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One ~~[illegible]~~ example for $\chi^{(2)}$:

KDP = tetragonal

point group $D_{2d} = \bar{4}2m$ $\qquad$ β-BBO = C_{3v}

$AgGaSe_2$ or $AgGaS_2$ $\qquad$ Quartz = D_3

$$S_4 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad C_2 = \begin{pmatrix} -1 & & \emptyset \\ & -1 & \\ \emptyset & & 1 \end{pmatrix} \qquad \sigma_d = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

examine C_2: 111 → −111 = 0; 222 → −222 = 0; 333 → 333 $\quad$ 112, 212 etc. $\quad$ even 1, 2. needed any 3: 113 → 113, 223 → 223 $\quad$ 123 + all permutations

examine S_4: 113 → −223 ⇒ 113 + 223 = 0

123 → 213 $\quad$ (2 × −1)
312 → 321 $\quad$ (1 × −1)
~~213 → 123~~ $\quad$ (2 × −1)
132 → 231

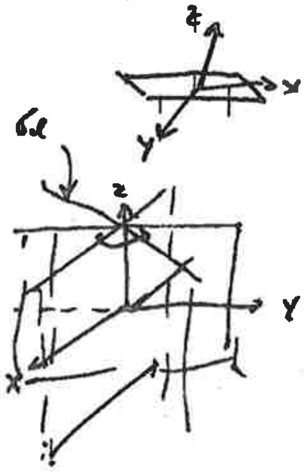
113 =

Thus:

$$\boxed{\begin{aligned} xyz &= yxz \\ zxy &= zyx \\ xzy &= yzx \end{aligned}}$$

Tetragonal C_{4v} is often taken as a model for an

~~An~~ isotropic surface:



~~Cyl.~~: C_{4v}: C_2 C_4 σ_v σ_d

rotations 90°; 180°

$$C_2 = \begin{pmatrix} -1 & & \emptyset \\ & -1 & \\ \emptyset & & 1 \end{pmatrix}$$

diagonal 333
+ odd × ~~223~~
appearance of 1, 2

$$C_4 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

333 $\qquad$ zzz
113 = 223 $\qquad$ xxz = yyz
131 = 232 $\qquad$ xzx = yzy
322 = 311 $\qquad$ zxx = zyy

113 → 223
123 → −213
223 → 113

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KDP

$$D(C_2) = \begin{pmatrix} -1 & & 0 \\ & -1 & \\ 0 & & 1 \end{pmatrix}$$

even numbers of (1,2) are necessary:

$\left\{ \begin{array}{l} 113,\ 223 + \text{permutations} \\ 123,\ 132 + \text{permutations} \\ 333 \end{array} \right.$

$$D(\sigma_d) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

does not limit C_2 more than S_4 already did

$123 \to 213$

$$D(S_{4z}) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$113 \longrightarrow -223$

$123 \longrightarrow 213$

$312 \longrightarrow 321$

$132 \longrightarrow 231$

this limits the selection done by $C_2(z)$ – we cross them out

$\left\{ \begin{array}{l} \cancel{113},\ \cancel{223} + \cancel{\text{permutations}} \\ 123,\ 132 + \text{permutations} \\ \cancel{333} \end{array} \right.$

$\Rightarrow$ final result for KDP

$$\boxed{\begin{array}{l} xyz = yxz \\ zxy = zyx \\ xzy = yzx \end{array}}$$

Another way of solving it:

$\chi_{123}, \chi_{213}, \chi_{312}, \chi_{321}, \chi_{132}, \chi_{213}$ are non-zero because we need a combination of xyz that gives +1 when multiplying the matrix elements in $D(S_4), D(C_2), D(\sigma_d)$

e.g. $\chi^{(2)}_{123} = D_{12}\, D_{21}\, D_{33}\, \chi^{(2)}_{213}$

$-1 \quad +1 \quad -1 \quad (S_4)$

$+1 \quad +1 \quad +1 \quad (\sigma_d)$