水素化ダイヤモンド表面 CH の SFG テンソル

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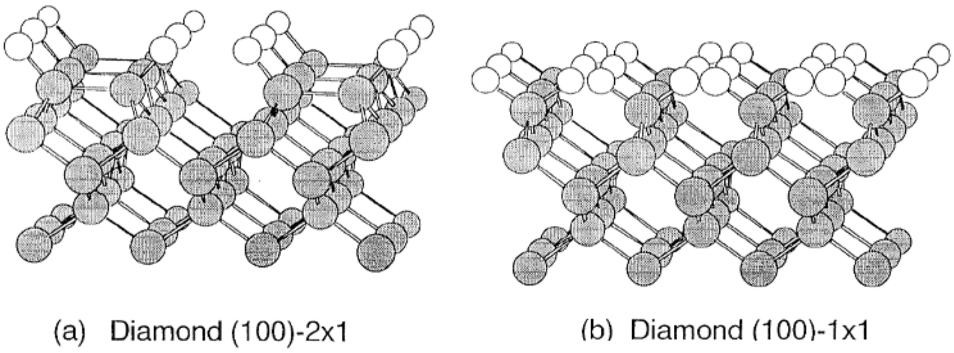

1．序論

水素化ダイヤモンド表面の CH 伸縮振動を例にとって、単結晶表面の化学結合からの SFG スペクトルの解析に有効な事項について記す。

最初に、水素化 C(100) 表面についてまとめておこう。一般に言われているのは、as cut 表面の C 原子から出ている２本のダングリングボンド（dangling bond）のうちの１本が隣の C 原子のダングリングボンドと単結合を形成して（再構成表面の形成）、残る１本が水素化する（上の図の (a)、以後、monohydride モ

デルと呼ぶ)、というものである。しかし、as cut 表面のままで、２本のダングリングボンドの両方が水素化することも（上の図の (b) 、以後、dihydride モデルと呼ぶ）考えとしては可能である。図から明らかなように、CH 結合に注目すると、前者では HCCH がユニットになり、後者では CH_2 がユニットになる。そして、これらのユニットが表面上での広がりを持つために、表面単位胞の対称性は裸の表面の対称性と異なる。本稿では、HCCH および CH_2 ユニットに付随する SFG テンソルについて考察する。

ダイヤモンド結晶の格子定数は 3.567 Å であるから、C—C 結合距離は 1.545 Å である。そして、表面に出ている C 原子間の距離は、as cut 表面で 2.51 Å である。再構成表面については、表面単位胞のサイズが 2.51 × 5.1 Å であるとの報告がある（R. E. Stallcup et al., *Appl. Phys. Lett.* 66, 2331(1995)）。再構成によって形成される C—C 結合の原子間隔を 2.0 Å と仮定すると、非結合炭素原子の間隔は 3.1 Å になる。

C—H 結合距離は 1.1 ~ 1.2 Å である。表面 CH_2 基が図 (b) の配向を取っているときには、隣りあう CH_2 基の H 原子の間隔が 0.7 Å 程度になる。また、表面 HCCH ユニットが図 (a) のような配向を取るときには、隣りあうユニットの H 原子間隔が 2 Å 程度になる（CH 結合が表面法線に対してなす角を 30° と仮定したときの値、これを 55° のままとするときにはもっと短い）。

ところで、水素原子の間には反発力働く。この反発力がが働きはじめる距離の目安が H 原子のファンデルワールス半径で、その値は 1.20 Å である。よって、水素原子の中心の間の距離が 2.4 Å 程度以下になると、立体障害が働くはずである。図 (b) の状況がこれに該当することは明らかであろう。また、図 (a) のケースでも、隣りあう HCCH ユニットの H 原子の間隔がかなり短いから、立体障害の存在が十分疑われる。従って、立体障害を解消するために、表面 CH 結合の配向に何らかの歪みが生じる可能性が高い。

立体障害を解消するには、角を突き合わせている H 原子が、表面から等距離を保ったまま前後にずれた状態と、どちらか一方の H 原子が表面側に潜り、他方の H 原子が上方にずれた状態が考えられる。CH_2 基で言えば、C_2 軸周りの回転または分子面の傾斜による方法と、分子面に垂直な軸の周りでの回転である。また、HCCH 基で言えば、表面法線の周りでの CH 結合の回転、HCC 結合角の増減、あるいは、分子面の傾斜（平面を保つ）またはねじれ（分子面がよじれる）が考えられる。いずれにせよ、立体障害の解消は隣りあうユニットに属する CH 結合の間で行われる。これによってユニットに生じる変化には、表面の上でのユニットの並び方も絡むはずである。

HCCH ユニットの対称性について考えると、C_{2v} 対称と C_2 対称が考えられる。C_{2v} 対称は、H 原子が立体障害を受けない場合、そして、立体障害による「逃げ」が分子面が平面のままで、表面に対する傾斜がユニットごとに互い違いになっているときのものである。これに対して C_2 対称は、「逃げ」に際して生じる左右の CH 結合のずれが、もともとの HCCH 面に関して反対方向になるときのものである。

CH_2 ユニットは、3 原子分子の特性として平面のままである。そして、2 個の H 原子は等価であるから、C_{2v} 対称が保たれる。

2. 分子固定座標系と空間固定座標系

1.　分子に固定した座標系：(abc) 系と表す。

CH_2 基では、C_2 対称軸に沿って外向きに c 軸を取り、分子面内に a 軸を取る。

HCCH 基では、C_2 対称軸に沿って外向きに c 軸をとり、平面形（C_{2v} 対称）では分子面内に a 軸を、ねじれ形（C_2 対称）では２つの CCH 面を２等分する平面（すなわち CCC 面）上に a 軸を取る。

2a.　表面に固定した座標系：(xyz) 系と表す。

2b.　空間に固定した座標系：(XYZ) 系と表す。

3.　分子の配向：オイラー角 (χ, θ, ϕ) の定義を、分子固定 (abc) 系を表面固定 (xyz) 系に重ねるときのものとする。

用いるオイラー角 (χ, θ, ϕ) は、次のように表現される。

(1) 内部回転角 ϕ：ac **面（ここで考えている** CH_2 **基及び** HCCH **基では分子面）の（表面に対する）ねじれ角である。**c **軸まわりの回転で** ac **面を表面と垂直にするために必要な回転角、あるいは** a **軸が** z **軸の** ab **面への射影に重なるまでの回転角でもある。（**a **軸に沿ったベクトルと** x **軸に沿ったベクトルの内積がプラスになる方向で重ねる。）**ac **面が表面に垂直なときには** $\phi = 0$ or π **であり、**ac **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。分子がランダムな内部回転角を取っている場合には** ϕ **は** $0 \sim 2\pi$ **の任意の値を等しいウェイトで取る。**
(2) 傾き角・tilt 角 θ_{tilt}：通常の定義に合わせて、c **軸と外向きの法線** (-z) **の間の角を傾き角と定義し、**N **軸（**z **軸と** c **軸の両方に垂直な直線、**ab **面と** xy **面の交線）まわりの回転で** c **軸を外向きの法線に重ねる方向をプラス回転とする。**z **軸は下向きの法線であるから、オイラー角** θ **は** $\pi - \theta_{tilt}$ **である。**
(3) 面内配向角 $\chi_{in\text{-}plane}$ (χ_{ip} と略記する)：z **軸まわりの回転で** c **軸の** xy **面への射影を** x **軸に重ねるための回転角と定義する。ここでの** z **軸の向きでは、**x **軸の方向に見て射影が左側にあるときがプラスになる。**z **軸を基板の内部に向けて取っているので、対応するオイラー角** χ **は** $\pi/2 + \chi_{ip}$ **である。分子の面内配向がランダムなときには、**χ_{ip} **は** $0 \sim 2\pi$ **の任意の値を等しいウェイトで取る。**

3. 分子固定 (abc) 系におけるテンソル成分

対称性の考察から、ゼロ以外の値を持つテンソル成分を摘出することが出来る。C_{2v} **分子（**CH_2 **基と平面形** HCCH **基）では、**β_{aac}、β_{bbc}、β_{ccc};、$\beta_{caa} = \beta_{aca}$、$\beta_{cbb} = \beta_{bcb}$ **であり、**C_2 **分子（ねじれ形** HCCH **基）では、**β_{aac}、β_{bbc}、β_{ccc}、$\beta_{abc} = \beta_{bac}$、$\beta_{caa} = \beta_{aca}$、$\beta_{bca} = \beta_{cba}$、$\beta_{cbb} = \beta_{bcb}$、$\beta_{cab} = \beta_{acb}$ **である。それぞれの値の目安として、**CH **結合のテンソル成分がそのまま転用できると仮定したときの値は、ファイル「オイラー角」と「分子固定から空間固定へ」を参照して導くことができる。**

CH_2 基；

ファイル「オイラー角」の Eu-5 **式により、(1) ２個の** CH **結合では角** χ **が互いに** π **だけ違っているので、**$\sin\chi$、$\sin3\chi$、$\cos\chi$、$\cos3\chi$ **が掛っている項の和はゼロになる。また、**$\chi = 0$ **と** π **であるから、**$\sin2\chi = 0$、$\cos2\chi = +1$ **となり、**$\sin2\chi$ **と** $(1 - \cos2\chi)$ **が掛る項もゼロである。 (2) 角** ϕ **は ゼロ であるから、**$\sin\phi = \sin2\phi = \sin3\phi = 0$、$\cos\phi = \cos2\phi = \cos3\phi = +1$ **となり、**$\sin\phi$、$\sin2\phi$、$\sin3\phi$、$(1 - \cos2\phi)$ **が掛かる項もゼロになる。これらのことを考慮して、ファイル「分子固定から空間固定へ」により２個の** CH **結合についてとったテンソル成分の和は、下のようになる。**

$$\beta_{aac} = 2\{\beta_{\xi\xi\zeta}\cos^3(\alpha/2) + \beta_{\zeta\zeta\zeta}[\cos(\alpha/2) - \cos^3(\alpha/2)]\} \quad (3\text{-}1a)$$
$$\beta_{bbc} = 2\beta_{\eta\eta\zeta}\cos(\alpha/2) \quad (3\text{-}1b)$$
$$\beta_{ccc} = 2\{\beta_{\xi\xi\zeta}[\cos(\alpha/2) - \cos^3(\alpha/2)] + \beta_{\zeta\zeta\zeta}\cos^3(\alpha/2)\} \quad (3\text{-}1c)$$
$$\beta_{caa} = \beta_{aca} = -2(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})[\cos(\alpha/2) - \cos^3(\alpha/2)] \quad (3\text{-}2)$$
$$\beta_{cbb} = \beta_{bcb} = 0 \quad (3\text{-}3)$$

(CH **伸縮振動は** b **軸方向の成分を持たないので、下付きの右端が** b **のテンソル成分はゼロになる。**)

HCH **角を** 4 **面体角にとると、**$\cos\alpha = -1/3$、$\sin\alpha = 2\sqrt{2}/3$ **であるから、**$\cos(\alpha/2) = \sqrt{1/3}$ **となり、**

$$\beta_{aac} = (2\sqrt{3}/9)(\beta_{\xi\xi\zeta} + 2\beta_{\zeta\zeta\zeta}) \quad (3\text{-}4a)$$
$$\beta_{bbc} = (2\sqrt{3}/9)(3\beta_{\eta\eta\zeta}) \quad (3\text{-}4b)$$
$$\beta_{ccc} = (2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta}) \quad (3\text{-}4c)$$
$$\beta_{caa} = \beta_{aca} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta}) \quad (3\text{-}5)$$

を得る。CH 基自体と違って、$\beta_{aac} \sim \beta_{ccc}$ であることに注意しよう。

HCCH 基（平面形）;

上と同様な筋道での導出になる。ファイル「オイラー角」の (Eu-6) 式と (Eu-5) 式の違いは、$(\alpha/2)$ の代りに $\alpha - \pi/2$ が入る、ということである。（ただし、ここの α は HCC 角である）よって、下式が得られる。

$$\beta_{aac} = 2[\beta_{\xi\xi\zeta}\sin^3\alpha + \beta_{\zeta\zeta\zeta}(\sin\alpha - \sin^3\alpha)] \quad \text{(3-6a)}$$
$$\beta_{bbc} = 2\beta_{\eta\eta\zeta}\sin\alpha \quad \text{(3-6b)}$$
$$\beta_{ccc} = 2[\beta_{\xi\xi\zeta}(\sin\alpha - \sin^3\alpha) + \beta_{\zeta\zeta\zeta}\sin^3\alpha] \quad \text{(3-6c)}$$
$$\beta_{caa} = \beta_{aca} = -2(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\sin\alpha - \sin^3\alpha) \quad \text{(3-7)}$$

HCC 角を４面体角にとると、$\cos\alpha = -1/3$、$\sin\alpha = 2\sqrt{2}/3$ であるから、

$$\beta_{aac} = (4\sqrt{2}/37)(8\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta}) \quad \text{(3-8a)}$$
$$\beta_{bbc} = (4\sqrt{2}/37)(9\beta_{\eta\eta\zeta}) \quad \text{(3-8b)}$$
$$\beta_{ccc} = (4\sqrt{2}/37)(\beta_{\xi\xi\zeta} + 8\beta_{\zeta\zeta\zeta}) \quad \text{(3-8c)}$$
$$\beta_{caa} = \beta_{aca} = -(4\sqrt{2}/37)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta}) \quad \text{(3-9)}$$

ここでは、$\beta_{aac} < \beta_{ccc}, \beta_{caa}$ であることに注意しよう。

HCCH 基（ねじれ形）;

ファイル「オイラー角」の (Eu-8) 式、(Eu-10) 式、(Eu-10) 式により、オイラー角を使った表式がまず得られる。次に、オイラー角を HCC 角および２面角と結び付ける、という面倒な手続きが必要である。

ファイル「分子固定から空間固定へ」により得られるオイラー角を使った表式は、下のようになる。

$$\begin{aligned}\beta_{aac} = &(\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta})\cos\theta \\ &- (1/2)(\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta} - 2\beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)(1 + \cos2\chi) \\ &- (1/2)(\beta_{\xi\xi\zeta} - \beta_{\eta\eta\zeta})\{[\cos\theta(1 - \cos2\chi) - \cos^3\theta(1 + \cos2\chi)]\cos2\phi + 2\cos^2\theta\sin2\chi\sin2\phi\}\end{aligned} \quad \text{(3-10a)}$$

$$\begin{aligned}\beta_{bbc} = &(\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta})\cos\theta \\ &- (1/2)(\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta} - 2\beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)(1 - \cos2\chi) \\ &- (1/2)(\beta_{\xi\xi\zeta} - \beta_{\eta\eta\zeta})\{[\cos\theta(1 + \cos2\chi) - \cos^3\theta(1 - \cos2\chi)]\cos2\phi - 2\cos^2\theta\sin2\chi\sin2\phi\}\end{aligned} \quad \text{(3-10b)}$$

$$\begin{aligned}\beta_{ccc} = &(\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta})\cos\theta \\ &- (\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta} - 2\beta_{\zeta\zeta\zeta})\cos^3\theta \\ &+ (\beta_{\xi\xi\zeta} - \beta_{\eta\eta\zeta})(\cos\theta - \cos^3\theta)\cos2\phi\end{aligned} \quad 1 \quad \text{(3-10c)}$$

$$\begin{aligned}\beta_{abc} = \beta_{bac} = &(1/2)(\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta} - 2\beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)\sin2\chi \\ &- (1/2)(\beta_{\xi\xi\zeta} - \beta_{\eta\eta\zeta})[(\cos\theta + \cos^3\theta)\sin2\chi\cos2\phi + 2\cos^2\theta\cos2\chi\sin2\phi]\end{aligned} \quad \text{(3-10d)}$$

$$\begin{aligned}\beta_{caa} = \beta_{aca} = &-(1/2)(\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta} - 2\beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)(1 + \cos2\chi) \\ &- (1/2)(\beta_{\xi\xi\zeta} - \beta_{\eta\eta\zeta})[(\cos\theta - \cos^3\theta)(1 + \cos2\chi)\cos2\phi - \sin^2\theta\sin2\chi\sin2\phi]\end{aligned} \quad \text{(3-11a)}$$

$$\begin{aligned}\beta_{bca} = \beta_{cba} = &(1/2)(\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta} - 2\beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)\sin2\chi \\ &+ (1/2)(\beta_{\xi\xi\zeta} - \beta_{\eta\eta\zeta})[(\cos\theta - \cos^3\theta)\sin2\chi\cos2\phi + \sin^2\theta\,(1 + \cos2\chi)\sin2\phi]\end{aligned} \quad \text{(3-11b)}$$

$$\beta_{cbb} = \beta_{bcb} = -(1/2)(\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta} - 2\beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$$

$$- (1/2)(\beta_{\xi\xi\zeta} - \beta_{\eta\eta\zeta})[(\cos\theta - \cos^3\theta)(1 - \cos 2\chi)\cos 2\phi + \sin^2\theta \sin 2\chi \sin 2\phi] \quad (3\text{-}12a)$$

$$\beta_{cab} = \beta_{acb} = (1/2)(\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta} - 2\beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)\sin 2\chi$$
$$+ (1/2)(\beta_{\xi\xi\zeta} - \beta_{\eta\eta\zeta})[(\cos\theta - \cos^3\theta)\sin 2\chi \cos 2\phi - \sin^2\theta\,(1 - \cos 2\chi)\sin 2\phi] \quad (3\text{-}12b)$$

これを α と τによる表式に変えるにあたり、単純な置き換えをしてから式を整理すると、下記のようになる。

$$\beta_{aac} = 2(\beta_{\xi\xi\zeta}\sin^2\alpha + \beta_{\zeta\zeta\zeta}\cos^2\alpha)\sin\alpha\cos(\tau/2) \quad (3\text{-}13a)$$
$$\beta_{bbc} = 2[\beta_{\xi\xi\zeta}\cos^2\alpha\sin^2(\tau/2) + \beta_{\eta\eta\zeta}\cos^2(\tau/2) + \beta_{\zeta\zeta\zeta}\sin^2\alpha\sin^2(\tau/2)]\sin\alpha\cos(\tau/2) \quad (3\text{-}13b)$$
$$\beta_{ccc} = 2[\beta_{\xi\xi\zeta}\cos^2\alpha\cos^2(\tau/2) + \beta_{\eta\eta\zeta}\sin^2(\tau/2) + \beta_{\zeta\zeta\zeta}\sin^2\alpha\cos^2(\tau/2)]\sin\alpha\cos(\tau/2) \quad (3\text{-}13c)$$
$$\beta_{abc} = \beta_{bac} = 2(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})[\sin\alpha\cos\alpha\sin(\tau/2)]\sin\alpha\cos(\tau/2) \quad (3\text{-}13d)$$
$$\beta_{caa} = \beta_{aca} = -2(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\alpha\cos^2\alpha\cos(\tau/2) \quad (3\text{-}14a)$$
$$\beta_{bca} = \beta_{cba} = -2[\beta_{\xi\xi\zeta}\cos^2\alpha - \beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta}\sin^2\alpha]\cos\alpha\sin(\tau/2)\cos(\tau/2) \quad (3\text{-}14b)$$
$$\beta_{cbb} = \beta_{bcb} = +2[\beta_{\xi\xi\zeta}\cos^2\alpha - \beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta}\sin^2\alpha]\sin\alpha\sin^2(\tau/2)\cos(\tau/2) \quad (3\text{-}15a)$$
$$\beta_{cab} = \beta_{acb} = -2(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin^2\alpha\cos\alpha\cos(\tau/2) \quad (3\text{-}15b)$$

HCC 角を四面体角にとると、$\cos\alpha = -1/3$、$\sin\alpha = 2\sqrt{2}/3$ であるから、

$$\beta_{aac} = (4\sqrt{2}/27)(8\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\cos(\tau/2) \quad (3\text{-}16a)$$
$$\beta_{bbc} = (4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2) + 9\beta_{\eta\eta\zeta}]\cos(\tau/2) \quad (3\text{-}16b)$$
$$\beta_{ccc} = (4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\cos^2(\tau/2) + 9\beta_{\eta\eta\zeta}]\cos(\tau/2) \quad (3\text{-}16c)$$
$$\beta_{abc} = \beta_{bac} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(2\sqrt{2})\sin(\tau/2)\cos(\tau/2) \quad (3\text{-}16d)$$
$$\beta_{caa} = \beta_{aca} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos(\tau/2) \quad (3\text{-}17a)$$
$$\beta_{bca} = \beta_{cba} = +(2/27)[\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta}]\sin(\tau/2)\cos(\tau/2) \quad (3\text{-}17b)$$
$$\beta_{cbb} = \beta_{bcb} = +(4\sqrt{2}/27)[\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta}]\sin^2(\tau/2)\cos(\tau/2) \quad (3\text{-}18a)$$
$$\beta_{cab} = \beta_{acb} = +(8/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos(\tau/2) \quad (3\text{-}18b)$$

4. 表面固定 (xyz) 系における HCCH 基のテンソル成分

典型的な配向について、表面固定系でのテンソル成分を求めておこう。なお、一般的な配向に対する表式を付録 A に記してあるので、個別のオイラー角を当てはめれば以下で示す表式が求まる。

なお、下で出てくる τ は、分子面（ac 面）と表面（xy 面）の間の２面角である。

4a. 傾いた平面形 HCCH 基

分子面 [ac 面] が表面から角 τ だけ傾いているとして、２つある傾き方に対するオイラー角は（ファイル「オイラー角」の (Eu-4) 式を参照して）次のようになる。α は CCH 結合角である。

$R_z(\chi = -\pi/2)\ R_{b'}(\theta = -\tau)\ R_c(\phi = \pi/2)$、　$R_z(\chi = -\pi/2)\ R_{b'}(\theta = +\tau)\ R_c(\phi = \pi/2)$、$\tau = \pi/2 - \theta$

$\sin\chi = -1$、$\sin 2\chi = 0$、$\sin 3\chi = +1$　　$\cos\chi = 0$、$\cos 2v = -1$、$\cos 3\chi = 0$

$\sin\phi = +1$、$\sin 2\phi = 0$、$\sin 3v = -1$　　$\cos\phi = 0$、$\cos 2\phi = -1$、$\cos 3\phi = 0$

$\sin\theta = -(\pm)\sin\tau$、　　$\cos\theta = \cos\tau$　　(4a-1)

（隣り合う HCCH 基は交互に -τ と +τ を取る。）

により、

［対称伸縮振動］

(ppp) $\chi_{xxz} = \beta_{aac}\text{cost}$

$\chi_{zzz} = -(\beta_{bbc} - \beta_{ccc})\cos^3\tau + \beta_{bbc}\cos\tau$

(spp) $\chi_{yzz} = \pm(\beta_{bbc} - \beta_{ccc})(\sin\tau - \sin^3\tau)$

(ssp) $\chi_{yyz} = (\beta_{bbc} - \beta_{ccc})\cos^3\tau + \beta_{ccc}\cos\tau$

(psp) $\chi_{zyz} = \pm(\beta_{bbc} - \beta_{ccc})(\sin\tau - \sin^3\tau)$

(sps) $\chi_{yzy} = -(\beta_{bbc} - \beta_{ccc})(\cos\tau - \cos^3\tau)$

(pps) $\chi_{xxy} = -(\pm)\beta_{aac}\sin\tau$

$\chi_{zzy} = -(\pm)\beta_{bbc}\sin^3\tau - (\pm)\beta_{ccc}(\sin\tau - \sin^3\tau)$

(pss) $\chi_{zyy} = -(\beta_{bbc} - \beta_{ccc})(\cos\tau - \cos^3\tau)$

(sss) $\chi_{yyy} = -(\pm)\beta_{bbc}(\sin\tau - \sin^3\tau) - (\pm)\beta_{ccc}\sin^3\tau$ (4a-2)

［逆対称伸縮振動］

(ppp) $\chi_{zxx} = \beta_{caa}\cos\tau$

$\chi_{xzx} = \beta_{caa}\cos\tau$

(spp) $\chi_{yxx} = -(\pm)\beta_{caa}\sin\tau$

(ssp) none

(psp) $\chi_{xyx} = -(\pm)\beta_{caa}\sin\tau$

(sps) none

(pps) none

(pss) none

(sss) none (4a-3)

CH 基のテンソル成分による表式 (3-6) 式に Td 角を仮定した (3-8) 式を使用すると、下記の表式を得る。

［対称伸縮振動］

(ppp) $\chi_{xxz} = (4\sqrt{2}/27)(8\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\cos\tau$

$\chi_{zzz} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\cos^3\tau$

(spp) $\chi_{yzz} = -(\pm)(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})(\sin\tau - \sin^3\tau)$

(ssp) $\chi_{yyz} = (4\sqrt{2}/27)[-(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})(\cos\tau - \cos^3\tau) + 9\beta_{\eta\eta\zeta}\cos\tau]$

(psp) $\chi_{zyz} = -(\pm)(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})(\sin\tau - \sin^3\tau)$

(sps) $\chi_{yzy} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})(\cos\tau - \cos^3\tau)$

(pps) $\chi_{xxy} = -(\pm)(4\sqrt{2}/27)(9\beta_{\eta\eta\zeta})\sin\tau$

$\chi_{zzy} = -(\pm)(4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})(\sin\tau - \sin^3\tau) - 9\beta_{\eta\eta\zeta}\sin\tau]$

(pss) $\chi_{zyy} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})(\cos\tau - \cos^3\tau)$

(sss) $\chi_{yyy} = -(\pm)(4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^3\tau + 9\beta_{\eta\eta\zeta}\sin\tau]$ (4a-4)

［逆対称伸縮振動］

(ppp) $\chi_{zxx} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau$

$\chi_{xzx} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau$

(spp) $\chi_{yxx} = (\pm)(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau$

(ssp) none

(psp) $\chi_{xxx} = -(\pm)(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau$
(sps) none
(pps) none
(pss) none
(sss) none (4a-5)

4b. ねじれ形 HCCH 基

ねじれ形 HCCH **基の** ac **面は** xz **面と重なっていると見なせるから、上の** (3-10) **式** ~ (3-18) **式で左辺の下付き** (abc) **を** (xyz) **に読み替えたものがそのまま当てはまる。**α **は** CCH **結合角、**τ **は２個の** CCH **面の間の２面角である。**

$$R_z(\chi = 0)\ R_{b'}(\theta = 0)\ R_c(\phi = 0)、\tau = 0 \tag{4b-1}$$

により、下記の表式を得る。なお、CH **基のテンソル成分による表式** (3-13) **式を使って整理したものも示す。**

［**対称伸縮振動**］

(ppp) $\chi_{xxz} = \beta_{aac} = 2(\beta_{\xi\xi\zeta}\sin^2\alpha + \beta_{\zeta\zeta\zeta}\cos^2\alpha)\sin\alpha\cos(\tau/2)$
$\chi_{zzz} = \beta_{ccc} = 2[\beta_{\xi\xi\zeta}\cos^2\alpha\cos^2(\tau/2) + \beta_{\eta\eta\zeta}\sin^2(\tau/2) + \beta_{\zeta\zeta\zeta}\sin^2\alpha\cos^2(\tau/2)]\sin\alpha\cos(\tau/2)$
(spp) $\chi_{yxz} = \beta_{abc} = 2(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})[\sin\alpha\cos\alpha\sin(\tau/2)]\sin\alpha\cos(\tau/2)$
(ssp) $\chi_{yyz} = \beta_{bbc} = 2[\beta_{\xi\xi\zeta}\cos^2\alpha\sin^2(\tau/2) + \beta_{\eta\eta\zeta}\cos^2(\tau/2) + \beta_{\zeta\zeta\zeta}\sin^2\alpha\sin^2(\tau/2)]\sin\alpha\cos(\tau/2)$
(psp) $\chi_{xyz} = \beta_{abc} = 2(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})[\sin\alpha\cos\alpha\sin(\tau/2)]\sin\alpha\cos(\tau/2)$
(sps) none
(pps) none
(pss) none
(sss) none (4b-2)

［**逆対称伸縮振動**］

(ppp) $\chi_{zxx} = \beta_{caa} = -2(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\alpha\cos^2\alpha\cos(\tau/2)$
$\chi_{xzx} = \beta_{caa} = -2(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\alpha\cos^2\alpha\cos(\tau/2)$
(spp) $\chi_{yzx} = \beta_{bca} = -2(\beta_{\xi\xi\zeta}\cos^2\alpha - \beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta}\sin^2\alpha)\cos\alpha\sin(\tau/2)\cos(\tau/2)$
(ssp) none
(psp) $\chi_{zyx} = \beta_{bca} = -2(\beta_{\xi\xi\zeta}\cos^2\alpha - \beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta}\sin^2\alpha)\cos\alpha\sin(\tau/2)\cos(\tau/2)$
(sps) $\chi_{yzy} = \beta_{cbb} = +2(\beta_{\xi\xi\zeta}\cos^2\alpha - \beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta}\sin^2\alpha)\sin\alpha\sin2(\tau/2)\cos(\tau/2)$
(pps) $\chi_{zxy} = \beta_{cab} = -2(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin^2\alpha\cos\alpha\cos(\tau/2)$
$\chi_{xzy} = \beta_{cab} = -2(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin^2\alpha\cos\alpha\cos(\tau/2)$
(pss) $\chi_{zyy} = \beta_{cbb} = +2(\beta_{\xi\xi\zeta}\cos^2\alpha - \beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta}\sin^2\alpha)\sin\alpha\sin^2(\tau/2)\cos(\tau/2)$
(sss) none (4b-3)

さらに、Td **角を仮定すると** $\cos\alpha = -1/3$, $\sin\alpha = 2\sqrt{2}/3$ **であるから、**

［**対称伸縮振動**］

(ppp)　$\chi_{xxz} = \beta_{aac} = (4\sqrt{2}/27)(8\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta})\cos(\tau/2)$

　　　$\chi_{zzz} = \beta_{ccc} = (4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\cos^2(\tau/2) + 9\beta_{\eta\eta\zeta}]\cos(\tau/2)$

(spp)　$\chi_{yxz} = \beta_{abc} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(2\sqrt{2})\sin(\tau/2)\cos(\tau/2)$

(ssp)　$\chi_{yyz} = \beta_{bbc} = (4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2) + 9\beta_{\eta\eta\zeta}]\cos(\tau/2)$

(psp)　$\chi_{xyz} = \beta_{abc} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(2\sqrt{2})\sin(\tau/2)\cos(\tau/2)$

(sps)　none

(pps)　none

(pss)　none

(sss)　none　(4b-4)

［**逆対称伸縮振動**］

(ppp)　$\chi_{zxx} = \beta_{caa} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos(\tau/2)$

　　　$\chi_{xzx} = \beta_{caa} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos(\tau/2)$

(spp)　$\chi_{yzx} = \beta_{bca} = (2/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin(\tau/2)\cos(\tau/2)$

(ssp)　none

(psp)　$\chi_{zyx} = \beta_{bca} = (2/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin(\tau/2)\cos(\tau/2)$

(sps)　$\chi_{yzy} = \beta_{cbb} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2)\cos(\tau/2)$

(pps)　$\chi_{zxy} = \beta_{cab} = (8/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos(\tau/2)$

　　　$\chi_{xzy} = \beta_{cab} = (8/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos(\tau/2)$

(pss)　$\chi_{zyy} = \beta_{cbb} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2)\cos(\tau/2)$

(sss)　none　(4b-5)

5. 表面固定 (xyz) 系における CH_2 基のテンソル成分

5a. ねじれた CH_2 基

立体障害を解消するために C_2 **軸まわりで角** γ **だけねじれるとき、ファイル「オイラー角」の** (Eu-1) **式により下式が得られる。**α **は** HCH **結合角である。**

$R_z(\chi = \gamma)\ R_{b'}(\theta = 0)\ R_c(\phi = 0)$、$R_z(\chi = -\gamma)\ R_{b'}(\theta = 0)\ R_c(\phi = 0)$、$\tau = \pi/2$

$\sin\chi = \sin\gamma$、$\sin2\chi = \sin2\gamma$、$\sin3\chi = \sin3\gamma$　　$\cos\chi = \cos\gamma$、$\cos2\chi = -\cos2\gamma$、$\cos3\chi = \cos3\gamma$

$\sin\phi = 0$、$\sin2\phi = 0$、$\sin3\phi = 0$　　$\cos\phi = 1$、$\cos2\phi = 1$、$\cos3\phi = 1$　(5a-1)

　　$(\sin\gamma/-\sin\gamma)$、$(\sin2\gamma/-\sin2\gamma)$、$(\sin3\gamma/-\sin3\gamma)$　pairs

（隣り合う CH_2 **基はともに** $+\gamma$ **または** $-\gamma$ **のどちらかを取り、互い違いにはならない。）**

により、

［**対称伸縮振動**］

(ppp)　$\chi_{xxz} = (1/2)[\beta_{aac}(1 + \cos2\chi) + \beta_{bbc}(1 - \cos2\chi)]$

　　　$\chi_{zzz} = \beta_{ccc}$

(spp)　$\chi_{yxz} = -(1/2)(\beta_{aac} - \beta_{bbc})\sin2\chi$

(ssp)　$\chi_{yyz} = (1/2)[(\beta_{aac}(1 - \cos2\chi) + \beta_{bbc}(1 + \cos2\chi)]$

(psp)　$\chi_{xyz} = -(1/2)(\beta_{aac} - \beta_{bbc})\sin2\chi$

(sps)　none

(pps)　none

(pss)　none

(sss)　none　(5a-2)

［逆対称伸縮振動］

(ppp)　$\chi_{zxx} = (1/2)\beta_{caa}(1 + \cos 2\chi)$

$\chi_{xzx} = (1/2)\beta_{caa}(1 + \cos 2\chi)$

(spp)　$\chi_{yzx} = -(1/2)\beta_{caa}\sin 2\chi$

(ssp)　none

(psp)　$\chi_{zyx} = -(1/2)\beta_{caa}\sin 2\chi$

(sps)　$\chi_{yzy} = (1/2)\beta_{caa}(1 - \cos 2\chi)$

(pps)　$\chi_{zxy} = -(1/2)\beta_{caa}\sin 2\chi$

$\chi_{xzy} = -(1/2)\beta_{caa}\sin 2\chi$

(pss)　$\chi_{zyy} = (1/2)\beta_{caa}(1 - \cos 2\chi)$

(sss)　none　(5a-3)

CH 基のテンソル成分による表式に Td 角を仮定すると、(3-4) 式と (3-5) 式によりさらに整理される。

［対称伸縮振動］

(ppp)　$\chi_{xxz} = (\sqrt{3}/9)[(\beta_{\xi\xi\zeta} + 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta}) + (\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos 2\chi]$

$\chi_{zzz} = (2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})$

(spp)　$\chi_{yxz} = -(\sqrt{3}/9)(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\sin 2\chi$

(ssp)　$\chi_{yyz} = (\sqrt{3}/9)[(\beta_{\xi\xi\zeta} + 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta}) - (\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos 2\chi]$

(psp)　$\chi_{xyz} = -(\sqrt{3}/9)(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\sin 2\chi$

(sps)　none

(pps)　none

(pss)　none

(sss)　none　(5a-4)

［逆対称伸縮振動］

(ppp)　$\chi_{zxx} = -(\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(1 + \cos 2\chi)$

$\chi_{xzx} = -(\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(1 + \cos 2\chi)$

(spp)　$\chi_{yzx} = (\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\beta_{caa}\sin 2\chi$

(ssp)　none

(psp)　$\chi_{zyx} = (\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin 2\chi$

(sps)　$\chi_{yzy} = -(\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(1 - \cos 2\chi)$

(pps)　$\chi_{zxy} = (\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin 2\chi$

$\chi_{xzy} = (\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin 2\chi$

(pss)　$\chi_{zyy} = -(\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(1 - \cos 2\chi)$

(sss)　none　(5a-5)

5b. のけぞった CH_2 基

分子面が xz 面から角 θ だけ ±y 軸方向にのけぞることで立体障害を解消しているときには、ファイル

「オイラー角」の (Eu-2a) 式により下しきが得られる。α は HCH 結合角である。

$R_z(\chi = -\pi/2)\ R_{b'}(-\theta)\ R_c(\phi = \pi/2)$、$R_z(\chi = -\pi/2)\ R_{b'}(\theta)\ R_c(\phi = \pi/2)$、$\tau = \pi/2 - \theta$

$\sin\chi = -1$、$\sin2\chi = 0$、$\sin3\chi = +1$　$\cos\chi = 0$、$\cos2\chi = -1$、$\cos3\chi = 0$

$\sin\phi = +1$、$\sin2\phi = 0$、$\sin3\phi = -1$　$\cos\phi = 0$、$\cos2\phi = -1$、$\cos3\phi = 0$

$$\sin\theta = -(\pm)\cos\tau,\ \cos\theta = \sin\tau \qquad (5b\text{-}1)$$

($\sin\theta$ / $-\sin\theta$) pair（隣り合う CH_2 基は交互に $+\theta$ と $-\theta$ をとる。）

により、

［対称伸縮振動］

(ppp)　$\chi_{xxz} = \beta_{aac}\cos\theta$

　$\chi_{zzz} = \beta_{bbc}(\cos\theta - \cos^3\theta) + \beta_{ccc}\cos^3\theta$

(spp)　$\chi_{yzz} = (\beta_{bbc} - \beta_{ccc})(\sin\theta - \sin^3\theta)$

(ssp)　$\chi_{yyz} = (\beta_{bbc} - \beta_{ccc})\cos^3\theta + \beta_{ccc}\cos\theta$

(psp)　$\chi_{zyz} = (\beta_{bbc} - \beta_{ccc})(\sin\theta - \sin^3\theta)$

(sps)　$\chi_{yzy} = -(\beta_{bbc} - \beta_{ccc})(\cos\theta - \cos^3\theta)$

(pps)　$\chi_{xxy} = -\beta_{aac}\sin\theta$

　$\chi_{zzy} = -(\beta_{bbc} - \beta_{ccc})\sin^3\theta - \beta_{ccc}\sin\theta$

(pss)　$\chi_{zyy} = -(\beta_{bbc} - \beta_{ccc})(\cos\theta - \cos^3\theta)$

(sss)　$\chi_{yyy} = -\beta_{bbc}\sin\theta + (\beta_{bbc} - \beta_{ccc})\sin^3\theta$　(5b-2)

［逆対称伸縮振動］

(ppp)　$\chi_{zxx} = \beta_{caa}\cos\theta$

　$\chi_{xzx} = \beta_{caa}\cos\theta$

(spp)　$\chi_{yxx} = -\beta_{caa}\sin\theta$

(ssp)　none

(psp)　$\chi_{xyx} = -\beta_{caa}\sin\theta$

(sps)　none

(pps)　none

(pss)　none

(sss)　none　(5b-3)

CH 基のテンソル成分による表式に Td 角を仮定すると、 (3-4) 式と (3-5) 式によりさらに整理される。

［対称伸縮振動］

(ppp)　$\chi_{xxz} = (2\sqrt{3}/9)(\beta_{\xi\xi\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\theta$

　$\chi_{zzz} = (2\sqrt{3}/9)[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\cos^3\theta + 3\beta_{\eta\eta\zeta}\cos\theta]$

(spp)　$\chi_{yzz} = -(2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})(\sin\theta - \sin^3\theta)$

(ssp)　$\chi_{yyz} = (2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta) + 3\beta_{\eta\eta\zeta}\cos\theta]$

(psp)　$\chi_{zyz} = -(2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})(\sin\theta - \sin^3\theta)$

(sps)　$\chi_{yzy} = (2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)$

(pps) $\chi_{xxy} = -(2\sqrt{3}/9)(\beta_{\xi\xi\zeta} + 2\beta_{\zeta\zeta\zeta})\sin\theta$

$\chi_{zzy} = -(2\sqrt{3}/9)[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})(\sin\theta - \sin^3\theta) + 3\beta_{\eta\eta\zeta}\sin\theta]$

(pss) $\chi_{zyy} = (2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)$

(sss) $\chi_{yyy} = -(2\sqrt{3}/9)[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^3\theta + 3\beta_{\eta\eta\zeta}\sin\theta]$ (5b-4)

［逆対称伸縮振動］

(ppp) $\chi_{zxx} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\theta$

$\chi_{xzx} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\theta$

(spp) $\chi_{yxx} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\theta$

(ssp) none

(psp) $\chi_{xyx} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\theta$

(sps) none

(pps) none

(pss) none

(sss) none (5b-5)

5c. 横ざまにかしいだ CH_2 基

分子面が xz 面内で角 θ だけ ±x 軸方向に横ざまにかしぐことで立体障害を解消しているとき、ファイル「オイラー角」の (Eu-2b) 式により下式が得られる。α は HCH 結合角である。

$R_z(\chi = \pi)\ R_{b'}(\theta)\ R_c(\phi = \pi)$ **または** $R_z(\chi = -\pi)\ R_{b'}(-\theta)\ R_c(\phi = \pi)$、$\tau = \pi/2$

$\sin\chi = 0$、$\sin2\chi = 0$、$\sin3\chi = 0$ $\cos\chi = -1$、$\cos2\chi = +1$、$\cos3\chi = -1$

$\sin\phi = 0$、$\sin2\phi = 0$、$\sin3\phi = 0$ $\cos\phi = -1$、$\cos2\phi = +1$、$\cos3\phi = -1$

$\sin\theta = \pm\sin\theta$、$\cos\theta = \cos\theta$ (5c-1)

either $\sin\theta$ /or - $\sin\theta$

（隣り合う CH_2 基は、交互に +θ または -θ のどちらかをとり、逆符号のものが隣り合わせにはならない。）

により、

［対称伸縮振動］

(ppp) $\chi_{xxx} = \beta_{aac}(\sin\theta - \sin^3\theta) + \beta_{ccc}\sin^3\theta$

$\chi_{xzz} = -(\beta_{aac} - \beta_{ccc})(\sin\theta - \sin^3\theta)$

$\chi_{zxz} = -(\beta_{aac} - \beta_{ccc})(\sin\theta - \sin^3\theta)$

$\chi_{zzx} = \beta_{aac}\sin^3\theta + \beta_{ccc}(\sin\theta - \sin^3\theta)$

$\chi_{xzx} = -(\beta_{aac} - \beta_{ccc})(\cos\theta - \cos^3\theta)$

$\chi_{zxx} = -(\beta_{aac} - \beta_{ccc})(\cos\theta - \cos^3\theta)$

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

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

(spp) none

(ssp) $\chi_{yyx} = \beta_{bbc}\sin\theta$

$\chi_{yyz} = \beta_{bbc}\cos\theta$

(psp) none

(sps) $\chi_{yzy} = -(\beta_{aac} - \beta_{ccc})(\cos\theta - \cos^3\theta)$

(pps) none

(pss) $\chi_{zyy} = -(\beta_{aac} - \beta_{ccc})(\cos\theta - \cos^3\theta)$

(sss) none (5c-2)

［逆対称伸縮振動］

(ppp) $\chi_{zxx} = \beta_{caa}\cos\theta$

$\chi_{xzx} = \beta_{caa}\cos\theta$

(spp) none

(ssp) none

(psp) none

(sps) $\chi_{yxy} = \beta_{caa}\sin\theta$

(pps) none

(pss) $\chi_{xyy} = \beta_{caa}\sin\theta$

(sss) none (5c-3)

CH 基のテンソル成分による表式に Td 角を仮定すると、(3-4) 式と (3-5) 式によりさらに整理される。

［対称伸縮振動］

(ppp) $\chi_{xxx} = -(2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\sin\theta - \sin^3\theta) - (2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\sin\theta]$

$\chi_{xzz} = (2\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\sin\theta - \sin^3\theta)$

$\chi_{zxz} = (2\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\sin\theta - \sin^3\theta)$

$\chi_{zzx} = (2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\sin\theta - \sin^3\theta) - (2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\sin\theta]$

$\chi_{xzx} = (2\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)$

$\chi_{zxx} = (2\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)$

$\chi_{xxz} = (2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta) - (2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\cos\theta]$

$\chi_{zzz} = -(2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta) - (2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\cos\theta]$

(spp) none

(ssp) $\chi_{yyx} = (6\sqrt{3}/9)\beta_{\eta\eta\zeta}\sin\theta$

$\chi_{yyz} = (6\sqrt{3}/9)\beta_{\eta\eta\zeta}\cos\theta$

(psp) none

(sps) $\chi_{yzy} = (2\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)$

(pps) none

(pss) $\chi_{zyy} = (2\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)$

(sss) none (5c-4)

［逆対称伸縮振動］

(ppp) $\chi_{zxx} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\theta$

$\chi_{xzx} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\theta$

(spp) none

(ssp) none

(psp) none

(sps) $\chi_{yxy} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\theta$

(pps) none

(pss) $\chi_{xyy} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\theta$

(sss) none (5c-5)

5d. z 軸まわりにねじれてからうしろにのけぞった CH_2 基

分子面が z 軸まわりに γ だけねじれると同時に xz 面から角 θ だけ ±y 軸方向にのけぞっているとき、ファイル「オイラー角」の (Eu-3a) 式により下式が得られる。α は HCH 結合角である。

$\sin\chi = -1$、$\sin2\chi = 0$、$\sin3\chi = -1$ $\cos\chi = 0$、$\cos2\chi = -1$、$\cos3\chi = 0$、

$\sin\phi = \cos\gamma = \cos\tau/\sin\theta$、 $\sin2\phi = \sin2\gamma = 2\cos\tau\sqrt{\sin^2\theta - \cos^2\tau}/\sin^2\theta$、

$\cos\phi = \sin\gamma = \sqrt{\sin^2\theta - \cos^2\tau}/\sin\theta$、 $\cos2\phi = -\cos2\gamma = (\sin^2\theta - 2\cos^2\tau)/\sin^2\theta$、

$1 + \cos2\phi = 1 - \cos2\gamma = 2(\sin^2\theta - \cos^2\tau)/\sin^2\theta$、 $1 - \cos\phi = 1 + \cos2\gamma = 2\cos^2\tau/\sin^2\theta$ (5d-1)

either ($\sin\gamma$, $\sin2\gamma$, $\sin3\gamma$) set or ($-\sin2\gamma$, $-\sin2\gamma$, $-\sin3\gamma$) set

($\sin\theta$ /$-\sin\theta$) pair

（隣り合う CH_2 基は同じく +γ または -γ のどちらかを取り、θ の符号が交互に交代する。）

により、

［対称伸縮振動］

(ppp) $\chi_{xxx} = -(1/2)(\beta_{aac} - \beta_{bbc})\sin\theta\cos\theta\sin2\phi$

$\chi_{xzz} = (1/2)(\beta_{aac} - \beta_{bbc})\sin\theta\cos\theta\sin2\phi$

$\chi_{zxz} = (1/2)(\beta_{aac} - \beta_{bbc})\sin\theta\cos\theta\sin2\phi$

$\chi_{xxz} = (1/2)[\beta_{aac}(1 - \cos2\phi) + \beta_{bbc}(1 + \cos2\phi)]\cos\theta$

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

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

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

$\chi_{yxz} = (1/2)(\beta_{aac} - \beta_{bbc})\cos^2\theta\sin2\theta$

(ssp) $\chi_{yyx} = (1/2)(\beta_{aac} - \beta_{bbc})\sin\theta\cos\theta\sin2\phi$

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

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

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

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

(pps) $\chi_{xxy} = -(1/4)(\beta_{aac} - \beta_{bbc})(1 - \cos2\phi) - (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta + (1/2)(\beta_{aac} - \beta_{ccc})\sin^3\theta$

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

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

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

(5d-2)

［逆対称伸縮振動］

(ppp) $\chi_{xxx} = -\beta_{caa}\sin\theta\cos\theta\sin2\phi$

$\chi_{zxx} = \beta_{caa}\cos\theta$

$\chi_{xzx} = \beta_{caa}\cos\theta$

(spp) $\chi_{yzz} = (1/2)\beta_{caa}(\sin\theta - 2\sin^3\theta)(1 + \cos2\phi)$

(ssp) none

(psp) none

(sps) $\chi_{yxy} = (1/2)\beta_{caa}\sin\theta\cos\theta\sin2\phi$

(pps) none

(pss) $\chi_{xyy} = (1/2)\beta_{caa}\sin\theta\cos\theta\sin2\phi$

(sss) $\chi_{yyy} = -(1/2)\beta_{caa}[(\sin\theta - \sin^3\theta)(1 + \cos2\phi) + \sin\theta\ (1 - \cos2\phi)]$ (5d-3)

CH 基のテンソル成分による表式に Td 角を仮定すると、(3-4) 式と (3-5) 式によりさらに整理される。

［対称伸縮振動］

(ppp) $\chi_{xxx} = -(2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\tau\sqrt{\sin^2\theta - \cos^2\tau}]\cos\theta$

$\chi_{xzz} = (2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\tau\sqrt{\sin^2\theta - \cos^2\tau}]\cos\theta$

$\chi_{zxz} = (2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\tau\sqrt{\sin^2\theta - \cos^2\tau}]\cos\theta$

$\chi_{xxz} = (2\sqrt{3}/9)[3\beta_{\eta\eta z} + (\beta_{\xi\xi\zeta} + 2\beta_{\zeta\zeta\zeta})\cos^2\tau/\sin^2\theta]\cos\theta$

$\chi_{zzz} = (2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos^2\tau/\sin^2\theta + 3\beta_{\eta\eta\zeta}](\cos\theta - \cos^3\theta)$

$+ (2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\cos^3\theta\}$

(spp) $\chi_{yxx} = (\sqrt{3}/9)[-(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})(1 + \cos^2\tau - 2\cos^2\tau/\sin^2\theta)$

$+ 3(\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\theta]\sin\theta$

$\chi_{yzz} = (2\sqrt{3}/9)[-(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos^2\tau/\sin^2\theta$

$- (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})](\sin\theta - \sin^3\theta)]$

$\chi_{yxz} = (2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\tau\sqrt{\sin^2\theta - \cos^2\tau}]\cos^2\theta/\sin\theta$

(ssp) $\chi_{yyx} = (2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\tau\sqrt{\sin^2\theta - \cos^2\tau}]\cos\theta$

$\chi_{yyz} = -(2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos^2\tau/\sin^2\theta$

$- (\beta_{\xi\xi\zeta} + 2\beta_{\zeta\zeta\zeta})]\cos^3\theta$

$- (2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)\}$

(psp) $\chi_{xyx} = -(\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})(1 + \cos^2\tau - 2\cos^2\tau/\sin^2\theta)$

$- 3(\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\theta]\sin\theta$

$\chi_{zyz} = -(2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos^2\tau/\sin^2\theta$

$+ (\beta_{\xi\xi\zeta} + 2\beta_{\zeta\zeta\zeta})](\sin\theta - \sin^3\theta)$

(sps) $\chi_{yzy} = (2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos^2\tau/\sin^2\theta$

$- 3(\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})](\cos\theta - \cos^3\theta)$

(pps) $\chi_{xxy} = -(2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})(\sin\theta - \sin^3\theta + \cos^2\tau/\sin^2\theta)$

$+ 6\beta_{\zeta\zeta\zeta}\sin\theta]$

$\chi_{zzy} = (2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos^2\tau\sin\theta$
$+ (\beta_{\xi\xi\zeta} + 2\beta_{\zeta\zeta\zeta})\sin^3\theta$
$+ (2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})(\sin\theta - \sin^3\theta)]$

(pss) $\chi_{zyy} = (2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos^2\tau/\sin^2\theta$
$- 3(\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})](\cos\theta - \cos^3\theta)$

(sss) $\chi_{yyy} = -(\sqrt{3}/9)\ [(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})(\sin\theta + \cos^2\tau\sin\theta)$
$+ (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin^3\theta$
$+ 6\beta_{\eta\eta\zeta}\sin\theta]$ (5d-4)

［逆対称伸縮振動］

(ppp) $\chi_{xxx} = (8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sqrt{\sin^2\theta - \cos^2\tau}\,\cos\theta$

$\chi_{zxx} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\theta$
$\chi_{xzx} = -(4\sqrt{3}/9\ 9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\theta$

(spp) $\chi_{yzz} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\sin\theta - 2\sin^3\tau)(1 - \cos^2\tau/\sin^2\theta)$

(ssp) none

(psp) none

(sps) $\chi_{yxy} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sqrt{\sin^2\theta - \cos^2\tau}\,\cos\theta$

(pps) none

(pss) $\chi_{xyy} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sqrt{\sin^2\theta - \cos^2\tau}\,\cos\theta$

(sss) $\chi_{yyy} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})[(\sin\theta - \sin^3\theta) + \cos^2\tau\sin\theta]$ (5d-5)

5e. z 軸まわりにねじれてから横ざまにかしいだ CH_2 基

分子面が z 軸まわりに γ だけねじれると同時に xz 面内で角 θ だけ ±x 軸方向に横ざまにかしいでいるとき、ファイル「オイラー角」の (Eu-3b) 式により下式が得られる。α は HCH 結合角である。

$\sin\chi = 0$、$\sin2\chi = 0$、$\sin3\chi = 0$　　$\cos\chi = -1$、$\cos2\chi = +1$、$\cos3\chi = -1$、

$\sin\phi = \sin\gamma = \cos\tau in\theta$、　　$\sin2\phi = -\sin2\gamma = -2\cos\tau\sqrt{\sin^2\theta - \cos^2\tau}\,/\sin^2\theta$、

$\cos\phi = -\cos\gamma = -\sqrt{\sin^2\theta - \cos^2\tau}\,/\sin\theta$、　　$\cos2\phi = \cos2\gamma = (\sin^2\theta - 2\cos^2\tau)/\sin^2\theta$、

$1 + \cos2\phi = 1 + \cos2\gamma = 2(\sin^2\theta - \cos^2\tau)/\sin^2\theta$、　$1 - \cos2\phi = 1 - \cos2\gamma = 2\cos^2\tau/\sin^2\theta$ (5e-1)

$(+\gamma, +\theta)$ set、$(+\gamma, -\theta)$ set、$(-\gamma, +\theta)$ set、or $(-\gamma, -\theta)$ set

（隣り合う CH_2 基は同じく $+\gamma$ または $-\gamma$ のどちらかを取り、θ も同じ符号を取る。）

により、

［対称伸縮振動］

(ppp) $\chi_{xxx} = (1/2)[\beta_{aac}(1 + \cos2\phi) + \beta_{bbc}(1 - \cos2\phi)](\sin\theta - \sin^3\theta) + \beta_{ccc}\sin^3\theta$
$\chi_{xzz} = -(1/2)[\beta_{aac}(1 + \cos2\phi) + \beta_{bbc}(1 - \cos2\phi)](\sin\theta - \sin^3\theta) + \beta_{ccc}(\sin\theta - \sin^3\theta)$

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

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

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

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

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

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

(spp) $\chi_{yxx} = -(1/2)(\beta_{aac} - \beta_{bbc})\sin\theta\cos\theta\sin 2\phi$

$\chi_{yzz} = (1/2)(\beta_{aac} - \beta_{bbc})\sin\theta\cos\theta\sin 2\phi$

$\chi_{yzx} = (1/2)(\beta_{aac} - \beta_{bbc})\sin^2\theta\sin 2\phi$

$\chi_{yxz} = -(1/2)(\beta_{aac} - \beta_{bbc})\cos^2\theta\sin 2\phi$

(ssp) $\chi_{yyx} = (1/2)[\beta_{aac}(1 - \cos 2\phi) + \beta_{bbc}(1 + \cos 2\phi)]\sin\theta$

$\chi_{yyz} = (1/2)[\beta_{aac}(1 - \cos 2\phi) + \beta_{bbc}(1 + \cos 2f)]\cos\theta$

(psp) $\chi_{xyx} = -(1/2)(\beta_{aac} - \beta_{bbc})\sin\theta\cos\theta\sin 2\phi$

$\chi_{zyz} = (1/2)(\beta_{aac} - \beta_{bbc})\sin\theta\cos\theta\sin 2\phi$

$\chi_{xyz} = -(1/2)(\beta_{aac} - \beta_{bbc})\cos^2\theta\sin 2\phi$

$\chi_{zyx} = (1/2)(\beta_{aac} - \beta_{bbc})\sin^2\theta\sin 2\phi$

(sps) none

(pps) none

(pss) none

(sss) none (5e-2)

［**逆対称伸縮振動**］

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

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

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

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

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

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

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

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

(spp) $\chi_{yxx} = -(1/2)\beta_{caa}\sin\theta\cos\theta\sin 2\phi$

$\chi_{yzz} = (1/2)\beta_{caa}\sin\theta\cos\theta\sin 2\phi$

$\chi_{yzx} = -(1/2)\beta_{caa}\cos^2\theta\sin 2\phi$

$\chi_{yxz} = (1/2)\beta_{caa}\sin^2\theta\sin 2\phi$

(ssp) none

(psp) $\chi_{xyx} = -(1/2)\beta_{caa}\sin\theta\cos\theta\sin 2\phi$

$\chi_{zyz} = (1/2)\beta_{caa}\sin\theta\cos\theta\sin 2\phi$

$\chi_{xyz} = (1/2)\beta_{caa}\sin^2\theta\sin 2\phi$

$\chi_{zyx} = -(1/2)\beta_{caa}\cos^2\theta\sin 2\phi$

(sps) $\chi_{yxy} = (1/2)\beta_{caa}\sin\theta(1 - \cos 2\phi)$

$\chi_{yzy} = (1/2)\beta_{caa}\cos\theta (1 - \cos 2\phi)$

(pps) $\chi_{xxy} = -\beta_{caa}\sin\theta\cos\theta\sin 2\phi$

$\chi_{zzy} = \beta_{caa}\sin\theta\cos\theta\sin 2\phi$

$\chi_{zxy} = (1/2)\beta_{caa}(1 - 2\cos^2\theta)\sin 2\phi$

$\chi_{xzy} = (1/2)\beta_{caa}(1 - 2\cos^2\theta)\sin 2\phi$

(pss) $\chi_{xyy} = (1/2)\beta_{caa}\sin\theta(1 - \cos 2\phi)$

$\chi_{zyy} = (1/2)\beta_{caa}\cos\theta(1 - \cos 2\phi)$

(sss) none (5e-3)

CH 基のテンソル成分による表式に Td 角を仮定すると、 (3-4) 式と (3-5) 式によりさらに整理される。

［対称伸縮振動］

(ppp) $\chi_{xxx} = (2\sqrt{3}/9)\{[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})(1 - \cos^2\tau/\sin^2\theta) + 3\beta_{\eta\eta\zeta}]\cos^2\theta + (2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\theta\}\sin\theta$

$\chi_{xzz} = -(2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})(1 - \cos^2\tau/\sin^2\theta) + (2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})]\sin\theta\cos^2\theta$

$\chi_{zxz} = -(2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})(1 - \cos^2\tau/\sin^2\theta) + (2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})]\sin\theta\cos^2\theta$

$\chi_{zzx} = -(2\sqrt{3}/9)\{[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})(1 - \cos^2\tau/\sin^2\theta) + 3\beta_{\eta\eta\zeta}]\sin^2\theta - (2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\cos^2\theta\}\sin\theta$

$\chi_{xzx} = -(2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})(1 - \cos^2\tau/\sin^2\theta) - (2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})]\sin^2\theta\cos\theta$

$\chi_{zxx} = -(2\sqrt{3}/9)[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})(1 - \cos^2\tau/\sin^2\theta) - (2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})]\sin^2\theta\cos\theta$

$\chi_{xxz} = (2\sqrt{3}/9)\{[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})(1 - \cos^2\tau/\sin^2\theta) + 3\beta_{\eta\eta\zeta}]\cos^2\theta + (2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\theta\}\cos\theta$

$\chi_{zzz} = (2\sqrt{3}/9)\{[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})(1 - \cos^2\tau/\sin^2\theta) + 3\beta_{\eta\eta\zeta}]\cos^2\theta + (2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\theta\}\cos\theta$

(spp) $\chi_{yxx} = (2\sqrt{3}/9)(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1 - \cos^2\tau/\sin^2\theta}\,\cos\theta$

$\chi_{yzza} = -(2\sqrt{3}/9)(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1 - \cos^2\tau/\sin^2\theta}\,n^2\theta)\sin\theta$

$\chi_{yxz} = (2\sqrt{3}/9)(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1 - \cos^2\tau/\sin^2\theta}\,\cos^2\theta/\sin\theta$

(ssp) $\chi_{yyx} = (2\sqrt{3}/9)\{[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos^2\tau/\sin^2\theta + 3\beta_{\eta\eta\zeta}]\sin\theta$

$\chi_{yyz} = (2\sqrt{3}/9)\{[(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos^2\tau/\sin^2\theta + 3\beta_{\eta\eta\zeta}]\cos\theta$

(psp) $\chi_{xyx} = (2\sqrt{3}/9)(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1 - \cos^2\tau/\sin^2\theta}\,\cos\theta$

$\chi_{zyz} = -(2\sqrt{3}/9)(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1 - \cos^2\tau/\sin^2\theta}\,\cos\theta$

$\chi_{xyz} = (2\sqrt{3}/9)(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1 - \cos^2\tau/\sin^2\theta}\,\cos^2\theta/\sin\theta$

$\chi_{zyx} = -(2\sqrt{3}/9)(\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1 - \cos^2\tau/\sin^2\theta}\,\sin\theta$

(sps) none

(pps) none

(pss) none

(sss) none (5e-4)

［逆対称伸縮振動］

(ppp) $\chi_{xxx} = -(8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\sin\theta - \sin^3\theta)(1 - \cos^2\tau/\sin^2\theta)$

$\chi_{xzz} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\sin\theta - 2\sin^3\theta)(1 - \cos^2\tau/\sin^2\theta)$

$\chi_{zxz} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\sin\theta - 2\sin^3\theta)(1 - \cos^2\tau/\sin^2\theta)$
$\chi_{zzx} = (8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\sin\theta - \sin^3\theta)(1 - \cos^2\tau/\sin^2\theta)$
$\chi_{zxx} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\cos\theta - 2\cos^3\theta)(1 - \cos^2\tau/\sin^2\theta)$
$\chi_{xzx} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\cos\theta - 2\cos^3\theta)(1 - \cos^2\tau/\sin^2\theta)$
$\chi_{xxz} = (8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)(1 - \cos^2\tau/\sin^2\theta)$
$\chi_{zzz} = (8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(\cos\theta - \cos^3\theta)(1 - \cos^2\tau/\sin^2\theta)$

(spp) $\chi_{yxx} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1-\cos^2\tau/\sin^2\theta}\,\cos\theta$

$\chi_{yzz} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1-\cos^2\tau/\sin^2\theta}\,\cos\theta$

$\chi_{yzx} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1-\cos^2\tau/\sin^2\theta}\,\cos^2\theta/\sin\theta$

$\chi_{yxz} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1-\cos^2\tau/\sin^2\theta}\,\sin\theta$

(ssp) none

(psp) $\chi_{xyx} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1-\cos^2\tau/\sin^2\theta}\,\cos\theta$

$\chi_{zyz} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1-\cos^2\tau/\sin^2\theta}\,\cos\theta$

$\chi_{xyz} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1-\cos^2\tau/\sin^2\theta}\,\sin\theta$

$\chi_{zyx} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1-\cos^2\tau/\sin^2\theta}\,\cos^2\theta/\sin\theta$

(sps) $\chi_{yxy} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\theta\cos^2\tau/\sin^2\theta$
$\chi_{yzy} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\theta\cos^2\tau/\sin^2\theta$

(pps) $\chi_{xxy} = (8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1-\cos^2\tau/\sin^2\theta}\,\cos\theta$

$\chi_{zzy} = -(8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sqrt{1-\cos^2\tau/\sin^2\theta}\,\cos\theta$

$\chi_{zxy} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(1 - 2\cos^2\theta)\cos\tau\sqrt{1-\cos^2\tau/\sin^2\theta}\,/\sin\theta$

$\chi_{xzy} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})(1 - 2\cos^2\theta)\cos\tau\sqrt{1-\cos^2\tau/\sin^2\theta}\,/\sin\theta$

(pss) $\chi_{xyy} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\theta\cos^2\tau/\sin^2\theta$
$\chi_{zyy} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\theta\cos^2\tau/\sin^2\theta$

(sss) none (5e-5)

5f. ねじれと傾きの両方を持つ CH_2 基

分子軸が z **軸から角** ±θ **だけ倒れ、さらに分子面が表面と２面角** τ **で傾くことで立体障害を解消しているときには、ファイル「オイラー角」の** (Eu-3c) **式により下式がを得られる。**α **は** HCH **結合角である。**

$R_z(\chi)\, R_{b'}(\theta)\, R_c(\phi)$, $R_z(\chi)\, R_{b'}(-\theta)\, R_c(\phi)$

($R_c(\phi)$)：b 軸が z 軸に垂直になるように — z 軸と c 軸が作る面に垂直に — する。）
($R_{b'}(\pm\theta)$)：c 軸を z 軸に重ねる — xy 面と ab 面を重ねる。）
($R_z(\chi)$)：b 軸を y 軸に重ねる — xz 面と分子面を重ねる。）
ケース 5e からの回転角を χ^* とする。

$\sin\chi = \sin\chi^*$、$\sin 2\chi = -\sin 2\chi^*$、$\sin 3\chi = \sin 3\chi^*$　　$\cos\chi = -\cos\chi^*$、$\cos 2c = +\cos 2\chi^*$、$\cos 3\chi = -\cos 3\chi^*$、
$\sin\phi = \sin\gamma = \cos\tau/\sin\theta$、　　$\sin 2\phi = -\sin 2\gamma = -2\cos\tau\sqrt{(\sin^2\theta - \cos^2\tau)}/\sin^2\theta$、
$\cos\phi = -\cos\gamma = -\sqrt{(\sin^2\theta - \cos^2\tau)}/\sin\theta$、　　$\cos 2\phi = \cos 2\gamma = (\sin^2\theta - 2\cos^2\tau)/\sin^2\theta$、
$1 + \cos 2\phi = 1 + \cos 2\gamma = 2(\sin^2\theta - \cos^2\tau)/\sin^2\theta$、　　$1 - \cos 2\phi = 1 - \cos 2\gamma = 2\cos^2\tau/\sin^2\theta$　　(5f-1)
for either one of the $(+\gamma, +\theta)$ set、$(+\gamma, -\theta)$ set、$(-\gamma, +\theta)$ set、or $(-\gamma, -\theta)$ set
（隣り合う CH_2 基は同じく $+\gamma$ または $-\gamma$ のどちらかを取り、θ も同じ符号を取る。χ^* の符号が交代する。）

により、

［対称伸縮振動］

(ppp)
$$\chi_{xxx} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi^* -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(3\cos\chi^* + \cos 3\chi^*) -(1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(\cos\chi^* - \cos 3\chi^*) - (\sin\theta - \sin^3\theta)(3\cos\chi^* + \cos 3\chi^*)]\cos 2\phi - 2\sin\theta\cos\theta(\sin\chi^* + \sin 3\chi^*)\sin 2\phi\}$$
$$\chi_{xzz} = -(1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi^* - (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\cos\chi^*\cos 2\phi + \sin\theta\cos\theta\sin\chi^*\sin 2\phi]$$
$$\chi_{zxz} = -(1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi^* - (1/3)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\cos\chi^*\cos 2\phi + \sin\theta\cos\theta\sin\chi^*\sin 2\phi]$$
$$\chi_{zzx} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi^* - (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\sin\theta - \sin^3\theta)\cos\chi^* +(1/2)(\beta_{aac} - \beta_{bbc})\cos\chi^*\sin^3\theta\cos 2\phi$$
$$\chi_{xzx} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos 2\chi^*) - (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 + \cos 2\chi^*)\cos 2\phi + \sin^2\theta\sin 2\chi^*\sin 2\phi]$$
$$\chi_{zxx} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos 2\chi^*) - (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 + \cos 2\chi^*)\cos 2\phi + \sin^2\theta\sin 2\chi^*\sin 2\phi]$$
$$\chi_{xxz} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta - (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos 2\chi^*) - (1/4)(\beta_{aac} - \beta_{bbc})\{[(\cos\theta - \cos^3\theta) - (\cos\theta + \cos^3\theta)\cos 2\chi^*]\cos 2\phi - 2\cos^2\theta\sin 2\chi^*\sin 2\phi\}$$
$$\chi_{zzz} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta - (1/2)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\cos^3\theta + (1/2)(\beta_{aac} - \beta_{bbc})(\cos\theta - \cos^3\theta)\cos 2\phi$$

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

$- (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi^*\cos 2\phi - \sin\theta\cos\theta\cos\chi^*\sin 2\phi]$

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

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

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

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

(ssp) $\chi_{yyx} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi^*$

$- (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi^* - \cos 3\chi^*)$

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

$+ 2\sin\theta\cos\theta(\sin\chi^* + \sin 3\chi^*)\sin 2\phi\}$

$\chi_{yyz} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$

$- (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos 2\chi^*)$

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

(psp) $\chi_{xyx} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi^* + \sin 3\chi^*)$

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

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

$- (1/2)(\beta_{aac} - \beta_{bbc})[(\sin\theta - \sin^3\theta)\sin\chi^*\cos 2\phi - \sin\theta\cos\theta\cos\chi^*\sin 2\phi]$

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

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

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

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

(sps) $\chi_{yxy} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi^* - \cos 3\chi^*)$

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

$\chi_{yzy} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos 2\chi^*)$

$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 - \cos 2\chi^*)\cos 2\phi - \sin^2\theta\sin 2\chi^*\sin 2\phi]$

(pps) $\chi_{xxy} = (1/2)(\beta_{aac} + \beta_{bbc})\sin q\sin\chi^*$

$- (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin c^* + \sin 3\chi^*)$

$+ (1/8)(\beta_{aac} - \beta_{bbc})\{[(\sin\theta - \sin^3\theta)(\sin c^* + \sin 3\chi^*) - \sin\theta(3\sin\chi^* - \sin 3\chi^*)\cos 2\phi]$

$\chi_{zzy} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi^*$

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

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

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

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

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

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

(pss) $\chi_{xyy} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi^* - \cos 3\chi^*)$

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

$\chi_{zyy} = -(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos 2\chi^*)$

$- (1/4)(\beta_{aac} - \beta_{bbc})[(\cos\theta - \cos^3\theta)(1 - \cos 2\chi^*)\cos 2\phi - \sin^2\theta\sin 2\chi^*\sin 2\phi]$

(sss) $\chi_{yyy} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi^*$
$- (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta\ (3\sin\chi^* - \sin3\chi^*)$
$- (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(\sin\chi^* + \sin3\chi^*) - (\sin\theta - \sin^3\theta)(3\sin\chi^* - \sin3\chi^*)]\cos2\phi$
$+ 2\sin\theta\cos\theta\ (\cos\chi^* - \cos3\chi^*)\sin2\phi\}$ (5f-2)

［逆対称伸縮振動］

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

(sss) $\chi_{yyy} = (1/4)\beta_{caa}\{[(\sin\theta - \sin^3\theta)(3\sin\chi^* - \sin3\chi^*)(1 + \cos2\phi) + \sin\theta(\sin\chi^* + \sin3\chi^*)(1 - \cos2\phi)]$
$- 2\sin\theta\ \cos\theta(\cos\chi^* - \cos3\chi^*)\sin2\phi\}$ (5f-3)

上の結果も、$1 \pm \cos2\phi$ と θ, τ を結びつける式及び CH 基のテンソル成分による表式に Td 角を仮定すると、(3-4) 式と (3-5) 式によりさらに整理されるが、あまり実りがなさそうなのでやめておく。

6. 実験室固定(XYZ)系におけるテンソル成分

光の光路にあわせて定義される実験室固定 (XYZ) 座標系におけるテンソル成分を導く。(XYZ) 座標系は表面固定 (xyz) 座標系を z 軸のまわりに角 χ だけ回転したものであるとして、ファイル「表面の回転」を参照している。

6a. 傾いた平面形 HCCH 基

［対称伸縮振動］

(ppp) $\chi_{XXX} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau - \beta_{bbc}]\sin\tau\sin^3\chi - \beta_{aac}\sin\tau\sin\chi\cos^2\chi$

$\chi_{XZZ} = (\beta_{bbc} - \beta_{ccc})\sin\tau\cos^2\tau\sin\chi$

$\chi_{ZXZ} = (\beta_{bbc} - \beta_{ccc})\sin\tau\cos^2\tau\sin\chi$

$\chi_{ZZX} = -[(\beta_{bbc} - \beta_{ccc})\sin\tau\cos^2\tau + \beta_{ccc}\sin\tau]\sin\chi$

$\chi_{ZXX} = -(\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\sin^2\chi$

$\chi_{XZX} = -(\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\sin^2\chi$

$\chi_{XXZ} = [(\beta_{bbc} - \beta_{ccc})\cos^2\tau + \beta_{ccc}]\cos\tau\sin^2\chi + \beta_{aac}\cos\tau\cos^2\chi$

$\chi_{ZZZ} = -[(\beta_{bbc} - \beta_{ccc})\cos^2\tau - \beta_{bbc}]\cos\tau$

(spp) $\chi_{YXX} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau + (\beta_{aac} - \beta_{bbc})]\sin\tau\sin^2\chi\cos\chi$

$\chi_{YZZ} = (\beta_{bbc} - \beta_{ccc})\sin\tau\cos^2\tau\cos\chi$

$\chi_{YZX} = (\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\sin\chi\cos\chi$

$\chi_{YXZ} = [(\beta_{bbc} - \beta_{ccc})\cos^2\tau - (\beta_{aac} - \beta_{ccc})]\cos\tau\sin\chi\cos\chi$

(ssp) $\chi_{YYX} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau + (\beta_{aac} - \beta_{bbc})]\sin\tau\sin\chi\cos^2\chi - \beta_{aac}\sin\tau\sin\chi$

$\chi_{YYZ} = [(\beta_{bbc} - \beta_{ccc})\cos^2\tau + \beta_{ccc}]\cos\tau\sin^2\chi + \beta_{aac}\cos\tau\cos^2\chi$

(psp) $\chi_{XYX} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau + (\beta_{aac} - \beta_{bbc})]\sin\tau\sin^2\chi\cos\chi$

$\chi_{ZYZ} = (\beta_{bbc} - \beta_{ccc})\sin\tau\cos^2\tau\cos\chi$

$\chi_{XYZ} = [(\beta_{bbc} - \beta_{ccc})\cos^2\tau - (\beta_{aac} - \beta_{ccc})]\cos\tau\sin\chi\cos\chi$

$\chi_{ZYX} = (\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\sin\chi\cos\chi$

(sps) $\chi_{YXY} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau + (\beta_{aac} - \beta_{bbc})]\sin\tau\sin\chi\cos^2\chi$

$\chi_{YZY} = -(\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\cos^2\chi$

(pps) $\chi_{XXY} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau + (\beta_{aac} - \beta_{bbc})]\sin\tau\sin^2\chi\cos\chi - \beta_{aac}\sin\tau\cos\chi$

$\chi_{ZZY} = -[(\beta_{bbc} - \beta_{ccc})\sin^2\tau + \beta_{ccc}]\sin\tau\cos\chi$

$\chi_{ZXY} = -(\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\sin\chi\cos\chi$

$\chi_{XZY} = -(\beta_{bbc} -\beta_{ccc})\sin^2\tau\cos\tau\sin\chi\cos\chi$

(pss) $\chi_{XYY} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau + (\beta_{aac} - \beta_{bbc})]\sin\tau\sin\chi\cos^2\chi$

$\chi_{ZYY} = -(\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\cos^2\chi$

(sss) $\chi_{YYY} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau - \beta_{bbc}]\sin\tau\cos^3\chi - \beta_{aac}\sin\tau\sin^2\chi\cos\chi$ (6a-1)

［**逆対称伸縮振動**］

(ppp) $\chi_{XXX} = 0$

$\chi_{XZZ} = 0$

$\chi_{ZXZ} = 0$

$\chi_{ZZX} = 0$

$\chi_{ZXX} = \beta_{caa}\cos\tau\cos^2\chi$

$\chi_{XZX} = \beta_{caa}\cos\tau\cos^2\chi$

$\chi_{XXZ} = 0$

$\chi_{ZZZ} = 0$

(spp) $\chi_{YXX} = 2\beta_{caa}\sin\tau\sin^2\chi\cos\chi$

$\chi_{YZZ} = 0$

$\chi_{YZX} = -\beta_{caa}\cos\tau\sin\chi\cos\chi$

$\chi_{YXZ} = 0$

(ssp) $\chi_{YYX} = 2\beta_{caa}\sin\tau\sin\chi\cos^2\chi$

$\chi_{YYZ} = 0$

(psp) $\chi_{XYX} = 2\beta_{caa}\sin\tau\sin^2\chi\cos\chi$

$\chi_{ZYZ} = 0$

$\chi_{XYZ} = 0$

$\chi_{ZYX} = -\beta_{caa}\cos\tau\sin\chi\cos\chi$

(sps) $\chi_{YXY} = 2\beta_{caa}\sin\tau\sin\chi\cos^2\chi$

$\chi_{YZY} = \beta_{caa}\cos\tau\sin^2\chi$

(pps) $\chi_{XXY} = 2\beta_{caa}\sin\tau\sin^2\chi\cos\chi$

$\chi_{ZZY} = 0$

$\chi_{ZXY} = -\beta_{caa}\cos\tau\sin\chi\cos\chi$

$\chi_{XZY} = -\beta_{caa}\cos\tau\sin\chi\cos\chi$

(pss) $\chi_{XYY} = 2\beta_{caa}\sin\tau\sin\chi\cos^2\chi$

$\chi_{ZYY} = \beta_{caa}\cos\tau\sin^2\chi$

(sss) $\chi_{YYY} = -2\beta_{caa}\sin\tau\sin^2\chi\cos\chi$ (6a-2)

(3-8) **式を使うと、**

［**対称伸縮振動**］

(ppp) $\chi_{XXX} = -(4\sqrt{2}/27)\{[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau - 9\beta_{\eta\eta\zeta}]\sin\tau\sin^3\chi + (8\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\sin\tau\sin\chi\cos^2\chi\}$

$\chi_{XZZ} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin\tau\cos^2\tau\sin\chi$

$\chi_{ZXZ} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin\tau\cos^2\tau\sin\chi$

$\chi_{ZZX} = (4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin\tau\cos^2\tau - (\beta_{\xi\xi\zeta} + 8\beta_{\zeta\zeta\zeta})\sin\tau]\sin\chi$

$\chi_{ZXX} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\sin^2\chi$

$\chi_{XZX} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\sin^2\chi$

$\chi_{XXZ} = -(4\sqrt{2}/27)\{[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\cos^2\tau - (\beta_{\xi\xi\zeta} + 8\beta_{\zeta\zeta\zeta})]\cos\tau\sin^2\chi$

$+ (8\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\cos\tau\cos^2\chi\}$

$\chi_{ZZZ} = (4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\cos^2\tau + 9\beta_{\eta\eta\zeta}]\cos\tau$

(spp) $\chi_{YXX} = -(4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau - (8\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})]\sin\tau\sin^2\chi\cos\chi$

$\chi_{YZZ} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin\tau\cos^2\tau\cos\chi$

$\chi_{YZX} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\sin\chi\cos\chi$

$\chi_{YXZ} = -(4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\cos^2\tau + (8\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})]\cos\tau\sin\chi\cos\chi$

(ssp) $\chi_{YYX} = -(4\sqrt{2}/27)\{[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau + (8\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})]\sin\tau\sin\chi\cos^2\chi$

$+ (8\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\sin\tau\sin\chi\}$

$\chi_{YYZ} = -(4\sqrt{2}/27)\{[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\cos^2\tau - (\beta_{\xi\xi\zeta} + 8\beta_{\zeta\zeta\zeta})]\cos\tau\sin^2\chi - (8\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\cos\tau\cos^2\chi\}$

(psp) $\chi_{XYX} = -(4\sqrt{2}/27)\{[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau - (8\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})]\sin\tau\sin\chi\cos^2\chi$

$\chi_{ZYZ} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin\tau\cos^2\tau\cos\chi$

$\chi_{XYZ} = -(4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\cos^2\tau + (8\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})]\cos\tau\sin\chi\cos\chi$

$\chi_{ZYX} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\sin\chi\cos\chi$

(sps) $\chi_{YXY} = -(4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau - (8\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})]\sin\tau\sin\chi\cos^2\chi$

$\chi_{YZY} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\cos^2\chi$

(pps) $\chi_{XXY} = -(4\sqrt{2}/27)\{[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau - (8\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})]\sin\tau\sin^2\chi\cos\chi$

$+ (8\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\sin\tau\cos\chi\}$

$\chi_{ZZY} = (4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta}) - (\beta_{\xi\xi\zeta} + 8\beta_{\zeta\zeta\zeta})]\sin\tau\cos\chi$

$\chi_{ZXY} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\sin\chi\cos\chi$

$\chi_{XZY} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\sin\chi\cos\chi$

(pss) $\chi_{XYY} = -(4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau - (8\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})]\sin\tau\sin\chi\cos^2\chi$

$\chi_{ZYY} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\cos^2\chi$

(sss) $\chi_{YYY} = -(4\sqrt{2}/27)\{[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2\tau + 9\beta_{\eta\eta\zeta}]\sin\tau\cos^3\chi + (8\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\sin\tau\sin^2\chi\cos\chi\}$

(6a-3)

［**逆対称伸縮振動**］

(ppp) $\chi_{XXX} = 0$

$\chi_{XZZ} = 0$

$\chi_{ZXZ} = 0$

$\chi_{ZZX} = 0$

$\chi_{ZXX} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\cos^2\chi$

$\chi_{XZX} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\cos^2\chi$

$\chi_{XXZ} = 0$
$\chi_{ZZZ} = 0$

(spp) $\chi_{YXX} = -(8\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin^2\chi\cos\chi$
$\chi_{YZZ} = 0$
$\chi_{YZX} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sin\chi\cos\chi$
$\chi_{YXZ} = 0$
(ssp) $\chi_{YYX} = -(8\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin\chi\cos^2\chi$
$\chi_{YYZ} = 0$
(psp) $\chi_{XYX} = -(8\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin^2\chi\cos\chi$
$\chi_{ZYZ} = 0$
$\chi_{XYZ} = 0$
$\chi_{ZYX} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sin\chi\cos\chi$
(sps) $\chi_{YXY} = -(8\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin\chi\cos^2\chi$
$\chi_{YZY} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sin^2\chi$
(pps) $\chi_{XXY} = -(8\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin^2\chi\cos\chi$
$\chi_{ZZY} = 0$
$\chi_{ZXY} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sin\chi\cos\chi$
$\chi_{XZY} = (4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sin\chi\cos\chi$
(pss) $\chi_{XYY} = -(6\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin\chi\cos^2\chi$
$\chi_{ZYY} = -(4\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sin^2\chi$
(sss) $\chi_{YYY} = (8\sqrt{2}/27)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin^2\chi\cos\chi$ (6a-4)

6b. ねじれ形 HCCH 基

［対称伸縮振動］

(ppp) $\chi_{XXZ} = \beta_{aac}\cos^2\chi + \beta_{bbc}\sin^2\chi + 2\beta_{abc}\sin\chi\cos\chi$
$\chi_{ZZZ} = \beta_{ccc}$
(spp) $\chi_{YXZ} = -(\beta_{aac} - \beta_{bbc})\sin\chi\cos\chi + \beta_{abc}(\cos^2\chi - \sin^2\chi)$
(ssp) $\chi_{YYZ} = \beta_{aac}\sin^2\chi + \beta_{bbc}\cos^2\chi - 2\beta_{abc}\sin\chi\cos\chi$
(psp) $\chi_{XYZ} = -(\beta_{aac} - \beta_{bbc})\sin\chi\cos\chi + \beta_{abc}(\cos^2\chi - \sin^2\chi)$
(sps) none
(pps) none
(pss) none
(sss) none (6b-1)

［逆対称伸縮振動］

(ppp) $\chi_{ZXX} = \beta_{caa}\cos^2\chi + \beta_{cbb}\sin^2\chi + (\beta_{cab} + \beta_{bca})\sin\chi\cos\chi$
$\chi_{XZX} = \beta_{caa}\cos^2\chi + \beta_{cbb}\sin^2\chi + (\beta_{cab} + \beta_{bca})\sin\chi\cos\chi$
(spp) $\chi_{YZX} = -(\beta_{caa} - \beta_{cbb})\sin\chi\cos\chi + (\beta_{bca}\cos^2\chi - \beta_{cab}\sin^2\chi)$
(ssp) none
(psp) $\chi_{ZYX} = -(\beta_{caa} - \beta_{cbb})\sin\chi\cos\chi + (\beta_{bca}\cos^2\chi - \beta_{cab}\sin^2\chi)$

(sps) $\chi_{YZY} = \beta_{caa}\sin^2\chi + \beta_{cbb}\cos^2\chi - (\beta_{cab} + \beta_{bca})\sin\chi\cos\chi$

(pps) $\chi_{ZXY} = -(\beta_{caa} - \beta_{cbb})\sin\chi\cos\chi + (\beta_{bca}\cos^2\chi - \beta_{cab}\sin^2\chi)$

$\chi_{XZY} = -(\beta_{caa} - \beta_{cbb})\sin\chi\cos\chi + (\beta_{bca}\cos^2\chi - \beta_{cab}\sin^2\chi)$

(pss) $\chi_{ZYY} = \beta_{caa}\sin^2\chi + \beta_{cbb}\cos^2\chi - (\beta_{cab} + \beta_{bca})\sin\chi\cos\chi$

(sss) $\chi_{YYY} = 0$ (6b-2)

(3-16) 式 ～ (3-18) 式を使うと、

［対称伸縮振動］

(ppp) $\chi_{XXZ} = (4\sqrt{2}/27)\{(8\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta})\cos^2\chi + [(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2) + 9\beta_{\eta\eta\zeta}]\sin^2\chi$
$- 4\sqrt{2}\ (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin(\tau/2)\sin\chi\cos\chi\}\cos(\tau/2)$

$\chi_{ZZZ} = (4\sqrt{2}/27)[(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\cos^2(\tau/2) + 9\beta_{\eta\eta\zeta}]\cos(\tau/2)$

(spp) $\chi_{YXZ} = -(4\sqrt{2}/27)\{[(8\beta_{\xi\xi\zeta} - 8\beta_{\eta\eta\zeta}) - (\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2)]\sin\chi\cos\chi$
$- 2\sqrt{2}\ (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin(\tau/2)(\cos^2\chi - \sin^2\chi)\}\cos(\tau/2)$

(ssp) $\chi_{YYZ} = (4\sqrt{2}/27)\{(8\beta_{\xi\xi\zeta} + \beta_{\eta\eta\zeta})\sin^2\chi + [(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2) + 9\beta_{\eta\eta\zeta}]\cos^2\chi$
$+4\sqrt{2}\ (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin(\tau/2)\sin\chi\cos\chi\}\cos(\tau/2)$

(psp) $\chi_{XYZ} = -(4\sqrt{2}/27)\{[(8\beta_{\xi\xi\zeta} - 8\beta_{\eta\eta\zeta}) - (\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2)]\sin\chi\cos\chi$
$- 2\sqrt{2}\ (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin(\tau/2)(\cos^2\chi - \sin^2\chi)\}\cos(\tau/2)$

(sps) none

(pps) none

(pss) none

(sss) none (6b-3)

［逆対称伸縮振動］

(ppp) $\chi_{ZXX} = (4\sqrt{2}/27)\{-(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos^2\chi + (\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2)\sin^2\chi$
$+ [(\sqrt{2}/4)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin(\tau/2) + \sqrt{2}\ (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})]\sin\chi\cos\chi\}\cos(\tau/2)$

$\chi_{XZX} = (4\sqrt{2}/27)\{-(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos^2\chi + (\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2)\sin^2\chi$
$+ [(\sqrt{2}/4)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin(\tau/2) + \sqrt{2}\ (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})]\sin\chi\cos\chi\}\cos(\tau/2)$

(spp) $\chi_{YZX} = (4\sqrt{2}/27)\{[(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})+(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2)]\sin\chi\cos\chi$
$- [(\sqrt{2}/4)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin(\tau/2)\cos^2\chi - \sqrt{2}\ (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin^2\chi]\}\cos(\tau/2)$

(ssp) none

(psp) $\chi_{ZYX} = (4\sqrt{2}/27)\{[(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})+(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2)]\sin\chi\cos\chi$
$- [(\sqrt{2}/4)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin(\tau/2)\cos^2\chi - \sqrt{2}\ (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin^2\chi]\}\cos(\tau/2)$

(sps) $\chi_{YZY} = (4\sqrt{2}/27)\{-(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin^2\chi + (\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2)\cos^2\chi$
$- [(\sqrt{2}/4)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin(\tau/2) + \sqrt{2}\ (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})]\sin\chi\cos\chi\}\cos(\tau/2)$

(pps) $\chi_{ZXY} = (4\sqrt{2}/27)\{[(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})+(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2)]\sin\chi\cos\chi$
$- [(\sqrt{2}/4)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin(\tau/2)\cos^2\chi - \sqrt{2}\ (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin^2\chi]\}\cos(\tau/2)$

$\chi_{XZY} = (4\sqrt{2}/27)\{[(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})+(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2)]\sin\chi\cos\chi$
$- [(\sqrt{2}/4)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin(\tau/2)\cos^2\chi - \sqrt{2}\ (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin^2\chi]\}\cos(\tau/2)$

(pss) $\chi_{ZYY} = (4\sqrt{2}/27)\{-(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin^2\chi + (\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin^2(\tau/2)\cos^2\chi$
$- [(\sqrt{2}/4)(\beta_{\xi\xi\zeta} - 9\beta_{\eta\eta\zeta} + 8\beta_{\zeta\zeta\zeta})\sin(\tau/2) + \sqrt{2}\ (\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})]\sin\chi\cos\chi\}\cos(\tau/2)$

(sss) none (6b-4)

6c. のけぞった CH_2 基

分子固定座標で表したものは (6a-1) **式および** (6a-2) **式と同じ方式になる。**CH **固定テンソルで近似する段階で違いが出る。**

［**対称伸縮振動**］

(ppp) $\chi_{XXX} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau - \beta_{bbc}]\sin\tau\sin^3\chi - \beta_{aac}\sin\tau\sin\chi\cos^2\chi$

$\chi_{XZZ} = (\beta_{bbc} - \beta_{ccc})\sin\tau\cos^2\tau\sin\chi$

$\chi_{ZXZ} = (\beta_{bbc} - \beta_{ccc})\sin\tau\cos^2\tau\sin\chi$

$\chi_{ZZX} = -[(\beta_{bbc} - \beta_{ccc})\sin\tau\cos^2\tau + \beta_{ccc}\sin\tau]\sin\chi$

$\chi_{ZXX} = -(\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\sin^2\chi$

$\chi_{XZX} = -(\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\sin^2\chi$

$\chi_{XXZ} = [(\beta_{bbc} - \beta_{ccc})\cos^2\tau + \beta_{ccc}]\cos\tau\sin^2\chi + \beta_{aac}\cos\tau\cos^2\chi$

$\chi_{ZZZ} = -[(\beta_{bbc} - \beta_{ccc})\cos^2\tau - \beta_{bbc}]\cos\tau$

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

$\chi_{YZZ} = (\beta_{bbc} - \beta_{ccc})\sin\tau\cos^2\tau\cos\chi$

$\chi_{YZX} = (\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\sin\chi\cos\chi$

$\chi_{YXZ} = [(\beta_{bbc} - \beta_{ccc})\cos^2\tau - (\beta_{aac} - \beta_{ccc})]\cos\tau\sin\chi\cos\chi$

(ssp) $\chi_{YYX} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau + (\beta_{aac} - \beta_{bbc})]\sin\tau\sin\chi\cos^2\chi - \beta_{aac}\sin\tau\sin\chi$

$\chi_{YYZ} = [(\beta_{bbc} - \beta_{ccc})\cos^2\tau + \beta_{ccc}]\cos\tau\sin^2\chi + \beta_{aac}\cos\tau\cos^2\chi$

(psp) $\chi_{XYX} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau + (\beta_{aac} - \beta_{bbc})]\sin\tau\sin^2\chi\cos\chi$

$\chi_{ZYZ} = (\beta_{bbc} - \beta_{ccc})\sin\tau\cos^2\tau\cos\chi$

$\chi_{XYZ} = [(\beta_{bbc} - \beta_{ccc})\cos^2\tau - (\beta_{aac} - \beta_{bbc})]\cos\tau\sin\chi\cos\chi$

$\chi_{ZYX} = (\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\sin\chi\cos\chi$

(sps) $\chi_{YXY} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau + (\beta_{aac} - \beta_{bbc})]\sin\tau\sin\chi\cos^2\chi$

$\chi_{YZY} = -(\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\cos^2\chi$

(pps) $\chi_{XXY} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau + (\beta_{aac} - \beta_{bbc})]\sin\tau\sin^2\chi\cos\chi - \beta_{aac}\sin\tau\cos\chi$

$\chi_{ZZY} = -[(\beta_{bbc} - \beta_{ccc})\sin^2\tau + \beta_{ccc}]\sin\tau\cos\chi$

$\chi_{ZXY} = -(\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\sin\chi\cos\chi$

$\chi_{XZY} = -(\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\sin\chi\cos\chi$

(pss) $\chi_{XYY} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau + (\beta_{aac} - \beta_{bbc})]\sin\tau\sin\chi\cos^2\chi$

$\chi_{ZYY} = -(\beta_{bbc} - \beta_{ccc})\sin^2\tau\cos\tau\cos^2\chi$

(sss) $\chi_{YYY} = [(\beta_{bbc} - \beta_{ccc})\sin^2\tau - \beta_{bbc})]\sin\tau\cos^3\chi - \beta_{aac}\sin\tau\sin^2\chi\cos\chi$ (6c-1)

［**逆対称伸縮振動**］

(ppp) $\chi_{XXX} = 0$

$\chi_{XZZ} = 0$

$\chi_{ZXZ} = 0$

$\chi_{ZZX} = 0$

$\chi_{ZXX} = \beta_{caa}\cos\tau\cos^2\chi$

$\chi_{XZX} = \beta_{caa}\cos\tau\cos^2\chi$

$\chi_{XXZ} = 0$

$\chi_{ZZZ} = 0$

(spp) $\chi_{YXX} = 2\beta_{caa}\sin\tau\sin^2\chi\cos\chi$

$\chi_{YZZ} = 0$

$\chi_{YZX} = -\beta_{caa}\cos\tau\sin\chi\cos\chi$

$\chi_{YXZ} = 0$

(ssp) $\chi_{YYX} = 2\beta_{caa}\sin\tau\sin\chi\cos^2\chi$

$\chi_{YYZ} = 0$

(psp) $\chi_{XYX} = 2\beta_{caa}\sin\tau\sin^2\chi\cos\chi$

$\chi_{ZYZ} = 0$

$\chi_{XYZ} = 0$

$\chi_{ZYX} = -\beta_{caa}\cos\tau\sin\chi\cos\chi$

(sps) $\chi_{YXY} = 2\beta_{caa}\sin\tau\sin\chi\cos^2\chi$

$\chi_{YZY} = \beta_{caa}\cos\tau\sin^2\chi$

(pps) $\chi_{XXY} = 2\beta_{caa}\sin\tau\sin^2\chi\cos\chi$

$\chi_{ZZY} = 0$

$\chi_{ZXY} = -\beta_{caa}\cos\tau\sin\chi\cos\chi$

$\chi_{XZY} = -\beta_{caa}\cos\tau\sin\chi\cos\chi$

(pss) $\chi_{XYY} = 2\beta_{caa}\sin\tau\sin\chi\cos^2\chi$

$\chi_{ZYY} = \beta_{caa}\cos\tau\sin^2\chi$

(sss) $\chi_{YYY} = -2\beta_{caa}\sin\tau\sin^2\chi\cos\chi$ (6c-2)

(3-4) **式と** (3-5) **式を使うと、**

［**対称伸縮振動**］

(ppp) $\chi_{XXX} = (2\sqrt{3}/9)\{[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau - 3\beta_{\eta\eta\zeta}]\sin\tau\sin^3\chi - (\beta_{\xi\xi\zeta} + 2\beta_{\zeta\zeta\zeta})\sin\tau\sin\chi\cos^2\chi\}$

$\chi_{XZZ} = (2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin\tau\cos^2\tau\sin\chi$

$\chi_{ZXZ} = (2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin\tau\cos^2\tau\sin\chi$

$\chi_{ZZX} = -(2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin\tau\cos^2\tau + (2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})\sin\tau$

$\chi_{ZXX} = -(2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\sin^2\chi$

$\chi_{XZX} = -(2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\sin^2\chi$

$\chi_{XXZ} = (2\sqrt{3}/9)\{[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\cos^2\tau + (2\beta_{\xi\xi\zeta} + \beta_{\zeta\zeta\zeta})]\cos\tau\sin^2\chi + (\beta_{\xi\xi\zeta} + 2\beta_{\zeta\zeta\zeta})\cos\tau\cos^2\chi\}$

$\chi_{ZZZ} = -(2\sqrt{3}/9)[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\cos^2\tau - 3\beta_{\eta\eta\zeta}]\cos\tau$

(spp) $\chi_{YXX} = (2\sqrt{3}/9)[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau + (\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})]\sin\tau\sin^2\chi\cos\chi$

$\chi_{YZZ} = (2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin\tau\cos^2\tau\cos\chi$

$\chi_{YZX} = (2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\sin\chi\cos\chi$

$\chi_{YXZ} = (2\sqrt{3}/9)[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\cos^2\tau + (\beta_{\xi\xi\zeta} - 3\beta_{\zeta\zeta\zeta})]\cos\tau\sin\chi\cos\chi$

(ssp) $\chi_{YYX} = (2\sqrt{3}/9)\{[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau + (\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})]\sin\tau\sin\chi\cos^2\chi$

$- (\beta_{\xi\xi\zeta} + 2\beta_{\zeta\zeta\zeta})\sin\tau\sin\chi\}$

$\chi_{YYZ} = (2\sqrt{3}/9)[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\cos^2\tau + (2\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})]\cos\tau\sin^2\chi + (\beta_{\xi\xi\zeta} + 2\beta_{\zeta\zeta\zeta})_c\cos\tau\cos^2\chi\}$

(psp) $\chi_{XYX} = (2\sqrt{3}/9)[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau + (\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})]\sin\tau\sin^2\chi\cos\chi$

$\chi_{ZYZ} = (2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin\tau\cos^2\tau\cos\chi$

$$\chi_{XYZ} = (2\sqrt{3}/9)[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\cos^2\tau - (\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})]\cos\tau\sin\chi\cos\chi$$

$$\chi_{ZYX} = (2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\sin\chi\cos\chi$$

(sps) $$\chi_{YXY} = (2\sqrt{3}/9)[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau + (\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})]\sin\tau\sin\chi\cos^2\chi$$

$$\chi_{YZY} = -(2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\cos^2\chi$$

(pps) $$\chi_{XXY} = (2\sqrt{3}/9)[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau + (\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})]\sin\tau\sin^2\chi\cos\chi - (\beta_{\xi\xi\zeta} + 2\beta_{\zeta\zeta\zeta})\sin\tau\cos\chi\}$$

$$\chi_{ZZY} = -(2\sqrt{3}/9)[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau + (2\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})]\sin\tau\cos\chi$$

$$\chi_{ZXY} = -(2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\sin\chi\cos\chi$$

$$\chi_{XZY} = -(2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\sin\chi\cos\chi$$

(pss) $$\chi_{XYY} = (2\sqrt{3}/9)[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau + (\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + 2\beta_{\zeta\zeta\zeta})]\sin\tau\sin\chi\cos^2\chi$$

$$\chi_{ZYY} = -(2\sqrt{3}/9)(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau\cos\tau\cos^2\chi$$

(sss) $$\chi_{YYY} = (2\sqrt{3}/9)\{[(2\beta_{\xi\xi\zeta} - 3\beta_{\eta\eta\zeta} + \beta_{\zeta\zeta\zeta})\sin^2\tau - 3\beta_{\eta\eta\zeta}]\sin\tau\cos^3\chi - [(\beta_{\xi\xi\zeta} + 2\beta_{\zeta\zeta\zeta})\sin\tau\sin^2\chi\cos\chi\}$$

(6c-3)

［逆対称伸縮振動］

(ppp) $$\chi_{XXX} = 0$$

$$\chi_{XZZ} = 0$$

$$\chi_{ZXZ} = 0$$

$$\chi_{ZZX} = 0$$

$$\chi_{ZXX} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\cos^2\chi$$

$$\chi_{XZX} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\cos^2\chi$$

$$\chi_{XXZ} = 0$$

$$\chi_{ZZZ} = 0$$

(spp) $$\chi_{YXX} = -(8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin^2\chi\cos\chi$$

$$\chi_{YZZ} = 0$$

$$\chi_{YZX} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sin\chi\cos\chi$$

$$\chi_{YXZ} = 0$$

(ssp) $$\chi_{YYX} = -(8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin\chi\cos^2\chi$$

$$\chi_{YYZ} = 0$$

(psp) $$\chi_{XYX} = -(8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin^2\chi\cos\chi$$

$$\chi_{ZYZ} = 0$$

$$\chi_{XYZ} = 0$$

$$\chi_{ZYX} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sin\chi\cos\chi$$

(sps) $$\chi_{YXY} = -(8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin\chi\cos^2\chi$$

$$\chi_{YZY} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sin^2\chi$$

(pps) $$\chi_{XXY} = -(8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin^2\chi\cos\chi$$

$$\chi_{ZZY} = 0$$

$$\chi_{ZXY} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sin\chi\cos\chi$$

$$\chi_{XZY} = (4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sin\chi\cos\chi$$

(pss) $$\chi_{XYY} = -(8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin\chi\cos^2\chi$$

$$\chi_{ZYY} = -(4\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\cos\tau\sin^2\chi$$

(sss) $\chi_{YYY} = (8\sqrt{3}/9)(\beta_{\xi\xi\zeta} - \beta_{\zeta\zeta\zeta})\sin\tau\sin^2\chi\cos\chi$ (6c-4)

6d. z 軸まわりにねじれてからうしろにのけぞった CH_2 基

未着手である。

付録 A C(100) 面の dihydride および monohydride pair の SFG テンソル

分子固定 (abc) **系がオイラー角** (χ,θ,ϕ) **によって空間固定** (XYZ) **系に重なるものとして、**(XYZ) **系でのテンソル成分を求めると下のようになる。**

CH_2 基および平面 HCCH 基 (C_{2v} 対称)

［**対称伸縮振動**］

(ppp)

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

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

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

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

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

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

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

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

(spp)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

［逆対称伸縮振動］

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

ねじれ HCCH 基（C_2 対称）

［**対称伸縮振動**］

(ppp) $\chi_{XXX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$

$+ (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(3\cos\chi + \cos3\chi)$

$+ (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\cos2\phi$

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

$+ (1/4)\beta_{abc}\{[\sin\theta(\cos\chi - \cos3\chi) - (\sin\theta - \sin^3\theta)(3\cos\chi + \cos3\chi)]\sin2\phi$

$- 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\cos2\phi\}$

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

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

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

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

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

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

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

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

$- (1/2)(\beta_{aac} - \beta_{bbc})\cos\chi\sin^3\theta\cos2\phi$

$- \beta_{abc}(2\sin\theta - \sin^3\theta)\cos\chi\sin2\phi$

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

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

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

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

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

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

$\chi_{XXZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$

$- (1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 + \cos2\chi)$

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

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

$\chi_{ZZZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$

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

$+ (1/2)(\beta_{aac} - \beta_{bbc})(\cos\theta - \cos^3\theta)\cos2\phi$

$+ \beta_{abc}(\cos\theta - \cos^3\theta)\sin2\phi$

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

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

$+ (1/2)\beta_{abc}[2(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\sin2\phi - \sin\theta\cos\theta(\cos\chi + \cos3\chi)\cos2\phi]$

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

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

$- \beta_{abc}[(\sin\theta - \sin^3\theta)\sin\chi\sin2\phi - \sin\theta\cos\theta\cos\chi\cos2\phi]$

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

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

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

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

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

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

(ssp) $\chi_{YYX} = -(1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\cos\chi$

$+ (1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\cos\chi - \cos3\chi)$

$+ (1/8)(\beta_{aac} - \beta_{bbc})\{[\sin\theta(3\cos\chi + \cos3\chi) - (\sin\theta - \sin^3\theta)(\cos\chi - \cos3\chi)]\cos2\phi$

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

$+ (1/4)\beta_{abc}\{[4 \sin\theta\cos\chi - (2\sin\theta - \sin^3\theta)]\sin2\phi + 2\sin\theta\cos\theta(\sin\chi + \sin3\chi)\cos2\phi\}$

$\chi_{YYZ} = (1/2)(\beta_{aac} + \beta_{bbc})\cos\theta$

$-(1/4)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})(\cos\theta - \cos^3\theta)(1 - \cos2\chi)$

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

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

(psp) $\chi_{XYX} = -(1/8)(\beta_{aac} + \beta_{bbc} - 2\beta_{ccc})\sin^3\theta(\sin\chi + \sin3\chi)$

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

$+ (1/4)\beta_{abc}[(2\sin\theta - \sin^3\theta)(\sin\chi + \sin3\chi)\sin2\phi - 2\sin\theta\cos\theta(\cos\chi + \cos3\chi)\cos2\phi$

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

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

$- \beta_{abc}[(\sin\theta - \sin^3\theta)\sin\chi\sin2\phi - \sin\theta\cos\theta\cos\chi\cos2\phi]$

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

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

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

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

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

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

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

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

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

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

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

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

(pps) $\chi_{XXY} = (1/2)(\beta_{aac} + \beta_{bbc})\sin\theta\sin\chi$

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

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

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

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

(pss)

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

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

(sss)

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

［逆対称伸縮振動］

(ppp)

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

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

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

$+ (\beta_{bca} - \beta_{cab})\sin\theta\cos\theta\sin\chi\}$

$\chi_{ZZX} = (\beta_{caa} + \beta_{cbb})(\sin\theta - \sin^3\theta)\cos\chi$

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

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

$- (\beta_{bca} - \beta_{cab})\sin\theta\cos\theta\sin\chi\sin 2\phi$

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

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

$- (\beta_{bca} + \beta_{cab})[2(\cos\theta - \cos^3\theta) - \cos^3\theta\cos 2\chi]\sin 2\phi + (1 - 3\cos^2\theta)\cos 2\phi\sin 2\chi]$

$+ (\beta_{bca} - \beta_{cab})\sin^2\theta\sin 2\chi\}$

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

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

$- (\beta_{bca} + \beta_{cab})[2(\cos\theta - \cos^3\theta) - \cos^3\theta\cos 2\chi]\sin 2\phi + (1 - 3\cos^2\theta)\cos 2\phi\sin 2\chi]$

$+ (\beta_{bca} - \beta_{cab})\sin^2\theta\sin 2\chi\}$

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

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

$+ (\beta_{bca} + \beta_{cab})[(\cos\theta - \cos^3\theta)(1 + \cos 2\chi)\sin 2\phi + \sin^2\theta\sin 2\chi\cos 2\phi]$

$+ (\beta_{bca} - \beta_{cab})\sin^2\theta\sin 2\chi\}$

$\chi_{ZZZ} = (\beta_{caa} + \beta_{cbb})(\cos\theta - \cos^3\theta)$

$+ (\beta_{caa} - \beta_{cbb})(\cos\theta - \cos^3\theta)\cos 2\phi$

$+ (\beta_{bca} + \beta_{cab})(\cos\theta - \cos^3\theta)\sin 2\phi$

(spp) $\chi_{YXX} = (1/4)\{(\beta_{caa} + \beta_{cbb})[2\sin\theta\sin\chi - \sin^3\theta(\sin\chi + \sin 3\chi)]$

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

$- (\beta_{bca} + \beta_{cab})[\sin\theta(\sin\chi - \sin 3\chi)\sin 2\phi + 2\sin\theta\cos\theta\cos 3\chi\cos 2\phi]$

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

$\chi_{YZZ} = -(1/2)\{(\beta_{caa} + \beta_{cbb})(\sin\theta - 2\sin^3\theta)\sin\chi$

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

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

$- (\beta_{bca} - \beta_{cab})\sin\theta\cos\theta\cos\chi\}$

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

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

$+ (\beta_{bca} + \beta_{cab})[2\cos^3\theta\ \cos 2\phi in 2\chi\cos 2\phi - \sin^2\theta(1 - \cos 2\chi) + 2\cos^2\theta]$

$+ (\beta_{bca} - \beta_{cab})[\sin^2\theta(1 - \cos 2\chi) + 2\cos^2\theta\cos 2\chi]\cos 2\phi\}$

$\chi_{YXZ} = (1/2)\{(\beta_{caa} + \beta_{cbb})(\cos\theta - \cos^3\theta)\sin 2\chi$

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

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

$- (\beta_{bca} - \beta_{cab})\sin^2\theta\cos 2\chi\}$

(ssp) $\chi_{YYX} = (1/4)\{(\beta_{caa} + \beta_{cbb})\sin^3\theta(\cos\chi - \cos 3\chi)$

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

$- (\beta_{bca} + \beta_{cab})(2\sin\theta - \sin^3\theta)(\cos\chi - \cos 3\chi)\sin 2\phi$

$+ (\beta_{bca} - \beta_{cab})[2\sin 2\theta(\sin\chi + \sin 3\chi)\cos 2\phi]\}$

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

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

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

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

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

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

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