha(\sin\theta-\sin^3\theta)\cos\chi
                 \chi_{ZZX} = -2\beta_{aac}\cos\alpha\sin\theta\cos\chi
                          +(\beta_{ax}-\beta_{cx})(\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_{ax} - \beta_{cx})\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_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)
                 \chi_{ZXX} = (1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)(3 + \cos2\phi) - \sin^2\theta\sin2\chi\sin2\phi]
                          -(\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)
                \chi_{XXZ} = 2\beta_{aac}\cos\alpha\cos\theta
                        +(1/2)(\beta_{ax}-\beta_{cx})(\cos\alpha-\cos^3\alpha)\{-2\cos\theta+3(\cos\theta-\cos^3\theta)(1+\cos2\chi)\}
                                                     +\left[(\cos\theta-\cos^3\!\theta)-(\cos\theta+\cos^3\!\theta)\!\cos\!2\chi]\!\cos\!2\varphi+2\cos^2\!\theta\!\sin\!2\chi\!\sin\!2\varphi\right]
                          -(\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)(1 + \cos2\chi)
                \chi_{ZZZ} = -2\beta_{aac}\cos\alpha\cos\theta
                          +(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)[-\cos\theta + 3\cos^3\theta - (\cos\theta - \cos^3\theta)\cos2\phi]
                          -2(\beta_{\rm ax} - \beta_{\rm cx})\cos\alpha\cos^3\theta
                \chi_{\rm YXX} = (1/4)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)\}
(spp)
                                              + 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_{ax} - \beta_{cx})(\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_{ax} - \beta_{cx})\cos\alpha(\sin\theta - \sin^3\theta)\sin\alpha
                \chi_{YZX} = -(1/2)(\beta_{aac} - \beta_{cc})(\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_{\rm ax} - \beta_{\rm cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi
                 \chi_{\rm YXZ} = -(1/2)(\beta_{\rm ac} - \beta_{\rm cc})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\alpha\}
                                              -2\cos^2\theta\cos 2\gamma\sin 2\phi
                          + (\beta_{ax} - \beta_{cx})\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_{ax} - \beta_{cx})(\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_{ax} - \beta_{cx})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)
                \chi_{YYZ} = 2\beta_{aac}\cos\alpha\sin\theta\cos\chi
```

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

```
+(1/2)(\beta_{ax}-\beta_{cx})(\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)\cos 2\chi]\cos 2\phi - 2\cos^2\theta\sin 2\chi\sin 2\phi
                          -(\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)
                \chi_{XYX} = (1/4)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[3\sin^3\theta - (2\sin\theta - \sin^3\theta)\cos2\phi](\sin\chi + \sin3\chi)\}
(psp)
                                              + 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\sin2\phi
                          -(1/2)(\beta_{aac} - \beta_{cx})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)
                \chi_{\rm ZYZ} = (\beta_{\rm ax} - \beta_{\rm cx})(\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\alpha
                 \chi_{XYZ} = -(1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[3(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos2\phi]\sin2\alpha\}
                                              -2\cos^2\theta\cos 2\gamma\sin 2\phi
                          + (\beta_{aac} - \beta_{ccc})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                          + (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi
                 \chi_{\rm ZYX} = -(1/2)(\beta_{\rm ax} - \beta_{\rm cx})(\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_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                \chi_{\rm YXY} = (1/4)(\beta_{\rm ax} - \beta_{\rm cx})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)\}
(sps)
                                              -2\sin\theta\cos\theta(\sin\chi-\sin3\chi)\sin2\phi
                          + (1/2)(\beta_{aac} - \beta_{coc})\cos\alpha\sin^3\theta(\cos\chi - \cos3\chi)
                 \chi_{yzy} = (1/2)(\beta_{ax} - \beta_{cx})(\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_{coc})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)
                \chi_{XXY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\gamma
(pps)
                          +(1/4)(\beta_{a\alpha} - \beta_{c\alpha})(\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_{\rm ac} - \beta_{\rm cc})\cos\alpha\sin^3\theta(\sin\chi + \sin3\chi)
                \chi_{ZZY} = 2\beta_{aac}\cos\alpha\sin\theta\sin\alpha
                          +(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)[-\sin\theta + 3(\sin\theta - \sin^3\theta) - \sin^3\theta\cos2\phi]\sin\alpha
                          - 2(\beta_{ax} - \beta_{cx})\cos\alpha(\sin\theta - \sin^3\theta)\sin\alpha
                 \chi_{XZY} = -(1/2)(\beta_{ax} - \beta_{cx})(\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_{coc})\cos\alpha(\cos\theta - \cos^3\theta)\sin 2\chi
                 \chi_{ZXY} = -(1/2)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)\sin2\chi(3 + \cos2\phi) - \sin^2\theta(1 - \cos2\chi)\sin2\phi]
                            + (\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)\sin2\chi
                \chi_{XYY} = (1/4)(\beta_{ax} - \beta_{cx})(\cos\alpha - \cos^3\alpha)\{[-3\sin^3\theta + (2\sin\theta - \sin^3\theta)\cos2\phi](\cos\chi - \cos3\chi)\}
(pss)
                                              -2\sin\theta\cos\theta(\sin\chi-\sin3\chi)\sin2\phi
                          +(1/2)(\beta_{aac} - \beta_{coc})\cos\alpha\sin^3\theta(\cos\alpha - \cos3\alpha)
                \chi_{\text{ZYY}} = (1/2)(\beta_{\text{agc}} - \beta_{\text{coc}})(\cos\alpha - \cos^3\alpha)[(\cos\theta - \cos^3\theta)(1 - \cos2\chi)(3 + \cos2\phi) + \sin^2\theta\sin2\chi\sin2\phi]
                          -(\beta_{ax} - \beta_{cx})\cos\alpha(\cos\theta - \cos^3\theta)(1 - \cos2\chi)
```

$$\begin{split} \chi_{\rm YYY} &= 2\beta_{\rm aac} {\rm cos}\alpha {\rm sin}\theta {\rm sin}\chi \\ &+ (1/4)(\beta_{\rm aac} - \beta_{\rm ccc})({\rm cos}\alpha - {\rm cos}^3\alpha) \{-4{\rm sin}\theta {\rm sin}\chi + 3{\rm sin}^3\theta (3{\rm sin}\chi - {\rm sin}3\chi) \\ &+ [{\rm sin}\theta ({\rm sin}\chi + {\rm sin}3\chi) - ({\rm sin}\theta - {\rm sin}^3\theta)(3{\rm sin}\chi - {\rm sin}3\chi)]{\rm cos}2\varphi \\ &- 2{\rm sin}\theta {\rm cos}\theta ({\rm cos}\chi - {\rm cos}3\chi){\rm sin}2\varphi \} \\ &- (1/2)(\beta_{\rm aac} - \beta_{\rm ccc}){\rm cos}\alpha {\rm sin}^3\theta (3{\rm sin}\chi - {\rm sin}3\chi) \end{split}$$

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

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

$$\begin{split} (\text{spp}) \qquad \chi_{\text{YXX}} &= -(1/2)(\beta_{\text{aac}} - \beta_{\text{ccc}})(\cos\alpha - \cos^3\alpha) \{ [(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) \\ &+ \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\phi \} \\ \chi_{\text{YZZ}} &= (\beta_{\text{aac}} - \beta_{\text{ccc}})(\cos\alpha - \cos^3\alpha) [(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi] \\ \chi_{\text{YZX}} &= -(1/2)(\beta_{\text{aac}} - \beta_{\text{ccc}})(\cos\alpha - \cos^3\alpha) \{ 2[(\cos\theta - \cos^3\theta)(1 + \cos2\phi) - \cos2\phi\cos\theta]\sin2\chi \\ &+ [-\sin^2\theta + (1 - 3\cos^2\theta)\cos2\chi]\sin2\phi \} \\ \chi_{\text{YXZ}} &= -(\beta_{\text{aac}} - \beta_{\text{ccc}})(\cos\alpha - \cos^3\alpha) [(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\phi) + \sin^2\theta\cos2\chi\sin2\phi] \end{split}$$

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

$$\begin{split} (psp) \qquad \chi_{XYX} &= -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) \{ [(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\varphi) \\ &\quad + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\varphi)] + 2\sin\theta\cos\theta\cos3\chi\sin2\varphi \} \\ \chi_{ZYZ} &= (\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) [(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\varphi) + \sin\theta\cos\theta\cos\chi\sin2\varphi] \\ \chi_{XYZ} &= -(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) [(\cos\theta - \cos^3\theta)\sin2\chi(1 + \cos2\varphi) + \sin^2\theta\cos2\chi\sin2\varphi] \\ \chi_{ZYX} &= -(1/2)(\beta_{aac} - \beta_{ccc})(\cos\alpha - \cos^3\alpha) \{ 2 [(\cos\theta - \cos^3\theta)(1 + \cos2\varphi) - \cos2\varphi\cos\theta]\sin2\chi \} \} \end{split}$$

+ 
$$[-\sin^2\theta + (1 - 3\cos^2\theta)\cos 2\chi] \sin 2\phi$$

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

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

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

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

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

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

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

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

[縮重パンド]  $\beta_{\text{CCC}} >> \beta_{\text{EEC}}, \beta_{nnC}$  のときには  $\beta_{caa} \sim (4/9) \beta_{\text{CCC}}, \beta_{aaa} \sim (4\sqrt{2}/9) \beta_{\text{CCC}}$  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 (  $\beta_{ik}=\beta_{ik}$ ) にあてはまる一般式である。

$$\begin{split} \beta_{xxz} + \beta_{yyz} &= -\beta_{caa}(\cos\alpha - \cos^3\alpha)[2 \pm (\cos2\varphi_A + \cos2\varphi_B)] \\ &- (1/2)\beta_{aaa}\sin^3\alpha[(\cos3\varphi_A + \cos3\varphi_B) \pm (\cos\varphi_A + \cos\varphi_B)] \\ \beta_{xxz} - \beta_{yyz} &= -\beta_{caa}(\cos\alpha - \cos^3\alpha)[2 \pm (\cos2\varphi_A + \cos2\varphi_B)] \\ &+ (1/2)\beta_{aaa}(2\sin\alpha - \sin^3\alpha)[(\cos3\varphi_A + \cos3\varphi_B) \pm (\cos\varphi_A + \cos\varphi_B)] \\ \beta_{xxz} + \beta_{yyz} - 2\beta_{zzz} &= -6\beta_{caa}(\cos\alpha - \cos^3\alpha)[2 \pm (\cos2\varphi_A + \cos2\varphi_B)] \\ &- (3/2)\beta_{aaa}\sin^3\alpha[(\cos3\varphi_A + \cos3\varphi_B) \pm (\cos\varphi_A + \cos\varphi_B)] \\ \beta_{zxx} &= \beta_{xzx} &= -(1/2)\beta_{caa}(\cos\alpha - 2\cos^3\alpha)[2 \pm (\cos2\varphi_A + \cos2\varphi_B)] \\ &+ (1/2)\beta_{aaa}(\sin\alpha - \sin^3\alpha)[(\cos3\varphi_A + \cos3\varphi_B) \pm (\cos\varphi_A + \cos\varphi_B)] \end{split}$$

#### [対称 (a<sub>1</sub>) 振動、c軸に沿った振動]

$$\begin{split} (ppp) \qquad & \chi_{XXX} = -(1/2)(\beta_{aac} + \beta_{bbc})sin\theta cos\chi \\ & + (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})sin^3\theta(3cos\chi + cos3\chi) \\ & + (1/8)(\beta_{aac} + \beta_{bbc})\{[sin\theta(cos\chi - cos3\chi) - (sin\theta - sin^3\theta)(3cos\chi + cos3\chi)]cos2\varphi \\ & + 2sin\theta cos\theta(sin\chi + sin3\chi)sin2\varphi\} \\ & + (1/4)\beta_{abc}\{[sin\theta(cos\chi - cos3\chi) - (sin\theta - sin^3\theta)(3cos\chi + cos3\chi)]sin2\varphi \\ & - 2sin\theta cos\theta(sin\chi + sin3\chi)cos2\varphi\} \\ & + (1/2)\beta_{acc}[(cos\theta - cos^3\theta)(3cos\chi + cos3\chi)cos\varphi - sin^2\theta(sin\chi + sin3\chi)sin\varphi] \\ & + (1/2)\beta_{bcc}[(cos\theta - cos^3\theta)(3cos\chi + cos3\chi)sin\varphi + sin^2\theta(sin\chi + sin3\chi)cos\varphi] \\ & \chi_{XZZ} = (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(sin\theta - sin^3\theta)cos\chi \\ & + (1/2)(\beta_{aac} - \beta_{bbc})[(sin\theta - sin^3\theta)cos\chi cos2\varphi - sin\theta cos\theta sin\chi sin2\varphi] \\ & + \beta_{abc}[(sin\theta - sin^3\theta)cos\chi sin2\varphi + sin\theta cos\theta sin\chi cos2\varphi] \end{split}$$

```
- \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_{\rm ZXZ} = (1/2)(\beta_{\rm ac} + \beta_{\rm bbc} - 2\beta_{\rm cc})(\sin\theta - \sin^3\theta)\cos\chi
         + (1/2)(\beta_{ax} - \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}[(cosθ - 2cos<sup>3</sup>θ)cosχcosφ - sin<sup>2</sup>θsinχsinφ]
          -\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_{ax} + \beta_{bbc} - 2\beta_{cc})(\sin\theta - \sin^3\theta)\cos\chi
           -(1/2)(\beta_{aac} - \beta_{bbc})\cos \chi \sin^3 \theta \cos 2\phi
           - \beta_{abc}(2\sin\theta - \sin^3\theta)\cos\gamma\sin2\phi
           - 2\beta_{ac}(cosθ - 2\cos^3\theta)cosχcosφ
           - 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_{hcc}[(\sin\theta - 2\sin^3\theta)(1 + \cos2\chi)\sin\phi + \sin\theta\cos\theta\sin2\chi\cos\phi]
\chi_{\rm ZXX} = -(1/4)(\beta_{\rm ac} + \beta_{\rm bbc} - 2\beta_{\rm cc})(\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_{cc})(\cos\theta - \cos^3\theta)(1 + \cos2\chi)
           -(1/4)(\beta_{aac} - \beta_{bbc})\{[(\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\}
           -(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)\cos 2\phi
           + \beta_{abc}(\cos\theta - \cos^3\theta)\sin 2\phi
           +2\beta_{acc}(\sin\theta - \sin^3\theta)\cos\phi
           +2\beta_{bcc}(\sin\theta - \sin^3\theta)\sin\phi
\chi_{\rm YXX} = -(1/8)(\beta_{\rm ax} + \beta_{\rm bbc} - 2\beta_{\rm cx})\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]
```

 $-(1/2)\beta_{acc}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\cos\phi + \sin^2\theta(\cos\chi + \cos3\chi)\sin\phi]$ 

(spp)

```
-(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_{cc})(\sin\theta - \sin^3\theta)\sin\chi
                             -(1/2)(\beta_{ax} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi\cos 2\phi + \sin\theta\cos\theta\cos\chi\sin 2\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_{coc})(\cos\theta - \cos^3\theta)\sin 2\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)\cos 2\chi\cos\phi + \sin 2\theta(1 + \cos 2\chi)\sin\phi]
                           +(1/2)\beta_{hcc}[(\sin\theta - 2\sin^3\theta)\cos 2\chi\sin\phi - \sin 2\theta(1 + \cos 2\chi)\cos\phi]
                \chi_{\rm YXZ} = (1/4)(\beta_{\rm ac} + \beta_{\rm bbc} - 2\beta_{\rm cc}) (\cos\theta - \cos^3\theta)\sin 2\chi
                           -(1/4)(\beta_{ac} - \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_{ac}[(\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_{ax} - \beta_{bbc})\{[(\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\}
                           -(1/2)\beta_{abc}\{[(\cos\theta - \cos^3\theta) + (\cos\theta + \cos^3\theta)\cos 2\chi]\sin 2\phi + \cos^2\theta\sin 2\chi\cos 2\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_{XYX} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi)
(psp)
                             +(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_{hcc}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\sin\phi - \sin^2\theta(\cos\chi + \cos3\chi)\cos\phi]
                \chi_{\rm ZYZ} = -(1/2)(\beta_{\rm ac} + \beta_{\rm bbc} - 2\beta_{\rm cc})(\sin\theta - \sin^3\theta)\sin\chi
                             -(1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi\cos 2\phi + \sin\theta\cos\theta\cos\chi\sin 2\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)\sin 2\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\gamma\sin\phi - \sin\theta\cos\theta\cos2\gamma\cos\phi]
                \chi_{\rm ZYX} = (1/4)(\beta_{\rm ax} + \beta_{\rm bbc} - 2\beta_{\rm cx})(\cos\theta - \cos^3\theta)\sin 2\chi
                          +(1/4)(\beta_{ax} - \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_{\rm YXY} = (1/8)(\beta_{\rm ac} + \beta_{\rm bbc} - 2\beta_{\rm cc})\sin^3\theta(\cos\chi - \cos3\chi)
                          -(1/8)(\beta_{ax} - \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_{ax} - \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_{hcc}[(\sin\theta - 2\sin^3\theta)(1 - \cos2\chi)\sin\phi - \sin\theta\cos\theta\sin2\chi\cos2\phi]
                \chi_{XXY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi
(pps)
                          -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi)
                          +(1/8)(\beta_{ax} - \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 \sin 2\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_{ax} + \beta_{bbc} - 2\beta_{cx})(\cos\theta - \cos^3\theta)\sin 2\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\gamma\sin2\phi + \sin^2\theta(1 - \cos2\gamma)\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]
```

$$+ (1/2)\beta_{bcc}[(sinθ - 2sin^3θ)sin2\chi sinφ + sinθcosθ(1 - cos2\chi)cosφ]$$

$$\chi_{ZXY} = (1/4)(\beta_{ax} + \beta_{bbc} - 2\beta_{cw})(cosθ - cos^3θ)sin2\chi$$

$$+ (1/4)(\beta_{ax} - \beta_{bbc})[(cosθ - cos^3θ)sin2\chi sos2φ - sin^3θ(1 - cos2\chi)cos2φ]$$

$$+ (1/2)\beta_{abc}[(cosθ - cos^3θ)sin2\chi sin2φ + sin^3θ(1 - cos2\chi)cos2φ]$$

$$+ (1/2)\beta_{abc}[(sinθ - 2sin^3θ)sin2\chi cosφ - sinθcosθ(1 - cos2\chi)cosφ]$$

$$+ (1/2)\beta_{abc}[(sinθ - 2sin^3θ)sin2\chi sinφ + sinθcosθ(1 - cos2\chi)cosφ]$$

$$(pss) \quad \chi_{XYY} = (1/8)(\beta_{ax} + \beta_{bbc} - 2\beta_{cw})sin^3θ(cos\chi - cos3\chi)$$

$$- (1/8)(\beta_{ax} - \beta_{bbc})[(2sinθ - sin^3θ)(cos\chi - cos3\chi)cos2φ - 2sinθcosθ(sin\chi - sin3\chi)cos2φ]$$

$$- (1/4)\beta_{abc}[(2sinθ - sin^3θ)(cos\chi - cos3\chi)cosφ - sinθcosθ(sin\chi - sin3\chi)cos2φ]$$

$$+ (1/2)\beta_{acc}[(cosθ - cos^3θ)(cos\chi - cos3\chi)cosφ - sin^3θ(sin\chi - sin3\chi)cosφ]$$

$$\chi_{ZYY} = -(1/4)(\beta_{ax} + \beta_{bbc} - 2\beta_{cw})(cosθ - cos^3θ)(1 - cos2\chi)$$

$$- (1/4)(\beta_{ax} - \beta_{bbc})[(cosθ - cos^3θ)(1 - cos2\chi)cos2φ + sin^3θsin2\chi sin2φ]$$

$$- (1/2)\beta_{abc}[(cosθ - cos^3θ)(1 - cos2\chi)cos2φ + sin^3θsin2\chi cos2φ]$$

$$- (1/2)\beta_{abc}[(cosθ - cos^3θ)(1 - cos2\chi)cos2φ + sin^3θsin2\chi cos2φ]$$

$$- (1/2)\beta_{abc}[(sinθ - 2sin^3θ)(1 - cos2\chi)cos2φ + sinθcosθsin2\chi cosφ]$$

$$(sss) \quad \chi_{YYY} = (1/2)(\beta_{ax} + \beta_{bbc} - 2\beta_{cw})sin^3θ(sin\chi - sin3\chi)$$

$$- (1/8)(\beta_{ax} + \beta_{bbc})[sinθ(sin\chi + sin3\chi) - (sinθ - sin^3θ)(sin\chi - sin3\chi)]sin2φ$$

$$- 2sinθcosθ(cos\chi - cos3\chi)sin2φ + (1/2)\beta_{acc}[(cosθ - cos^3θ)(3sin\chi - sin3\chi)cosφ + sin^2θ(cos\chi - cos3\chi)sinφ]$$

$$- (1/2)\beta_{acc}[(cosθ - cos^3θ)(3sin\chi - sin3\chi)cosφ + sin^2θ(cos\chi - cos3\chi)sinφ]$$

$$- (1/2)\beta_{acc}[(cosθ - cos^3θ)(3sin\chi - sin3\chi)sinφ - sin^2θ(cos\chi - cos3\chi)sinφ]$$

$$- (1/2)\beta_{acc}[(cos\theta - cos^3θ)(3sin\chi - sin3\chi)sinφ - sin^2θ(cos\chi - cos3\chi)sinφ]$$

$$- (1/2)\beta_{acc}[(sinθ - sin^3θ)sin\chi - sin3\chi)sinφ - sin^2θ(cos\chi - cos3\chi)sinφ]$$

$$- (1/4)\beta_{acc}[(sinθ - sin^3θ)(3cos\chi + cos3\chi)(1 + cos2φ) + sinθ(cos\chi - cos3\chi)(1 - cos2φ)]$$

$$- (1/4)$$

$$\begin{split} \chi_{XXX} &= -(1/4)\beta_{caa}\{ [(\sin\theta - \sin^2\theta)(3\cos\chi + \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi - \cos3\chi)(1 - \cos2\phi)] \\ &- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\sin2\phi \} \\ &+ (1/4)\beta_{bca}\{ [\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\sin2\phi \\ &- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\cos2\phi \} \\ &+ (1/16)\beta_{aaa}[-(\cos\theta - \cos^3\theta)(3\cos\chi + \cos3\chi)(3\cos\phi + \cos3\phi) \\ &+ 4\cos\theta(3\cos\chi\cos\phi + \cos3\chi\cos3\phi) - 4(3\sin\chi\sin\phi + \sin3\chi\sin3\phi) \\ &+ 3\sin^2\theta(\sin\chi + \sin3\chi)(\sin\phi + \sin3\phi)] \\ &+ (1/16)\beta_{bba}[-(\cos\theta - \cos^3\theta)(3\cos\chi + \cos3\chi)(\cos\phi - \cos3\phi) \\ &+ 4\cos\theta(\cos\chi\cos\phi - \cos3\chi\cos3\phi) - 4(\sin\chi\sin\phi - \sin3\chi\sin3\phi) \\ &+ \sin^2\theta(\sin\chi + \sin3\chi)(\sin\phi - 3\sin3\phi)] \\ &+ \sin^2\theta(\sin\chi + \sin3\chi)(\sin\phi - 3\sin3\phi)] \\ &+ (1/4)\beta_{caa}[(\cos\theta - \cos^3\theta)(3\cos\chi + \cos3\chi)\cos\phi - \sin^2\theta(\sin\chi + \sin3\chi)\sin\phi] \\ \chi_{XZZ} &= (1/2)\beta_{caa}[(\sin\theta - 2\sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi] \end{split}$$

```
+ (1/2)\beta_{bca}[(\sin\theta - 2\sin^3\theta)\cos\chi\sin2\phi + \sin\theta\cos\theta\sin\chi(1 + \cos2\phi)]
         +(1/4)\beta_{aaa}[(\cos\theta - \cos^3\theta)\cos\chi(3\cos\phi + \cos3\phi) - \sin^2\theta\sin\chi(\sin\phi + \sin3\phi)]
         +(1/4)\beta_{bba}[(\cos\theta - \cos^3\theta)\cos\chi(\cos\phi - \cos3\phi) + \sin^2\theta\sin\chi(\sin\phi + \sin3\phi)]
         - \beta_{cca} (cosθ - cos<sup>3</sup>θ)cosχcosφ
\chi_{ZXZ} = (1/2)\beta_{con}[(\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\sin2\phi + \sin\theta\cos\theta\sin\chi(1 + \cos2\phi)]
         +(1/4)\beta_{320}[(\cos\theta - \cos^3\theta)\cos\chi(3\cos\phi + \cos3\phi) - \sin^2\theta\sin\chi(\sin\phi + \sin3\phi)]
         +(1/4)\beta_{bba}[(\cos\theta - \cos^3\theta)\cos\chi(\cos\phi - \cos3\phi) + \sin^2\theta\sin\chi(\sin\phi + \sin3\phi)]
         -\beta_{cca}(\cos\theta - \cos^3\theta)\cos\chi\cos\phi
\chi_{ZZX} = \beta_{caa} [(\sin\theta - \sin^3\theta)\cos\chi(1 + \cos2\phi) - \sin\theta\cos\theta\sin\chi\sin2\phi]
         +\beta_{bcs}[(\sin\theta - \sin^3\theta)\cos\gamma\sin2\phi - \sin\theta\cos\theta\sin\gamma(1 - \cos2\phi)]
         +(1/4)\beta_{aaa}[(\cos\theta - \cos^3\theta)\cos\chi(3\cos\phi + \cos3\phi) - \sin^2\theta\sin\chi(\sin\phi + \sin3\phi)]
         +(1/4)\beta_{hha}[(\cos\theta - \cos^3\theta)\cos\chi(\cos\phi - \cos3\phi) - \sin^2\theta\sin\chi(3\sin\phi - \sin3\phi)]
         + \beta_{coa}[\cos^3\theta\cos\chi\cos\phi - \cos^2\theta\sin\chi\sin\phi]
\chi_{ZXX} = (1/4)\beta_{cas} \{ 2[\cos\theta(1 + \cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1 + \cos2\chi)(1 + \cos2\phi) \}
                          + (1 - 3\cos^2\theta)\sin 2\chi \sin 2\phi
         -(1/4)\beta_{bca}\left\{2\left[(\cos\theta-\cos^3\theta)-\cos^3\theta\cos2\chi\right]\sin2\phi-\left[\sin^2\theta-(1-3\cos^2\theta)\cos2\phi\right]\sin2\chi\right\}
         +(1/8)\beta_{330}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)(3\cos\phi + \cos3\phi) + \sin\theta(1 - \cos2\chi)(\cos\phi - \cos3\phi)]
                          -2\sin\theta\cos\theta\sin2\chi(\sin\phi+\sin3\phi)]
         +(1/8)\beta_{bba}[(\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(\sin\phi-\sin3\phi)]
         +(1/2)\beta_{cca}[-(\sin\theta - \sin^3\theta)(1 + \cos2\gamma)\cos\phi + \sin\theta\cos\theta\sin2\gamma\sin\phi]
\chi_{XZX} = (1/4)\beta_{cos}\{2[\cos\theta(1+\cos2\chi\cos2\phi) - (\cos\theta - \cos^3\theta)(1+\cos2\chi)(1+\cos2\phi)]
                          + (1 - 3\cos^2\theta)\sin 2\chi \sin 2\phi
         -(1/4)\beta_{bcs}\left\{2\left[(\cos\theta-\cos^3\theta)-\cos^3\theta\cos2\chi\right]\sin2\phi-\left[\sin^2\theta-(1-3\cos^2\theta)\cos2\phi\right]\sin2\chi\right\}
         +(1/8)\beta_{330}[(\sin\theta - \sin^3\theta)(1 + \cos2\chi)(3\cos\phi + \cos3\phi) + \sin\theta(1 - \cos2\chi)(\cos\phi - \cos3\phi)]
                          - 2\sin\theta\cos\theta\sin2\chi(\sin\phi + \sin3\phi)]
         +(1/8)\beta_{bba}[(\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(\sin\phi - \sin3\phi)]
         +(1/2)\beta_{cg}[-(\sin\theta - \sin^3\theta)(1 + \cos2\chi)\cos\phi + \sin\theta\cos\theta\sin2\chi\sin\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]
            -(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_{330}[\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)(3cos\varphi+cos3\varphi)+(sin\theta-sin^3\theta)(1+cos2\chi)(cos\varphi-cos3\varphi)
                          + 2\sin\theta\cos\theta\sin2\chi \left(\sin\phi + \sin3\phi\right)
            +(1/2)\beta_{cea}\sin^3\theta(1+\cos2\chi)\cos\phi
\chi_{ZZZ} = \beta_{caa}(cos\theta - cos^3\theta)(1 + cos2\phi)
         + \beta_{bca}[(\cos\theta - \cos^3\theta)\sin 2\phi]
         +(1/4)\beta_{aaa}\sin^3\theta(3\cos\phi+\cos3\phi)
```

```
+\beta_{cca}(\sin\theta - \sin^3\theta)\cos\phi
              \chi_{\text{YXX}} = (1/4)\beta_{\text{cm}} \{ [(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)] \}
(spp)
                                         +2\sin\theta\cos\theta\cos3\gamma\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_{am}[(\cos\theta - \cos^3\theta)(\sin\gamma + \sin3\gamma)(3\cos\phi + \cos3\phi) - 4\cos\theta(\sin\gamma\cos\phi + \sin3\gamma\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_{co}[-(\cos\theta - \cos^3\theta)(\sin\chi + \sin^3\chi)\cos\phi + \sin^2\theta(\cos\chi - \cos^3\chi)\sin\phi]
               \chi_{YZZ} = -(1/2)\beta_{can}[(\sin\theta - 2\sin^3\theta)\sin\chi(1 + \cos2\phi) + \sin\theta\cos\theta\cos\chi\sin2\phi]
                           -(1/2)\beta_{hca}[(\sin\theta - 2\sin^3\theta)\sin2\chi\sin2\phi - \sin\theta\cos\theta\cos\chi(1 + \cos2\phi)]
                           -(1/4)\beta_{am}[(\cos\theta - \cos^3\theta)\sin\chi(3\cos\phi + \cos3\phi) + \sin^2\theta\cos\chi(\sin\phi + \sin3\phi)]
                           -(1/4)\beta_{hha}[(\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_{cso}\{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_{am}[\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)\sin 2\chi(\cos\phi - \cos 3\phi)
                        +(1/2)\beta_{cca}[(\sin\theta - \sin^3\theta)\sin2\chi\cos\phi - \sin\theta\cos\theta(1 - \cos2\chi)\sin\phi]
               \chi_{\text{YXZ}} = (1/2)\beta_{\text{cas}}[(\cos\theta - \cos^3\theta)\sin 2\chi(1 + \cos 2\phi) + \sin^2\theta\cos 2\chi\sin 2\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_{YYX} = (1/4)\beta_{caa}\{[-(\sin\theta - \sin^3\theta)(1 + \cos2\phi) + \sin\theta(1 - \cos2\phi)](\cos\chi - \cos3\chi)
(ssp)
                                         + 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_{hha}[-(\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_{cos}[(\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_{am}[\sin\theta(1+\cos2\chi)(\cos\phi-\cos3\phi)+(\sin\theta-\sin^3\theta)(1-\cos2\chi)(3\cos\phi+\cos3\phi)
```

 $+(1/4)\beta_{bba} \sin^3\theta(\cos\phi - \cos 3\phi)$ 

```
+ 2\sin\theta\cos\theta\sin2\chi(\sin\phi + \sin3\phi)]
                          +(1/8)\beta_{\text{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
              \chi_{XYX} = (1/4)\beta_{cas}\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 - \cos2\phi)]
(psp)
                                        +2\sin\theta\cos\theta\cos3\gamma\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_{am}[(\cos\theta - \cos^3\theta)(\sin\gamma + \sin3\gamma)(3\cos\phi + \cos3\phi) - 4\cos\theta(\sin\gamma\cos\phi + \sin3\gamma\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_{cm}[(\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_{am}[(\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_{cos}(\cos\theta - \cos^3\theta)\sin\chi\cos\phi
              \chi_{XYZ} = (1/2)\beta_{cm}[(\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_{am}[\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\cos2\chi(\sin\phi+\sin3\phi)]
                        - (1/2)β<sub>cca</sub>sin<sup>3</sup>θsin2χcosφ
              \chi_{\rm ZYX} = (1/4)\beta_{\rm cm} \{ 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_{hha}[\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_{ccs}[(\sin\theta - \sin^3\theta)\sin2\chi\cos\phi - \sin\theta\cos\theta(1 - \cos2\chi)\sin\phi]
              \chi_{\text{YXY}} = -(1/4)\beta_{\text{csa}} \{ [(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi) \}
(sps)
                                        + 2\sin\theta\cos\theta\sin3\gamma\sin2\phi}
                          + (1/4)\beta_{bca} \{ [2sin\theta cos\chi - (2sin\theta - sin^3\theta)(cos\chi - cos3\chi)]sin2\phi - 2sin\theta cos\theta(sin\chi - sin3\chi cos2\phi) \}
                          +(1/16)\beta_{ava}[-(\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_{bha}[-(\cos\theta-\cos^3\theta)(\cos\chi-\cos3\chi)(\cos\varphi-\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_{cos}[(\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_{ca} \{ 2[\cos\theta(1 - \cos2\phi\cos2\chi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\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_{am}[\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_{ccs}[(\sin\theta - \sin^3\theta)(1 - \cos2\gamma)\cos\phi - \sin\theta\cos\theta\sin2\gamma\sin\phi]
              \chi_{XXY} = (1/4)\beta_{ca} \{ [(\sin\theta - \sin^3\theta)(1 + \cos2\phi) - \sin\theta(1 - \cos2\phi)](\sin\chi + \sin3\chi) 
(pps)
                                        + 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_{am}[(\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_{coa}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\cos\phi + \sin^2\theta(3\cos\chi + \cos3\chi)\sin\phi]
              \chi_{ZZY} = -\beta_{cm}[(\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_{320}[(\cos\theta - \cos^3\theta)\sin\chi (3\cos\phi + \cos3\phi) + \sin^2\theta\cos\chi(\sin\phi + \sin3\phi)]
                        -(1/4)\beta_{bha}[(\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_{C33} \{ 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_{\rm bca}[2cos^3\theta sin2\chi sin2\varphi + sin^2\theta (1 + cos2\chi)(1 - cos2\varphi) - 2(1 - cos2\chi cos2\varphi)]
                        -(1/4)\beta_{nm}[\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\varphi-cos3\varphi)+(sin\theta-sin^3\theta)sin2\chi(cos\varphi-cos3\varphi)
                                        +2\sin\theta\cos\theta[2\sin\phi+\cos2\chi(\sin\phi-\sin3\phi)]
                      +(1/2)\beta_{cc}[(\sin\theta - \sin^3\theta)\sin2\chi\cos\phi + \sin\theta\cos\theta(1 + \cos2\chi)\sin\phi]
              \chi_{XZY} = (1/4)\beta_{cm} \{ 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_{nm}[\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_{XYY} = -(1/4)\beta_{cm}\{[(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 + \cos2\phi) + \sin\theta(\cos\chi + \cos3\chi)(1 - \cos2\phi)]
(pss)
                                        + 2\sin\theta\cos\theta\sin3\chi\sin2\phi
```

```
+ (1/4)\beta_{bca} \{ [2sin\theta cos\chi - (2sin\theta - sin^3\theta)(cos\chi - cos3\chi)] sin2\phi - 2sin\theta cos\theta(sin\chi - sin3\chi cos2\phi) \}
                                     +(1/16)\beta_{3m}[-(\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_{bha}[-(\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_{cos}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)\cos\phi + \sin^2\theta(\sin\chi + \sin3\chi)\sin\phi]
                         \chi_{\text{TYY}} = (1/4)\beta_{\text{cm}} \{ 2[\cos\theta(1 - \cos2\phi\cos2\chi) - (\cos\theta - \cos^3\theta)(1 - \cos2\chi)(1 + \cos2\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_{am}[\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]
                         \chi_{\text{YYY}} = (1/4)\beta_{\text{cas}} \left\{ \left[ (\sin\theta - \sin^3\theta)(3\sin\chi - \sin3\chi)(1 + \cos2\phi) + \sin\theta(\sin\chi + \sin3\chi)(1 - \cos2\phi) \right] \right\}
          (sss)
                                                  + 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_{379}[(\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_{hha}[(\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<sub>2</sub>) 振動、b 軸に沿った振動]
                         \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)]
          (ppp)
                                                  + 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_{adb}[-(\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 - \sin 3\chi \cos 3\phi) - 3\sin^2 \theta (\sin \chi + \sin 3\chi)(\cos \phi - \cos 3\phi)
                                  +(1/4)\beta_{cd}[(\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 - \sin 3\chi \sin 3\phi) + 3\sin^2 \theta (\sin \chi + \sin 3\chi)(\sin \phi - 3\sin 3\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 + \sin^2\theta\sin\chi(\cos\phi - \cos^3\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_{coh}(\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 + \sin^2\theta\sin\chi(\cos\phi - \cos^3\phi)]
        +(1/4)\beta_{bbb}[(\cos\theta - \cos^3\theta)\cos\chi(3\sin\phi - \sin^3\theta) + \sin^2\theta\sin\chi(\cos\phi - \cos^3\theta)]
        + \beta_{coh}(\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 + \sin^2\theta\sin\chi(3\cos\phi + \cos^3\phi)]
        +(1/4)\beta_{hhh}[(\cos\theta - \cos^3\theta)\cos\chi(3\sin\phi - \sin3\phi) + \sin^2\theta\sin\chi(\cos\phi - \cos3\phi)]
        - \beta_{cd} \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)\sin 2\gamma \sin 2\phi
         -(1/4)\beta_{csb}\left\{2\left[(\cos\theta-\cos^3\theta)-\cos^3\theta\cos2\chi\right]\sin2\phi+\left[\sin^2\theta+(1-3\cos^2\theta)\cos2\phi\right]\sin2\chi\right\}
         +(1/8)\beta_{ab}[(\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_{cb}[(\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)\sin 2\chi \sin 2\phi
         -(1/4)\beta_{csh}\left\{2\left[(\cos\theta-\cos^3\theta)-\cos^3\theta\cos2\chi\right]\sin2\phi+\left[\sin^2\theta+(1-3\cos^2\theta)\cos2\phi\right]\sin2\chi\right\}
         +(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_{coh}[(\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\gamma\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_{asb}[(\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)]
```

```
+ 2\sin\theta\cos\theta\sin2\chi(\cos\phi - \cos3\phi)]
                           +(1/2)\beta_{cd}sin^3\theta(1+cos2\chi)sin\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(\sin\phi-\sin3\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+\sin3\phi)
                         +(1/4)\beta_{bbb} \sin^3\theta(3\sin\phi - \sin 3\phi)
                        + \beta_{cch}(\sin\theta - \sin^3\theta)\sin\phi
                        +(1/2)\beta_{abb} \sin^3\theta(\cos\phi - \cos 3\phi)
(spp)
              \chi_{\rm YXX} = (1/4)\beta_{\rm cbb} \{ [(\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_{csb}\{[\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)
                         +(1/16)\beta_{adb}[(\cos\theta - \cos^3\theta)(\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-\cos3\phi)-4\cos^2\theta(\cos\chi\cos\phi-\cos3\chi\cos3\phi)]
                         +(1/16)\beta_{hbh}[(\cos\theta-\cos^3\theta)(\sin\chi+\sin3\chi)(3\sin\phi-\sin3\phi)-4\cos\theta(\sin\chi\sin\phi-\sin3\chi\sin3\phi)]
                                         -\sin^2\theta(\cos\chi + 3\cos3\chi)(\cos\phi - \cos3\phi) + 4(\cos\chi\cos\phi - \cos3\chi\cos3\phi)
                         -(1/4)\beta_{cob}[(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\sin\phi + \sin^2\theta(\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_{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(1-\cos2\phi)]
                        -(1/4)\beta_{ab}[(\cos\theta - \cos^3\theta)\sin\chi(\sin\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^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_{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)]
                         -(1/8)\beta_{aab}\{(2sin\theta - sin^3\theta)sin2\chi(sin\phi + sin3\phi) + 2sin\theta\cos\theta[2cos\phi - cos2\chi(cos\phi - cos3\phi)]\}
                         +(1/8)\beta_{hhh}[-(\sin\theta - \sin^3\theta)\sin2\chi(3\sin\phi - \sin3\phi) + \sin\theta\sin2\chi(\sin\phi + \sin3\phi)]
                                         +2\sin\theta\cos\theta\cos2\chi(\cos\phi-\cos3\phi)]
                         +(1/2)\beta_{cd}[(\sin\theta - \sin^3\theta)\sin2\chi\sin\phi + \sin\theta\cos\theta(1 - \cos2\chi)\cos\phi]
                         +(1/4)\beta_{abb}[-(\sin\theta - \sin^3\theta)\sin2\chi(\cos\phi - \cos3\phi) + \sin\theta\sin2\chi(\cos\phi + \cos3\phi)]
                                         -2\sin\theta\cos\theta(\sin\phi + \cos2\chi\sin3\phi)]
               \chi_{\text{YXZ}} = (1/2)\beta_{\text{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_{ab}[-(\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\cos2\chi(\cos\phi-\cos3\phi)]
```

```
+(1/8)\beta_{bbb}[-(\sin\theta - \sin^3\theta)\sin2\chi(3\sin\phi - \sin3\phi) + \sin\theta\sin2\chi(\sin\phi + \sin3\phi)]
                                        +2\sin\theta\cos\theta\cos2\chi(\cos\phi-\cos3\phi)]
                       -(1/2)\beta_{coh}\sin^3\theta\sin2\gamma\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_{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) \}
(ssp)
                                        -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]\}
                        +(1/16)\beta_{3ab}[-(\cos\theta-\cos^3\theta)(\cos\gamma-\cos3\gamma)(\sin\phi+\sin3\phi)+4\cos\theta(3\cos\gamma\sin\phi-\cos3\gamma\sin3\phi)]
                                        +\sin^2\theta(\sin\chi + 3\sin3\chi)(\cos\phi + \cos3\phi) + 4\cos^2\theta(3\sin\chi\cos\phi - \sin3\chi\cos3\phi)
                        +(1/16)\beta_{bbb}[-(\cos\theta-\cos^3\theta)(\cos\gamma-\cos3\gamma)(3\sin\phi-\sin3\phi)+4\cos\theta(\cos\gamma\sin\phi+\cos3\gamma\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_{crb}[(\cos\theta - \cos^3\theta)(\cos\chi - \cos3\chi)\sin\phi + \sin^2\theta(3\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_{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)]
                          + (1/8)\beta_{aab}[\sin\theta(1+\cos2\chi)(3\sin\varphi-\sin3\varphi) + (\sin\theta-\sin^3\theta)(1-\cos2\chi)(\sin\varphi+\sin3\varphi)
                                        + 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_{coh}\sin^3\theta(1-\cos2\chi)\sin\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(\sin\phi - \sin3\phi)]
              \chi_{xyx} = (1/4)\beta_{cbb}\{[(\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)(1 - \cos2\phi) + \sin\theta(\sin\chi - \sin3\chi)(1 + \cos2\phi)]
(psp)
                                        -2\sin\theta\cos\theta\cos3\chi\sin2\phi
                        -(1/4)\beta_{cab}\{[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_{aab}[(\cos\theta - \cos^3\theta)(\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-\cos3\phi)-4\cos^2\theta(\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(\sin\chi\sin\phi - \sin3\chi\sin3\phi)]
                                        -\sin^2\theta(\cos\chi + 3\cos3\chi)(\cos\phi - \cos3\phi) + 4(\cos\chi\cos\phi - \cos3\chi\cos3\phi)
                        -(1/4)\beta_{cob}[-(\cos\theta - \cos^3\theta)(\sin\chi + \sin3\chi)\sin\phi + \sin^2\theta(\cos\chi - \cos3\chi)\cos\eta\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\chi\sin\phi - \cos3\chi\sin3\phi)
              \chi_{\rm ZYZ} = -(1/2)\beta_{\rm 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)]
                      -(1/4)\beta_{ab}[(\cos\theta - \cos^3\theta)\sin\chi(\sin\phi + \sin^2\theta\cos\chi(3\cos\phi + \cos^3\phi))]
                        +(1/4)\beta_{hhh}[-(\cos\theta-\cos^3\theta)\sin\chi(3\sin\phi-\sin^2\theta)+\sin^2\theta\cos\chi(\cos\phi-\cos^2\theta)]
                       + \beta_{cd}(\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)\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_{ab}[\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_{coh}\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_{\rm ZYX} = (1/4)\beta_{\rm obh} \{ 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\gamma\sin2\phi - \sin^2\theta(1 - \cos2\gamma)(1 + \cos2\phi) + 2(1 - \cos2\gamma\cos2\phi)]
                        -(1/8)\beta_{ab}\{(2\sin\theta - \sin^3\theta)\sin 2\chi(\sin\phi + \sin 3\phi) + 2\sin\theta\cos\theta[2\cos 2\phi - \cos 2\chi(\cos\phi + \cos 3\phi)]\}
                       +(1/8)\beta_{hhh}[\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\gamma\sin\phi + \sin\theta\cos\theta(1 - \cos2\gamma)\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 \left(\sin\phi + \cos2\chi\sin3\phi\right)]
              \chi_{\rm YXY} = -(1/4)\beta_{\rm cbh} \{ [(\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)(1 - \cos2\phi) + \sin\theta(\cos\chi + \cos3\chi)(1 + \cos2\phi) ] 
(sps)
                                        -2\sin\theta\cos\theta\sin3\chi\sin2\phi
                        +(1/4)\beta_{csb}\{[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_{ab}[-(\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_{cd}[(\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)\sin 2\gamma \sin 2\phi
                        -(1/4)\beta_{cab}\{2[(cos\theta-cos^3\theta)+cos^3\theta cos2\chi]sin2\varphi-[sin^2\theta+(1-3cos^2\theta)cos2\varphi]sin2\chi\}
                        -(1/8)\beta_{ab}[\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_{hbh}[\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]
              \chi_{XXY} = (1/4)\beta_{cbb} \{ [(\sin\theta - \sin^3\theta)(1 - \cos2\phi) - \sin\theta(1 + \cos2\phi)](\sin\chi + \sin3\chi) 
(pps)
```

```
-2\sin\theta\cos\theta(\cos\chi+\cos3\chi)\sin2\phi
                        +(1/4)\beta_{coh}\{(2\sin\theta - \sin^3\theta)\sin 2\phi - 2\sin\theta\cos\theta[2\cos\chi - (\cos\chi + \cos3\chi)\cos 2\phi]\}
                        +(1/16)\beta_{ab}[(\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_{crb}[-(\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_{coh}[(\sin\theta - \sin^3\theta)\sin\gamma\sin2\phi - \sin\theta\cos\theta\cos\gamma(1 + \cos2\phi)]
                      +(1/4)\beta_{aab}[-(\cos\theta - \cos^3\theta)\sin\chi(\sin\phi + \sin^2\theta\cos\chi(3\cos\phi + \cos^3\phi)]
                      +(1/4)\beta_{hhh}[-(\cos\theta-\cos^3\theta)\sin\chi(3\sin\phi-\sin^3\theta)+\sin^2\theta\cos\chi(\cos\phi-\cos^3\phi)]
                       + \beta_{cd}[-\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_{c:b}[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_{ab}\{-(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\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_{a;b}\{-(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_{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)]
(pss)
                                        -2\sin\theta\cos\theta\sin3\gamma\sin2\phi
                        +(1/4)\beta_{csh}\{[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_{cob}[(\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_{\rm ZYY} = (1/4)\beta_{\rm 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)\sin 2\chi \sin 2\phi}
                       -(1/4)\beta_{cab}\left\{2\left[(\cos\theta-\cos^3\theta)-\cos^3\theta\cos2\chi\right]\sin2\phi-\left[\sin^2\theta+(1-3\cos^2\theta)\cos2\phi\right]\sin2\chi\right\}
                       +(1/8)\beta_{asb}[-\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_{hhh}[\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_{cd}[-(\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_{\rm YYY} = (1/4)\beta_{\rm 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_{ab}[(\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_{hbh}[(\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_{cd}[(\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)]
```