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Molecular Vibrations in Nonsymmorphic Crystals

II. Symmetry Coordinates for $P2_1/b$ $(C_{2h}{}^5)$

O. S. BORGEN, D. FREMSTAD, B. MESTVEDT and Ø. RA

Institute of Physical Chemistry, The Technical University of Norway, N-7034 Trondheim, Norway

$P2_1/b$ symmetry coordinates are listed for every wave vector associated with symmetry elements in the Brillouin zone. Free molecule symmmetry vectors for C_{2h} cases appear as a byproduct.

This is the second paper in a series aimed at the reporting of symmetry coordinates for molecular vibrations in nonsymmorphic crystals. Using the theory of multiplier representations, the induction of irreducible representations from little groups, the properties of projection operators; and adhering to the notation laid down in a previous article [1] we devote the present one to a study of

SPACE GROUP $P2_1/b$ (C_{2h})

G forms part of the monoclinic system. G/T is $2m$ (C_{2h}), and the vector group is simple Bravais. We write for the basic vectors of the direct lattice

$$\mathbf{a}_1 = (2{}^1{}_x, 2{}^1t_y, 0);\ \mathbf{a}_2 = (0, 2{}^2t_y, 0);\ \mathbf{a}_3 = (0,0,2{}^3t_z)$$

and for the fundamental periods in wave vector space

$$\mathbf{b}_1 = \pi({}^1t_x{}^{-1},0,0);\ \mathbf{b}_2 = \pi({}^1\bar{t}_y/{}^1t_x{}^2t_y, {}^2t_y{}^{-1}, 0);\ \mathbf{b}_3 = \pi(0,0,{}^3t_z{}^{-1})$$

Furthermore,

$$G/T = \{\mathbf{S}_1, \mathbf{S}_4, \mathbf{S}_{25}, \mathbf{S}_{28}\}$$

with

$$\mathbf{S}_4 = \begin{bmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{bmatrix},\ \mathbf{S}_{25} = \begin{bmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{bmatrix},\ \mathbf{S}_{28} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}$$

and

$$\mathbf{v}(S_4) = (0,0,{}^3t_z);\ \mathbf{v}(S_{25}) = ({}^1t_x, {}^1t_y, {}^3t_z);$$
$$\mathbf{v}(S_{28}) = ({}^1t_x, {}^1t_y, 0)$$

We have one general set composed of four positions, *i.e.*

$\mathbf{R}_1^{(1)} = (x,y,z)$; $\mathbf{R}_2^{(1)} = (\bar{x},\bar{y},z + {}^3t_z)$

$\mathbf{R}_3^{(1)} = (x + {}^1t_x, y + {}^1t_y, \bar{z})$; $\mathbf{R}_4^{(1)} = (\bar{x} - {}^1t_x, \bar{y} - {}^1t_y, \bar{z} - {}^3t_z)$

and four special sets; each one made up by two sites as follows

$\mathbf{R}_1^{(2)} = (\frac{1}{2}\,{}^1\bar{t}_x, \frac{1}{2}\,{}^1\bar{t}_y, \frac{1}{2}\,{}^3\bar{t}_z)$; $\mathbf{R}_2^{(2)} = (\frac{1}{2}\,{}^1t_x, \frac{1}{2}\,{}^1t_y, \frac{1}{2}\,{}^3t_z)$

$\mathbf{R}_1^{(3)} = (\frac{1}{2}\,{}^1\bar{t}_x, {}^2t_y - \frac{1}{2}\,{}^1t_y, \frac{1}{2}\,{}^3\bar{t}_z)$; $\mathbf{R}_2^{(3)} = (\frac{1}{2}\,{}^1t_x, {}^2\bar{t}_y + \frac{1}{2}\,{}^1t_y, \frac{1}{2}\,{}^3t_z)$

$\mathbf{R}_1^{(4)} = (\frac{1}{2}\,{}^1t_x, \frac{1}{2}\,{}^1t_y, \frac{1}{2}\,{}^3\bar{t}_z)$; $\mathbf{R}_2^{(4)} = (\frac{1}{2}\,{}^1\bar{t}_x, \frac{1}{2}\,{}^1\bar{t}_y, \frac{1}{2}\,{}^3t_z)$

$\mathbf{R}_1^{(5)} = (\frac{1}{2}\,{}^1t_x, {}^2t_y + \frac{1}{2}\,{}^1t_y, \frac{1}{2}\,{}^3\bar{t}_z)$; $\mathbf{R}_2^{(4)} = (\frac{1}{2}\,{}^1\bar{t}_x, {}^2\bar{t}_y - \frac{1}{2}\,{}^1t_y, \frac{1}{2}\,{}^3t_z)$

The nonvanishing blocks of monomial supermatrices constituting reducible representations of P_k can be obtained from

$$[S_4|v(S_4)] \rightarrow \begin{cases} \mathbf{R}_1^{(1)} & \mathbf{R}_2^{(1)} & \mathbf{R}_3^{(1)} & \mathbf{R}_4^{(1)} \\ \mathbf{R}_2^{(1)} & \mathbf{R}_1^{(1)} & \mathbf{R}_4^{(1)} & \mathbf{R}_3^{(1)} \end{cases} ; \quad \begin{matrix} \mathbf{R}_1^{(r)} & \mathbf{R}_2^{(r)} \\ \mathbf{R}_2^{(r)} & \mathbf{R}_1^{(r)} \end{matrix} \quad , r \in \{2,3,4,5\}$$

$$[S_{25}|v(S_{25})] \rightarrow \begin{cases} \mathbf{R}_1^{(1)} & \mathbf{R}_2^{(1)} & \mathbf{R}_3^{(1)} & \mathbf{R}_4^{(1)} \\ \mathbf{R}_4^{(1)} & \mathbf{R}_3^{(1)} & \mathbf{R}_2^{(1)} & \mathbf{R}_1^{(1)} \end{cases} ; \quad \begin{matrix} \mathbf{R}_1^{(r)} & \mathbf{R}_2^{(r)} \\ \mathbf{R}_1^{(r)} & \mathbf{R}_2^{(r)} \end{matrix} \quad , r \in \{2,3,4,5\}$$

$$[S_{28}|v(S_{28})] \rightarrow \begin{cases} \mathbf{R}_1^{(1)} & \mathbf{R}_2^{(1)} & \mathbf{R}_3^{(1)} & \mathbf{R}_4^{(1)} \\ \mathbf{R}_3^{(1)} & \mathbf{R}_4^{(1)} & \mathbf{R}_1^{(1)} & \mathbf{R}_2^{(1)} \end{cases} ; \quad \begin{matrix} \mathbf{R}_1^{(r)} & \mathbf{R}_2^{(r)} \\ \mathbf{R}_2^{(r)} & \mathbf{R}_1^{(r)} \end{matrix} \quad , r \in \{2,3,4,5\}$$

With the preliminaries set down we study first the

Symmetry at $\mathbf{k}_7 = (0,0,0)$.

$$P_{k_7} = G_{k_7}/T = \{S_1, S_4, S_{25}, S_{28}\}$$

$$\Gamma^{(1)} = 3\hat{\tau}_1 + 3\hat{\tau}_2 + 3\hat{\tau}_3 + 3\hat{\tau}_4$$

$$\Gamma^{(r)} = 3\hat{\tau}_2 + 3\hat{\tau}_4,\ r \in \{2,3,4,5\}$$

Evidently, every $d_j^{(r)}(S_f) = 1$ in this case. Symmetry combinations are given by

${}^1\hat{\tau}_1$	${}^2\hat{\tau}_1$	${}^3\hat{\tau}_1$	${}^1\hat{\tau}_2$	${}^2\hat{\tau}_2$	${}^3\hat{\tau}_2$	${}^1\hat{\tau}_3$	${}^2\hat{\tau}_3$	${}^3\hat{\tau}_3$	${}^1\hat{\tau}_4$	${}^2\hat{\tau}_4$	${}^3\hat{\tau}_4$
$\frac{1}{2}$	0	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	0	0
0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	0
0	0	$\bar{\frac{1}{2}}$	0	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$
$\bar{\frac{1}{2}}$	0	0	$\bar{\frac{1}{2}}$	0	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	0	0
0	$\bar{\frac{1}{2}}$	0	0	$\bar{\frac{1}{2}}$	0	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	0
0	0	$\bar{\frac{1}{2}}$	0	0	$\frac{1}{2}$	0	0	$\bar{\frac{1}{2}}$	0	0	$\bar{\frac{1}{2}}$
$\frac{1}{2}$	0	0	$\bar{\frac{1}{2}}$	0	0	$\bar{\frac{1}{2}}$	0	0	$\frac{1}{2}$	0	0
0	$\frac{1}{2}$	0	0	$\bar{\frac{1}{2}}$	0	0	$\bar{\frac{1}{2}}$	0	0	$\frac{1}{2}$	0
0	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	0	0	$\bar{\frac{1}{2}}$
$\bar{\frac{1}{2}}$	0	0	$\frac{1}{2}$	0	0	$\bar{\frac{1}{2}}$	0	0	$\frac{1}{2}$	0	0
0	$\bar{\frac{1}{2}}$	0	0	$\frac{1}{2}$	0	0	$\bar{\frac{1}{2}}$	0	0	$\frac{1}{2}$	0
0	0	$\frac{1}{2}$	0	0	$\frac{1}{2}$	0	0	$\bar{\frac{1}{2}}$	0	0	$\frac{1}{2}$

$= \{\mathbf{ES}_p^{(1)}(\mathbf{k}_7)\}$, and

$$\begin{array}{cccccc} {}^1\hat{\tau}_2 & {}^2\hat{\tau}_2 & {}^3\hat{\tau}_2 & {}^1\hat{\tau}_4 & {}^2\hat{\tau}_4 & {}^3\hat{\tau}_4 \end{array}$$

$$\begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 & 0 & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & 0 & 0 & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix} = \{\mathbf{ES}_p{}^{(2)}(\mathbf{k}_7)\},$$

and

$$\{\mathbf{ES}_p{}^{(r)}(\mathbf{k}_7)\} = \{\mathbf{ES}_p{}^{(2)}(\mathbf{k}_7)\} \text{ for } r \in \{3,4,5\}$$

Symmetry at $\mathbf{k}_{13} = \frac{1}{2}\mathbf{b}_2 = \pi(\frac{1}{2}\,{}^1\bar{t}_y/{}^1t_x{}^2t_y, \frac{1}{2}\,{}^2t_y{}^{-1}, 0)$

$$P_{k_7} = \{S_1,\ S_4,\ S_{25},\ S_{28}\}$$
$$\Gamma^{(1)} = 3\hat{\tau}_1 + 3\hat{\tau}_2 + 3\hat{\tau}_3 + 3\hat{\tau}_4;$$
$$\Gamma^{(r)} = 3\hat{\tau}_2 + 3\hat{\tau}_4 \text{ for } r \in \{2,4\}$$
$$\Gamma^{(r)} = 3\hat{\tau}_1 + 3\hat{\tau}_3 \text{ for } r \in \{3,5\}$$

Here $d_j{}^{(r)}(S_f) = -1$ for $r \in \{3,5\}$; $j \in \{1,2\}$; $f \in \{25,28\}$ whereas the remaining $d_j{}^{(r)}(S_f)$'s equal unity. Furthermore, we have $\{\mathbf{ES}_p{}^{(1)}(\mathbf{k}_{13})\} = \{\mathbf{ES}_p{}^{(1)}(\mathbf{k}_7)\}$, and $\{\mathbf{ES}_p{}^{(r)}(\mathbf{k}_{13})\} = \{\mathbf{ES}_p{}^{(2)}(\mathbf{k}_7)\}$ for $r \in \{2,4\}$. For $r \in \{3,5\}$ we can still use $\{\mathbf{ES}_p{}^{(2)}(\mathbf{k}_7)\}$ on the condition that the heading is changed into

$$\begin{array}{cccccc} {}^1\hat{\tau}_1 & {}^2\hat{\tau}_1 & {}^3\hat{\tau}_1 & {}^1\hat{\tau}_3 & {}^2\hat{\tau}_3 & {}^3\hat{\tau}_3 \end{array}$$

Symmetry at $\mathbf{k}_1 = \mu_1\mathbf{b}_1 + \mu_2\mathbf{b}_2 = \pi(\mu_1{}^1t_x{}^{-1} - \mu_2{}^1t_y/{}^1t_x{}^2t_y, \mu_2{}^2t_y{}^{-1}, 0)$

$$P_{k_1} = \{S_1,\ S_{28}\}$$
$$\Gamma^{(1)} = 6\hat{\tau}_1 + 6\hat{\tau}_2;\ \Gamma^{(r)} = 3\hat{\tau}_1 + 3\hat{\tau}_2,\ r = \{2,3,4,5\}$$
$$d_1{}^{(1)} = d_4{}^{(1)} = d_1{}^{(2)} = d_2{}^{(4)} = \eta_1 = \eta_2 = \eta_4{}^* = e^{-i\pi\mu_1};$$
$$d_2{}^{(1)} = d_3{}^{(1)} = d_2{}^{(2)} = d_1{}^{(4)} = \eta_1{}^* = \eta_2{}^* = \eta_4;$$
$$d_1{}^{(3)} = \eta_3 = e^{-i\pi(\mu_1 - 2\mu_2)};\quad d_2{}^{(3)} = \eta_3{}^*;$$
$$d_1{}^{(5)} = \eta_5 = e^{i\pi(\mu_1 + 2\mu_2)};\quad d_2{}^{(5)} = \eta_5{}^*.$$

With the convention that $\sigma(r)_\pm = \{2(1 \pm Re(\eta_r))^{\frac{1}{2}}\}^{-1}$ we have

$$\begin{array}{cccccc} {}^1\hat{\tau}_1 & {}^2\hat{\tau}_1 & {}^3\hat{\tau}_1 & {}^1\hat{\tau}_2 & {}^2\hat{\tau}_2 & {}^3\hat{\tau}_2 \end{array}$$

$$\begin{bmatrix} \sigma(r)_+(1+\eta_r) & 0 & 0 & \sigma(r)_-(1-\eta_r) & 0 & 0 \\ 0 & \sigma(r)_+(1+\eta_r) & 0 & 0 & \sigma(r)_-(1-\eta_r) & 0 \\ 0 & 0 & \sigma(r)_-(1-\eta_r) & 0 & 0 & \sigma(r)_+(1+\eta_r) \\ \sigma(r)_+(1+\eta^*_r) & 0 & 0 & \sigma(r)_-(1-\eta^*_r) & 0 & 0 \\ 0 & \sigma(r)_+(1+\eta^*_r) & 0 & 0 & \sigma(r)_-(1-\eta^*_r) & 0 \\ 0 & 0 & \sigma(r)_-(1-\eta^*_r) & 0 & 0 & \sigma(r)_+(1+\eta^*_r) \end{bmatrix}$$

$$= \{\mathbf{ES}_p{}^{(r)}(\mathbf{k}_1);\ r = 2,5\}$$

and

$$
\begin{array}{cccccccccccc}
{}^{1}\hat{r}_{1} & {}^{2}\hat{r}_{1} & {}^{3}\hat{r}_{1} & {}^{4}\hat{r}_{1} & {}^{5}\hat{r}_{1} & {}^{6}\hat{r}_{1} & {}^{1}\hat{r}_{2} & {}^{2}\hat{r}_{2} & {}^{3}\hat{r}_{2} & {}^{4}\hat{r}_{2} & {}^{5}\hat{r}_{2} & {}^{6}\hat{r}_{2}
\end{array}
$$

$$
\left[\begin{array}{cccccccccccc}
\sigma(1)_{+}(1+\eta_{1}) & 0 & 0 & 0 & 0 & 0 & \sigma(1)_{-}(1-\eta_{1}) & 0 & 0 & 0 & 0 & 0 \\
0 & \sigma(1)_{+}(1+\eta_{1}) & 0 & 0 & 0 & 0 & 0 & \sigma(1)_{-}(1-\eta_{1}) & 0 & 0 & 0 & 0 \\
0 & 0 & \sigma(1)_{-}(1-\eta_{1}) & 0 & 0 & 0 & 0 & 0 & \sigma(1)_{+}(1+\eta_{1}) & 0 & 0 & 0 \\
0 & 0 & 0 & \sigma(1)_{+}(1+\eta^{*}_{1}) & 0 & 0 & 0 & 0 & 0 & \sigma(1)_{-}(1-\eta^{*}_{1}) & 0 & 0 \\
0 & 0 & 0 & 0 & \sigma(1)_{+}(1+\eta^{*}_{1}) & 0 & 0 & 0 & 0 & 0 & \sigma(1)_{-}(1-\eta^{*}_{1}) & 0 \\
0 & 0 & 0 & 0 & 0 & \sigma(1)_{-}(1-\eta^{*}_{1}) & 0 & 0 & 0 & 0 & 0 & \sigma(1)_{+}(1+\eta^{*}_{1}) \\
\sigma(1)_{+}(1+\eta^{*}_{1}) & 0 & 0 & 0 & 0 & 0 & \sigma(1)_{-}(1-\eta^{*}_{1}) & 0 & 0 & 0 & 0 & 0 \\
0 & \sigma(1)_{+}(1+\eta^{*}_{1}) & 0 & 0 & 0 & 0 & 0 & \sigma(1)_{-}(1-\eta^{*}_{1}) & 0 & 0 & 0 & 0 \\
0 & 0 & \sigma(1)_{-}(1-\eta^{*}_{1}) & 0 & 0 & 0 & 0 & 0 & \sigma(1)_{+}(1+\eta^{*}_{1}) & 0 & 0 & 0 \\
0 & 0 & 0 & \sigma(1)_{+}(1+\eta_{1}) & 0 & 0 & 0 & 0 & 0 & \sigma(1)_{-}(1-\eta_{1}) & 0 & 0 \\
0 & 0 & 0 & 0 & \sigma(1)_{+}(1+\eta_{1}) & 0 & 0 & 0 & 0 & 0 & \sigma(1)_{-}(1-\eta_{1}) & 0 \\
0 & 0 & 0 & 0 & 0 & \sigma(1)_{-}(1-\eta_{1}) & 0 & 0 & 0 & 0 & 0 & \sigma(1)_{+}(1+\eta_{1})
\end{array}\right]
$$

$$= \{\mathbf{ES}_{\mathrm{p}}{}^{(1)}(\mathbf{k}_{1})\}$$

Symmetry at $\mathbf{k}_2 = \mu_1\mathbf{b}_1 + \mu_2\mathbf{b}_2 + \frac{1}{2}\mathbf{b}_3 = \pi(\mu_1{}^1t_x^{-1} - \mu_2{}^1t_y/{}^1t_x{}^2t_y,\ \mu_2{}^2t_y^{-1},\ \frac{1}{2}{}^3t_z^{-1})$

The $\mathbf{k}_1$ results extend to this case without amendments.

Symmetry at $\mathbf{k}_3 = \mu_3\mathbf{b}_3 = \pi(0,0,\mu_3{}^3t_z^{-1})$

$$P_{\mathbf{k}_3} = \{\mathbf{S}_1, \mathbf{S}_4\}$$

$$\Gamma^{(1)} = 6\hat{\tau}_1 + 6\hat{\tau}_2;\ \Gamma^{(r)} = 3\hat{\tau}_1 + 3\hat{\tau}_2,\ r \in \{2,3,4,5\}$$

$$d_4^{(1)} = d_1^{(r)} = \eta^* = e^{-i\pi\mu_3};\ r \in \{1,2,3,4,5\}$$

$$d_3^{(1)} = d_2^{(r)} = \eta;\ r = \{1,2,3,4,5\}$$

Defining $\sigma_\pm = \{2(1 \pm \cos(\pi\mu_3))^{\frac{1}{2}}\}^{-1}$, the symmetry coordinates read

$$\begin{array}{cccccc}
{}^1\hat{\tau}_1 & {}^2\hat{\tau}_1 & {}^3\hat{\tau}_1 & {}^1\hat{\tau}_2 & {}^2\hat{\tau}_2 & {}^3\hat{\tau}_2
\end{array}$$

$$\left[\begin{array}{cccccc}
\sigma_-(1-\eta^*) & 0 & 0 & \sigma_+(1+\eta^*) & 0 & 0 \\
0 & \sigma_-(1-\eta^*) & 0 & 0 & \sigma_+(1+\eta^*) & 0 \\
0 & 0 & \sigma_+(1+\eta^*) & 0 & 0 & \sigma_-(1-\eta^*) \\
\sigma_-(1-\eta) & 0 & 0 & \sigma_+(1+\eta) & 0 & 0 \\
0 & \sigma_-(1-\eta) & 0 & 0 & \sigma_+(1+\eta) & 0 \\
0 & 0 & \sigma_+(1+\eta) & 0 & 0 & \sigma_-(1-\eta)
\end{array}\right] = \{\mathbf{ES}_p^{(r)}(\mathbf{k}_3);\ r = 2,5\}$$

and

$$\begin{array}{cccccccccccc}
{}^1\hat{\tau}_1 & {}^2\hat{\tau}_1 & {}^3\hat{\tau}_1 & {}^4\hat{\tau}_1 & {}^5\hat{\tau}_1 & {}^6\hat{\tau}_1 & {}^1\hat{\tau}_2 & {}^2\hat{\tau}_2 & {}^3\hat{\tau}_2 & {}^4\hat{\tau}_2 & {}^5\hat{\tau}_2 & {}^6\hat{\tau}_2
\end{array}$$

$$\left[\begin{array}{cccccccccccc}
\sigma_-(1-\eta^*) & 0 & 0 & 0 & 0 & 0 & \sigma_+(1+\eta^*) & 0 & 0 & 0 & 0 & 0 \\
0 & \sigma_-(1-\eta^*) & 0 & 0 & 0 & 0 & 0 & \sigma_+(1+\eta^*) & 0 & 0 & 0 & 0 \\
0 & 0 & \sigma_+(1+\eta^*) & 0 & 0 & 0 & 0 & 0 & \sigma_-(1-\eta^*) & 0 & 0 & 0 \\
\sigma_-(1-\eta) & 0 & 0 & 0 & 0 & 0 & \sigma_+(1+\eta) & 0 & 0 & 0 & 0 & 0 \\
0 & \sigma_-(1-\eta) & 0 & 0 & 0 & 0 & 0 & {}_{+}\sigma(1+\eta) & 0 & 0 & 0 & 0 \\
0 & 0 & \sigma_+(1+\eta) & 0 & 0 & 0 & 0 & 0 & \sigma_-(1-\eta) & 0 & 0 & 0 \\
0 & 0 & 0 & \sigma_-(1-\eta) & 0 & 0 & 0 & 0 & 0 & \sigma_+(1+\eta) & 0 & 0 \\
0 & 0 & 0 & 0 & \sigma_-(1-\eta) & 0 & 0 & 0 & 0 & 0 & \sigma_+(1+\eta) & 0 \\
0 & 0 & 0 & 0 & 0 & \sigma_+(1+\eta) & 0 & 0 & 0 & 0 & 0 & \sigma_-(1-\eta) \\
0 & 0 & 0 & \sigma_-(1-\eta^*) & 0 & 0 & 0 & 0 & 0 & \sigma_+(1+\eta^*) & 0 & 0 \\
0 & 0 & 0 & 0 & \sigma_-(1-\eta^*) & 0 & 0 & 0 & 0 & 0 & \sigma_+(1+\eta^*) & 0 \\
0 & 0 & 0 & 0 & 0 & \sigma_+(1+\eta^*) & 0 & 0 & 0 & 0 & 0 & \sigma_-(1-\eta^*)
\end{array}\right]$$

$$= \{\mathbf{ES}_p^{(1)}(\mathbf{k}_3)\}$$

Symmetry at $\mathbf{k}_4 = \frac{1}{2}\mathbf{b}_1 + \mu_3\mathbf{b}_3 = \pi(\frac{1}{2}{}^1t_x^{-1},0,\mu_3{}^3t_z^{-1})$

This case is already covered by the $\mathbf{k}_3$ results; which statement holds true also for

$$\mathbf{k}_5 = \tfrac{1}{2}\mathbf{b}_2 + \mu_3\mathbf{b}_3 = \pi(\tfrac{1}{2}{}^1\bar{t}_y/{}^1t_x{}^2t_y, \tfrac{1}{2}{}^2t_y^{-1},\ \mu_3{}^3t_z^{-1})$$

and

$$\mathbf{k}_6 = \tfrac{1}{2}\mathbf{b}_1 + \tfrac{1}{2}\mathbf{b}_2 + \mu_3\mathbf{b}_3 = \pi(\tfrac{1}{2}[{}^1t_x^{-1} - {}^1t_y/{}^1t_x{}^2t_y],\ \tfrac{1}{2}{}^2t_y^{-1},\ \mu_3{}^3t_z^{-1})$$

Symmetry at $\mathbf{k}_8 = \frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_3 = \pi(\frac{1}{2}\,{}^1t_x^{-1}, 0, \frac{1}{2}\,{}^3t_z^{-1})$

$$P_{\mathbf{k}_8} = \{\mathbf{S}_1, \mathbf{S}_4, \mathbf{S}_{25}, \mathbf{S}_{28}\}$$

$$\Gamma^{(1)} = 3\hat{\tau}_1 + 3\hat{\tau}_2 + 3\hat{\tau}_3 + 3\hat{\tau}_4;$$

$$\Gamma^{(r)} = 3\hat{\tau}_1 + 3\hat{\tau}_3,\ r \in \{2,3\};\ \Gamma^{(r)} = 3\hat{\tau}_2 + 3\hat{\tau}_4,\ r \in \{4,5\}$$

$d_j^{(r)}(S_f) = -i$ for (r,j,f) = (1,1,4), (1,4,4), (1,1,28), (1,4,28), (2,1,4), (2,1,28), (3,1,4), (3,1,28), (4,1,4), (4,2,28), (5,1,4), (5,2,28).
$d_j^{(r)}(S_f) = i$ for (r,j,f) = (1,2,4), (1,3,4), (1,2,28), (1,3,28), (2,2,4), (2,2,28), (3,2,4), (3,2,28), (4,2,4), (4,1,28), (5,2,4), (5,1,28).
$d_j^{(r)}(S_f) = -1$ for (r,j,f) = (1,1,25), (1,2,25), (1,3,25), (1,4,25), (2,1,25), (2,2,25), (3,1,25), (3,2,25).
$d_j^{(r)}(S_f) = 1$ for (r,j,f) = (4,1,25), (4,2,25), (5,1,25), (5,2,25).
The symmetry combinations can be chosen as given on p. 2597
and

$$\begin{array}{cccccc} {}^1\hat{\tau}_1 & {}^2\hat{\tau}_1 & {}^3\hat{\tau}_1{}^3 & {}^1\hat{\tau}_3 & {}^2\hat{\tau}_3 & {}^3\hat{\tau}_3 \end{array}$$

$$\begin{bmatrix} \frac{1}{2}(1+i) & 0 & 0 & \frac{1}{2}(1-i) & 0 & 0 \\ 0 & \frac{1}{2}(1+i) & 0 & 0 & \frac{1}{2}(1-i) & 0 \\ 0 & 0 & \frac{1}{2}(1-i) & 0 & 0 & \frac{1}{2}(1+i) \\ \frac{1}{2}(1-i) & 0 & 0 & \frac{1}{2}(1+i) & 0 & 0 \\ 0 & \frac{1}{2}(1-i) & 0 & 0 & \frac{1}{2}(1+i) & 0 \\ 0 & 0 & \frac{1}{2}(1+i) & 0 & 0 & \frac{1}{2}(1-i) \end{bmatrix} = \{\mathbf{ES}_p^{(r)}(\mathbf{k}_8);\ r = 2,3\}$$

$\{\mathbf{ES}_p^{(r)}(\mathbf{k}_8);\ r = 4,5\}$ follows from $\{\mathbf{ES}_p^{(r)}(\mathbf{k}_8);\ r = 2,3\}$ on substituting

$$\begin{array}{cccccc} {}^1\hat{\tau}_2 & {}^2\hat{\tau}_2 & {}^3\hat{\tau}_2 & {}^1\hat{\tau}_4 & {}^2\hat{\tau}_4 & {}^3\hat{\tau}_4 \end{array}$$

for the previous heading.

Symmetry at $\mathbf{k}_{10} = \frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2 + \frac{1}{2}\mathbf{b}_3 = \pi(\frac{1}{2}[{}^1t_x^{-1} - {}^1t_y/{}^1t_x{}^2t_y],\ \frac{1}{2}\,{}^2t_y^{-1},\ \frac{1}{2}\,{}^3t_z^{-1})$

$$P_{\mathbf{k}_{10}} = \{\mathbf{S}_1, \mathbf{S}_4, \mathbf{S}_{25}, \mathbf{S}_{28}\}$$

$$\Gamma^{(1)} = 3\hat{\tau}_1 + 3\hat{\tau}_2 + 3\hat{\tau}_1 + 3\hat{\tau}_4;$$

$$\Gamma^{(r)} = 3\hat{\tau}_1 + 3\hat{\tau}_3,\ r \in \{2,5\};\ \Gamma^{(r)} = 3\hat{\tau}_2 + 3\hat{\tau}_4,\ r \in \{3,4\}$$

When allowance is made for the swapping of special set headings required by the Γ-decompositions, the $\mathbf{k}_8$ results apply at $\mathbf{k}_{10}$ as well.

Symmetry at $\mathbf{k}_9 = \frac{1}{2}\mathbf{b}_2 + \frac{1}{2}\mathbf{b}_3 = \pi(\frac{1}{2}\,{}^1\bar{t}_y/{}^1t_x{}^2t_y,\ \frac{1}{2}\,{}^2t_y^{-1},\ \frac{1}{2}\,{}^3t_z^{-1})$

$$P_{\mathbf{k}_9} = \{\mathbf{S}_1, \mathbf{S}_4, \mathbf{S}_{25}, \mathbf{S}_{28}\}$$

$\Gamma^{(1)} = 6\hat{\tau}$; $\Gamma^{(r)} = 3\hat{\tau}$, $r \in \{2,3,4,5\}$ where $\hat{\tau}$ is two-dimensional.
$d_j^{(r)}(S_f) = -i$ for (r,j,f) = (1,1,4), (1,4,4), (1,1,25), (1,4,25), (2,1,4), (2,1,25), (3,1,4), (3,2,25), (4,1,4), (4,1,25), (5,1,4), (5,2,25).
$d_j^{(r)}(S_f) = i$ for (r,j,f) = (1,2,4), (1,3,4), (1,2,25), (1,3,25), (2,2,4), (2,2,25), (3,2,4), (3,1,25), (4,2,4), (4,2,25), (5,2,4), (5,1,25).
$d_j^{(r)}(S_f) = 1$ for (r,j,f) = (1,1,28), (1,2,28), (1,3,28), (1,4,28), (2,1,28), (2,2,28), (4,1,28), (4,2,28).
$d_j^{(r)}(S_f) = -1$ for (r,j,f) = (3,1,28), (3,2,28), (5,1,28), (5,2,28).

$$
\begin{array}{cccccccccccc}
{}^1f_1 & {}^2f_1 & {}^3f_1 & {}^1f_2 & {}^2f_2 & {}^3f_2 & {}^1f_3 & {}^2f_3 & {}^3f_3 & {}^1f_4 & {}^2f_4 & {}^3f_4
\end{array}
$$

$$
\left[\begin{array}{cccccccccccc}
\frac{\sqrt{2}}{4}(1+i) & 0 & 0 & \frac{\sqrt{5}}{10}(2+i) & 0 & 0 & \frac{\sqrt{2}}{4}(1-i) & 0 & 0 & \frac{\sqrt{5}}{10}(2-i) & 0 & 0 \\
0 & \frac{\sqrt{2}}{4}(1+i) & 0 & 0 & \frac{\sqrt{5}}{10}(2+i) & 0 & 0 & \frac{\sqrt{2}}{4}(1-i) & 0 & 0 & \frac{\sqrt{5}}{10}(2-i) & 0 \\
0 & 0 & \frac{\sqrt{2}}{4}(1-i) & 0 & 0 & \frac{\sqrt{5}}{10}(2+i) & 0 & 0 & \frac{\sqrt{2}}{4}(1+i) & 0 & 0 & \frac{\sqrt{5}}{10}(2-i) \\
\frac{\sqrt{2}}{4}(1-i) & 0 & 0 & \frac{\sqrt{5}}{10}(1-2i) & 0 & 0 & \frac{\sqrt{2}}{4}(1+i) & 0 & 0 & \frac{\sqrt{5}}{10}(1+2i) & 0 & 0 \\
0 & \frac{\sqrt{2}}{4}(1-i) & 0 & 0 & \frac{\sqrt{5}}{10}(1-2i) & 0 & 0 & \frac{\sqrt{2}}{4}(1+i) & 0 & 0 & \frac{\sqrt{5}}{10}(1+2i) & 0 \\
0 & 0 & \frac{\sqrt{2}}{4}(1+i) & 0 & 0 & \frac{\sqrt{5}}{10}(\bar{1}+2i) & 0 & 0 & \frac{\sqrt{2}}{4}(1-i) & 0 & 0 & \frac{\sqrt{5}}{10}(\bar{1}-2i) \\
\frac{\sqrt{2}}{4}(1-i) & 0 & 0 & \frac{\sqrt{5}}{10}(\bar{1}+2i) & 0 & 0 & \frac{\sqrt{2}}{4}(1+i) & 0 & 0 & \frac{\sqrt{5}}{10}(\bar{1}-2i) & 0 & 0 \\
0 & \frac{\sqrt{2}}{4}(1-i) & 0 & 0 & \frac{\sqrt{5}}{10}(\bar{1}+2i) & 0 & 0 & \frac{\sqrt{2}}{4}(1+i) & 0 & 0 & \frac{\sqrt{5}}{10}(\bar{1}-2i) & 0 \\
0 & 0 & \frac{\sqrt{2}}{4}(1+i) & 0 & 0 & \frac{\sqrt{5}}{10}(1-2i) & 0 & 0 & \frac{\sqrt{2}}{4}(1-i) & 0 & 0 & \frac{\sqrt{5}}{10}(1+2i) \\
\frac{\sqrt{2}}{4}(1+i) & 0 & 0 & \frac{\sqrt{5}}{10}(\bar{2}-i) & 0 & 0 & \frac{\sqrt{2}}{4}(1-i) & 0 & 0 & \frac{\sqrt{5}}{10}(\bar{2}+i) & 0 & 0 \\
0 & \frac{\sqrt{2}}{4}(1+i) & 0 & 0 & \frac{\sqrt{5}}{10}(\bar{2}-i) & 0 & 0 & \frac{\sqrt{2}}{4}(1-i) & 0 & 0 & \frac{\sqrt{5}}{10}(\bar{2}+i) & 0 \\
0 & 0 & \frac{\sqrt{2}}{4}(1-i) & 0 & 0 & \frac{\sqrt{5}}{10}(\bar{2}-i) & 0 & 0 & \frac{\sqrt{2}}{4}(1+i) & 0 & 0 & \frac{\sqrt{5}}{10}(\bar{2}+i)
\end{array}\right]
$$

$$= \{\mathbf{ES}_p{}^{(1)}(\mathbf{k}_8)\}$$

$$\begin{array}{cccccc} {}^1\hat{\tau}_{(1)} & {}^2\hat{\tau}_{(1)} & {}^3\hat{\tau}_{(1)} & {}^1\hat{\tau}_{(2)} & {}^2\hat{\tau}_{(2)} & {}^3\hat{\tau}_{(2)} \end{array}$$

$$\begin{bmatrix} \frac{1}{2}(1+i) & 0 & 0 & \frac{1}{2}(1-i) & 0 & 0 \\ 0 & \frac{1}{2}(1+i) & 0 & 0 & \frac{1}{2}(1-i) & 0 \\ 0 & 0 & \frac{1}{2}(1-i) & 0 & 0 & \frac{1}{2}(\bar{1}-i) \\ \frac{1}{2}(1-i) & 0 & 0 & \frac{1}{2}(1+i) & 0 & 0 \\ 0 & \frac{1}{2}(1-i) & 0 & 0 & \frac{1}{2}(1+i) & 0 \\ 0 & 0 & \frac{1}{2}(1+i) & 0 & 0 & \frac{1}{2}(\bar{1}+i) \end{bmatrix} = \{\mathbf{ES}_p^{(r)}(\mathbf{k}_9);\ r\in\{2,4\}\}$$

To recover $\{\mathbf{ES}_p^{(r)}(\mathbf{k}_9);\ r\in\{3,5\}\}$ from the above matrix it suffices to apply the new heading

$$\begin{array}{cccccc} {}^1\hat{\tau}_{(1)} & {}^2\hat{\tau}_{(1)} & {}^3\hat{\tau}_{(1)} & -{}^1\hat{\tau}_{(2)} & -{}^2\hat{\tau}_{(2)} & -{}^3\hat{\tau}_{(2)} \end{array}$$

$$\begin{array}{cccccccccccc} {}^1\hat{\tau}_{(1)} & {}^2\hat{\tau}_{(1)} & {}^3\hat{\tau}_{(1)} & {}^4\hat{\tau}_{(1)} & {}^5\hat{\tau}_{(1)} & {}^6\hat{\tau}_{(1)} & {}^1\hat{\tau}_{(2)} & {}^2\hat{\tau}_{(2)} & {}^3\hat{\tau}_{(2)} & {}^4\hat{\tau}_{(2)} & {}^5\hat{\tau}_{3(2)} & {}^6\hat{\tau}_{(2)} \end{array}$$

$$\begin{bmatrix} \frac{1}{2}(1+i) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(1-i) & 0 & 0 \\ 0 & \frac{1}{2}(1+i) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(1-i) & 0 \\ 0 & 0 & \frac{1}{2}(1-i) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(\bar{1}-i) \\ \frac{1}{2}(1-i) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(1+i) & 0 & 0 \\ 0 & \frac{1}{2}(1-i) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(1+i) & 0 \\ 0 & 0 & \frac{1}{2}(1+i) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(\bar{1}+i) \\ 0 & 0 & 0 & \frac{1}{2}(1-i) & 0 & 0 & \frac{1}{2}(1+i) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}(1-i) & 0 & 0 & \frac{1}{2}(1+i) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(1+i) & 0 & 0 & \frac{1}{2}(\bar{1}+i) & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2}(1+i) & 0 & 0 & \frac{1}{2}(1-i) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}(1+i) & 0 & 0 & \frac{1}{2}(1-i) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(1-i) & 0 & 0 & \frac{1}{2}(\bar{1}-i) & 0 & 0 & 0 \end{bmatrix}$$

$$= \{\mathbf{ES}_p^{(1)}\mathbf{k}_9)\}$$

Symmetry at $\mathbf{k}_{11} = \frac{1}{2}\mathbf{b}_3 = \pi(0,0,\frac{1}{2}\,{}^3t_z^{-1})$.
The symmetry vectors are given by

$$\{\mathbf{ES}_p^{(1)}\mathbf{k}_{11})\} = \{\mathbf{ES}_p^{(1)}(\mathbf{k}_9)\} \text{ and by}$$
$$\{\mathbf{ES}_p^{(r)}(\mathbf{k}_{11})\} = \{\mathbf{ES}_p^{(2)}(\mathbf{k}_9)\},\ r\in\{2,3,4,5\}$$

Symmetry at $\mathbf{k}_{12} = \frac{1}{2}\mathbf{b}_1 = \pi(\frac{1}{2}\,{}^1t_x^{-1},0,0)$.

$$P_{\mathbf{k}_{12}} = \{\mathbf{S}_1, \mathbf{S}_4, \mathbf{S}_{25}, \mathbf{S}_{28}\}$$

$\Gamma^{(1)} = 6\hat{\tau}$; $\Gamma^{(r)} = 3\hat{\tau}$, $r\in\{2,3,4,5\}$, where $\hat{\tau}$ is two-dimensional.
$d_j^{(r)}(S_f) = 1$ for $(r,j,f) = (1,1,4), (1,2,4), (1,3,4), (1,4,4), (2,1,4), (2,2,4), (3,1,4), (3,2,4), (4,1,4), (4,2,4), (5,1,4), (5,2,4)$.
$d_j^{(r)}(S_f) = i$ for $(r,j,f) = (1,2,25), (1,3,25), (1,2,28), (1,3,28), (2,2,25), (2,2,28), (3,2,25), (3,2,28), (4,1,25), (4,1,28), (5,1,25), (5,1,28)$.
$d_j^{(r)}(S_f) = -i$ for $(r,j,f) = (1,1,25), (1,4,25), (1,1,28), (1,4,28), (2,1,25), (2,1,28), (3,1,25), (3,1,28), (4,2,25), (4,2,28), (5,2,25), (5,2,28)$.
The obtained symmetry basis reads in the general case

$$\begin{array}{cccccccccccc}
{}^{1}\hat{\tau}_{(1)} & {}^{2}\hat{\tau}_{(1)} & {}^{3}\hat{\tau}_{(1)} & {}^{4}\hat{\tau}_{(1)} & {}^{5}\hat{\tau}_{(1)} & {}^{6}\hat{\tau}_{(1)} & {}^{1}\hat{\tau}_{(2)} & {}^{2}\hat{\tau}_{(2)} & {}^{3}\hat{\tau}_{(2)} & {}^{4}\hat{\tau}_{(2)} & {}^{5}\hat{\tau}_{(2)} & {}^{6}\hat{\tau}_{(2)}
\end{array}$$

$$\left[\begin{array}{cccccccccccc}
\frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\frac{i\sqrt{2}}{2}} & 0 & 0 \\
0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\frac{i\sqrt{2}}{2}} & 0 \\
0 & 2 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{i\sqrt{2}}{2} \\
\frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\frac{i\sqrt{2}}{2}} & 0 & 0 \\
0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\frac{i\sqrt{2}}{2}} & 0 \\
0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{\frac{i\sqrt{2}}{2}} \\
0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & \frac{i\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & \frac{i\sqrt{2}}{2} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & \overline{\frac{i\sqrt{2}}{2}} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & \frac{i\sqrt{2}}{2} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & \frac{i\sqrt{2}}{2} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & \frac{i\sqrt{2}}{2} & 0 & 0 & 0
\end{array}\right]$$

$$=\{\mathbf{ES}_{\mathrm{p}}{}^{(1)}(\mathbf{k}_{12})\}$$

For the special position symmetry sets we have

$$\begin{array}{cccccc}
{}^{1}\hat{\tau}_{(1)} & {}^{2}\hat{\tau}_{(1)} & {}^{3}\hat{\tau}_{(1)} & {}^{1}\hat{\tau}_{(2)} & {}^{2}\hat{\tau}_{(2)} & {}^{3}\hat{\tau}_{(2)}
\end{array}$$

$$\left[\begin{array}{cccccc}
\frac{\sqrt{2}}{2} & 0 & 0 & \frac{i\sqrt{2}}{2} & 0 & 0 \\
0 & \frac{\sqrt{2}}{2} & 0 & 0 & \frac{i\sqrt{2}}{2} & 0 \\
0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & \frac{i\sqrt{2}}{2} \\
\overline{\frac{\sqrt{2}}{2}} & 0 & 0 & \frac{i\sqrt{2}}{2} & 0 & 0 \\
0 & \overline{\frac{\sqrt{2}}{2}} & 0 & 0 & \frac{i\sqrt{2}}{2} & 0 \\
0 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & \overline{\frac{i\sqrt{2}}{2}}
\end{array}\right] = \{\mathbf{ES}_{\mathrm{p}}{}^{(\mathrm{r})}(\mathbf{k}_{12});\ \mathrm{r} = 2,3\}$$

For $\{\mathbf{ES}_p{}^{(r)}(\mathbf{k}_{12}); r=4,5\}$ we use the above result and insert

$$^1\hat{\tau}_{(1)} \quad ^2\hat{\tau}_{(1)} \quad ^3\hat{\tau}_{(1)} - {}^1\hat{\tau}_{(2)} - {}^2\hat{\tau}_{(2)} - {}^3\hat{\tau}_{(2)}$$

Symmetry at $\mathbf{k}_{14} = \frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2 = \pi(\frac{1}{2}[{}^1t_x{}^{-1} - {}^1t_y/{}^1t_x{}^2t_y], \frac{1}{2}{}^2t_y{}^{-1},0)$.

$$P_{k_{14}} = \{\mathbf{S}_1, \mathbf{S}_4, \mathbf{S}_{25}, \mathbf{S}_{28}\}$$

$$\Gamma^{(1)} = 6\hat{\tau};\ \Gamma^{(r)} = 3\hat{\tau},\ r \in \{2,3,4,5\}$$

where $\hat{\tau}$ is two-dimensional. This case is covered by the preceding one according to

$$\{\mathbf{ES}_p{}^{(1)}(\mathbf{k}_{14})\} = \{\mathbf{ES}_p{}^{(1)}(\mathbf{k}_{12})\}.$$

$$\{\mathbf{ES}_p{}^{(r)}(\mathbf{k}_{14})\} = \{\mathbf{ES}_p{}^{(2)}(\mathbf{k}_{12})\},\quad r \in \{2,5\}$$

$$\{\mathbf{ES}_p{}^{(r)}(\mathbf{k}_{14})\} = \{\mathbf{ES}_p{}^{(4)}(\mathbf{k}_{12})\},\quad r \in \{3,4\}$$

Connection with free molecule symmetry coordinates. It seems worth remarking that the $\mathbf{k}_7$-results provide (external) symmetry coordinates for all free molecules with point symmetry $2m$ (C_{2h}).

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