REPRESENTATIONS OF THE SPACE GROUPS OF THE CLASS D_{6h}

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The small representations for all the double space groups of the class D_{6h} and the degeneracy of representations due to the Time-Reversal symmetry are given.

In this paper we present the representations of the double space groups belonging to the class D_{6h}. Representations of all the space groups can be found in the book by Kovalyov [1] but in the first edition there are many errors.

Examples of substances crystallizing in structures of symmetries D_{6h}^{1-4} are given in Table I. The last investigated group, D_{6h}^{4}, is the symmetry group of the close-packed hexagonal structures. The group D_{6h}^{4} was also investigated in [2, 3, 4]; we consider this group in our paper for completeness.

TABLE I

Examples of structure types for the space groups D_{6h}^{1-4}

Symbol of space group		Name	Chemical symbol	Page in Landolt-Börnstein [11]
Schönflies	Hermann-Mauguin			
D_{6h}^{1}	$P6/mmm$		CoSn	31
D_{6h}^{2}	$P6/mcc$	beryl	$Be_3Al_2Si_6O_{18}$	75
D_{6h}^{3}	$P6_3/mcm$	tysonite	LaF_3	45
D_{6h}^{4}	$P6_3/mmc$	magnesium	Mg	17
		graphite	C	19

The space groups of the class D_{6h} have hexagonal lattice Γ_h. The three basic primitive translations are

$$\boldsymbol{a}_1 = (a, 0, 0), \quad \boldsymbol{a}_2 = \left(-\frac{a}{2}, \frac{a\sqrt{3}}{2}, 0\right), \quad \boldsymbol{a}_3 = (0, 0, c)$$

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(in the Cartesian coordinate system — Fig. 1). The basic vectors of the reciprocal lattice are

$$b_1 = \frac{4\pi}{a\sqrt{3}}\left(\frac{\sqrt{3}}{2}, \frac{1}{2}, 0\right), \quad b_2 = \frac{4\pi}{a\sqrt{3}}(0, 1, 0), \quad b_3 = \frac{2\pi}{c}(0, 0, 1).$$

The Brillouin zone for our groups is given in Fig. 2. The point group of our groups, D_{6h}, has its elements listed in Table II. In the second column of Table II we give in terms of the hexagonal coordinates ([5], p. 7) the position vectors [6] produced by the operation of

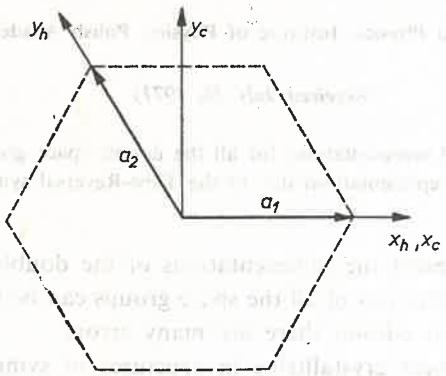

Fig. 1. Projection into the $x_c y_c$ plane of the central unit cells for the space groups of the class D_{6h}. x_h, y_h — hexagonal coordinate system, x_c, y_c — Cartesian coordinate system. The axes z_h and z_c are perpendicular to the plane of Figure

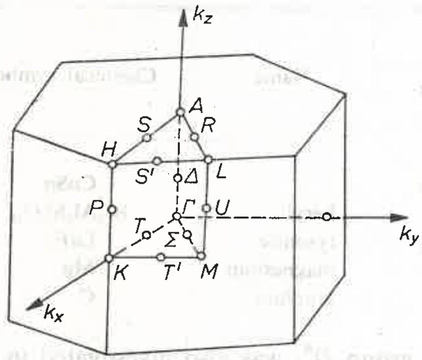

Fig. 2. The (first) Brillouin zone for the space groups of the class D_{6h}

a given group element upon the initial general position vector (x, y, z). Table II contains also the matrices corresponding to the elements of D_{6h} in configuration space (in the Cartesian system) and in spin space as well as the simplest fractional translations associated with the point operations in the space groups D_{6h}^{1-4} ([5], p. 298–304). To obtain the spinor matrices we have used the formulae given in [7]. We assume the convention that the sign "+" at the spinor matrices defines the "unbarred" elements of the double group D_{6h}.

TABLE II

Point group and fractional translations for the space groups D_{6h}^{1-4}

The point group element	Hexagonal coordinates of the equivalent general positions	Matrix in Cartesian system	Fractional translation	Spinor matrices
ε	(x, y, z)	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	0	$\pm\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
C_6	$(x-y, x, z)$	$\begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$	τ_1	$\pm\begin{bmatrix} \omega & 0 \\ 0 & \omega^* \end{bmatrix}$
C_3	$(\bar{y}, x-y, z)$	$\begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$	0	$\pm\begin{bmatrix} \omega^2 & 0 \\ 0 & (\omega^2)^* \end{bmatrix}$
C_2	$(\bar{x}, \bar{y}, z)$	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	τ_1	$\pm\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}$
C_3^{-1}	$(y-x, \bar{x}, z)$	$\begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$	0	$\pm\begin{bmatrix} (\omega^2)^* & 0 \\ 0 & \omega^2 \end{bmatrix}$
C_6^{-1}	$(y, y-x, z)$	$\begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$	τ_1	$\pm\begin{bmatrix} \omega^* & 0 \\ 0 & \omega \end{bmatrix}$
$C_2^{(1)}$	$(x-y, \bar{y}, \bar{z})$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	τ_2	$\pm\begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix}$
$C_2^{(2)}$	$(y, x, \bar{z})$	$\begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}$	τ_2	$\pm\begin{bmatrix} 0 & \omega^* \\ -\omega & 0 \end{bmatrix}$

Table II (continued)

The point group element	Hexagonal coordinates of the equivalent general positions	Matrix in Cartesian system	Fractional translation	Spinor matrices
$C_2^{(3)}$	$(\bar{x}, y-x, \bar{z})$	$\begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}$	τ_2	$\pm\begin{bmatrix} 0 & -\omega \\ \omega^* & 0 \end{bmatrix}$
$C_2'^{(1)}$	$(x, x-y, \bar{z})$	$\begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}$	τ_3	$\pm\begin{bmatrix} 0 & (\omega^2)^* \\ -\omega^2 & 0 \end{bmatrix}$
$C_2'^{(2)}$	$(y-x, y, \bar{z})$	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	τ_3	$\pm\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$
$C_2'^{(3)}$	$(\bar{y}, \bar{x}, \bar{z})$	$\begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}$	τ_3	$\pm\begin{bmatrix} 0 & -\omega^2 \\ (\omega^2)^* & 0 \end{bmatrix}$
I	$(\bar{x}, \bar{y}, \bar{z})$	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	0	$\pm\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
S_3^{-1}	$(y-x, \bar{x}, \bar{z})$	$\begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}$	τ_1	$\pm\begin{bmatrix} \omega & 0 \\ 0 & \omega^* \end{bmatrix}$
S_6^{-1}	$(y, y-x, \bar{z})$	$\begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}$	0	$\pm\begin{bmatrix} \omega^2 & 0 \\ 0 & (\omega^2)^* \end{bmatrix}$
σ_h	$(x, y, \bar{z})$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	τ_1	$\pm\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}$

Table II (continued)

The point group element	Hexagonal coordinates of the equivalent general positions	Matrix in Cartesian system	Fractional translation	Spinor matrices
S_6	$(x-y, \bar{x}, \bar{z})$	$\begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}$	0	$\pm\begin{bmatrix} (\omega^2)^* & 0 \\ 0 & \omega^2 \end{bmatrix}$
S_3	$(\bar{y}, x-y, \bar{z})$	$\begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}$	τ_1	$\pm\begin{bmatrix} \omega^* & 0 \\ 0 & \omega \end{bmatrix}$
σ_1	$(y-x, y, z)$	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	τ_2	$\pm\begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix}$
σ_2	$(\bar{y}, \bar{x}, z)$	$\begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$	τ_2	$\pm\begin{bmatrix} 0 & \omega^* \\ -\omega & 0 \end{bmatrix}$
σ_3	$(x, x-y, z)$	$\begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$	τ_2	$\pm\begin{bmatrix} 0 & -\omega \\ \omega^* & 0 \end{bmatrix}$
σ'_1	$(\bar{x}, y-x, z)$	$\begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$	τ_3	$\pm\begin{bmatrix} 0 & (\omega^2)^* \\ -\omega^2 & 0 \end{bmatrix}$
σ'_2	$(x-y, \bar{y}, z)$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	τ_3	$\pm\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$
σ'_3	(y, x, z)	$\begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 2 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$	τ_3	$\pm\begin{bmatrix} 0 & -\omega^2 \\ (\omega^2)^* & 0 \end{bmatrix}$

TABLE III

Point wave vector groups for the space groups of the class D_{6h}

Point	k	$\mathscr{P}_k$	Elements of $\mathscr{P}_k$
Γ A	$(0, 0, 0)$ $\left(0, 0, \frac{\pi}{c}\right)$	D_{6h}	ε, $C_2^{(1)}$, I, $C_2^{(1)}I = \sigma_1$, C_6, $C_6C_2^{(1)} = \overline{C_2'^{(1)}}$, $C_6I = S_3^{-1}$, $C_6C_2^{(1)}I = \sigma_1'$, $C_6^2 = C_3$, $C_6^2C_2^{(1)} = \overline{C_2^{(2)}}$, $C_6^2I = S_6^{-1}$, $C_6^2C_2^{(1)}I = \bar{\sigma}_2$, $C_6^3 = C_2$, $C_6^3C_2^{(1)} = C_2'^{(2)}$, $C_6^3I = \sigma_h$, $C_6^3C_3^{(1)}I = \sigma_2'$, $C_6^4 = \overline{C_3^{-1}}$, $C_6^4C_2^{(1)} = C_2^{(3)}$, $C_6^4I = \bar{S}_6$, $C_6^4C_2^{(1)}I = \sigma_3$, $C_6^5 = \overline{C_6^{-1}}$, $C_6^5C_2^{(1)} = C_2'^{(3)}$, $C_6^5I = \bar{S}_3$, $C_6^5C_2^{(1)}I = \sigma_3'$
K H	$\left(\frac{4\pi}{3a}, 0, 0\right)$ $\left(\frac{4\pi}{3a}, 0, \frac{\pi}{c}\right)$	D_{3h}	ε, $(S_3^{-1})^3 = \sigma_h$, $C_2^{(1)}$, $(S_3^{-1})^3C_2^{(1)} = \sigma_2'$, S_3^{-1}, $(S_3^{-1})^4 = \overline{C_3^{-1}}$, $S_3^{-1}C_2^{(1)} = \bar{\sigma}_1'$, $(S_3^{-1})^4C_2^{(1)} = C_2^{(3)}$, $(S_3^{-1})^2 = C_3$, $(S_3^{-1})^5 = \bar{S}_3$, $(S_3^{-1})^2C_2^{(1)} = \overline{C_2^{(2)}}$, $(S_3^{-1})^5C_2^{(1)} = \sigma_3'$
M L	$\left(\frac{\pi}{a}, \frac{\pi}{\sqrt{3}\,a}, 0\right)$ $\left(\frac{\pi}{a}, \frac{\pi}{\sqrt{3}\,a}, \frac{\pi}{c}\right)$	D_{2h}	ε, $C_2'^{(1)}$, I, $C_2'^{(1)}I = \sigma_1'$, C_2, $C_2C_2'^{(1)} = \overline{C_2^{(3)}}$, $C_2I = \sigma_h$, $C_2C_2'^{(1)}I = \bar{\sigma}_3$
Δ	$(0, 0, k)$	C_{6v}	ε, $C_6^3 = C_2$, σ_1, $\sigma_1C_6^3 = \bar{\sigma}_2'$, C_6, $C_6^4 = \overline{C_3^{-1}}$, $\sigma_1C_6 = \bar{\sigma}_3'$, $\sigma_1C_6^4 = \sigma_2$, $C_6^2 = C_3$, $C_6^5 = \overline{C_6^{-1}}$, $\sigma_1C_6^2 = \bar{\sigma}_3$, $\sigma_1C_6^5 = \sigma_1'$
P	$\left(\frac{4\pi}{3a}, 0, k\right)$	C_{3v}	ε, C_3, $\sigma_1'C_3 = \sigma_3'$, σ_1', $C_3^2 = \overline{C_3^{-1}}$, $\sigma_1'C_3^2 = \sigma_2'$
T S	$(k, 0, 0)$ $\left(k, 0, \frac{\pi}{c}\right)$	C_{2v}	ε, $C_2^{(1)}$, σ_h, $C_2^{(1)}\sigma_h = \bar{\sigma}_2'$
Σ R	$\left(k, \frac{k}{\sqrt{3}}, 0\right)$ $\left(k, \frac{k}{\sqrt{3}}, \frac{\pi}{c}\right)$	C_{2v}	ε, $C_2'^{(1)}$, σ_h, $C_2'^{(1)}\sigma_h = \sigma_3$
T' S'	$\left(\frac{4\pi}{3a} - \frac{k}{\sqrt{3}}, k, 0\right)$ $\left(\frac{4\pi}{a} - \frac{k}{\sqrt{3}}, k, \frac{\pi}{c}\right)$	C_{2v}	ε, $C_2^{(3)}$, σ_h, $C_2^{(3)}\sigma_h = \bar{\sigma}_1'$

Table III (continued)

Point	k	$\mathscr{P}_k$	Elements of $\mathscr{P}_k$			
U	$\left(\frac{\pi}{a}, \frac{\pi}{\sqrt{3}a}, k\right)$	C_{2v}	ε,	C_2,	σ_3,	$C_2\sigma_3 = \sigma_1'$
α	$(k, k', 0)$	C_s	ε,	σ_h		
β	$\left(k, k', \frac{\pi}{c}\right)$					
γ	$(k, 0, k')$	C_s	ε	σ_2'		
δ	$\left(k, \frac{k}{\sqrt{3}}, k'\right)$	C_s	ε,	σ_3		
ξ	$\left(\frac{4\pi}{3a} - \frac{k}{\sqrt{3}}, k, k'\right)$	C_s	ε,	σ_1'		

Our method of finding the representations of the space groups is based on the abstract definitions of the double group G^k of wave vector $\boldsymbol{k}$ and was described in [8, 9]. An abstract definition of the group D_{6h}, adapted for the double group D_{6h}, is given in terms of the generators $C_6, C_2^{(1)}, I$ (see Table II) by the relations

$$C_6^6 = \bar{\varepsilon}, \quad (C_6C_2^{(1)})^2 = \bar{\varepsilon},$$
$$(C_2^{(1)})^2 = \bar{\varepsilon}, \quad IC_6 = C_6I,$$
$$I^2 = \varepsilon, \quad IC_2^{(1)} = C_2^{(1)}I.$$

These relations can be obtained from the relations given in [12] using the explicit form of the spinor matrices (Tab. II) for the generators of the double point group.

The symmetry points, lines and planes of the Brillouin zone for our space groups are listed in Table III. The occurring point wave vector groups $\mathscr{P}^k$ are presented, the elements of the groups being expressed in terms of the generators of the groups. The relations giving elements of the point wave vector groups through generators are adapted there for the corresponding double groups.

The four-dimensional representations at the point A of the Brillouin zone, appearing for two space groups, have been obtained by multiplying one of the two-dimensional representations at $\boldsymbol{k} = \boldsymbol{k}_A$ by some representation at $\boldsymbol{k} = \boldsymbol{k}_\Gamma$ [10].

The small representations occurring for the double space groups D_{6h}^{1-4} are listed in Tables 1–23. Table IV indicates which among Tables 1–23 corresponds to the particular group G^k for a given group D_{6h}^{1-4}. We exhibit in our Tables only the matrices of the irreducible unitary representations for generators $\{\beta|\tau(\beta)\}$ of the wave vector groups G^k; here $\tau(\beta)$ is the simplest fractional translation associated with β in the group and is given in Table II. Below the Tables the Time-Reversal degeneracy is described, no comments meaning no T–R degeneracy.

TABLE IV

Tables of the irreducible representations for the space groups D_{6h}^{1-4}

	Γ	A	K	H	M	L	Δ	P	T	S	Σ	R	T'	S'	U	α	β	γ	δ	ξ
D_{6h}^1	1	1	5^a	5^a	7	7	11	12	13^a	13^a	15^a	15^a	17^a	17^a	19	20^a	20^a	21	22	23
D_{6h}^2	1	2	5^a	6^a	7	8	11	12	13^a	14^a	15^a	16^a	17^a	18^a	19	20^a	20^a	21	22	23
D_{6h}^3	1	3	5^a	5^b	7	9	11	12	13^a	13^b	15^a	16^b	17^a	17^b	19	20^a	20^b	21	22	23
D_{6h}^4	1	4	5^a	6^b	7	10	11	12	13^a	14^b	15^a	15^b	17^a	18^b	19	20^a	20^b	21	22	23

[1] The planes α, β, γ, δ and ξ are determined by the following pairs of lines $T-\Sigma$, $S-R$, $T-\Delta$, $\Sigma-\Delta$ and $P-U$, respectively.

TABLE 1

	$\{C_6\|\}$*	$\{C_2^{(1)}\|\}$	$\{I\|\}$
1, 2	1	1	± 1
3, 4	1	-1	± 1
5, 6	-1	1	± 1
7, 8	-1	-1	± 1
9, 10	$\begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$	$\pm\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
11,12	$\begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$	$\pm\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
13, 14	$\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$	$\pm\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
15, 16	$\begin{bmatrix} \omega & 0 \\ 0 & \omega^* \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$	$\pm\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
17, 18	$\begin{bmatrix} -\omega & 0 \\ 0 & -\omega^* \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$	$\pm\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

* In some Tables we omit for simplicity the simplest fractional translation associated with the rotational part of the given generator.

TABLE 2

	$\{C_6\|0\}$	$\{C_2^{(1)}\|\tau\}$	$\{I\|0\}$
1, 2	$\pm\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}$	$\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$	$\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$
3, 4	$\begin{bmatrix}\omega^2 & 0\\0 & (\omega^2)^*\end{bmatrix}$	$\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$	$\pm\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$
5, 6	$-\begin{bmatrix}\omega^2 & 0\\0 & (\omega^2)^*\end{bmatrix}$	$\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$	$\pm\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$
7, 8	$\begin{bmatrix}\omega & 0\\0 & \omega^*\end{bmatrix}$	$\begin{bmatrix}0 & 1\\-1 & 0\end{bmatrix}$	$\pm\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$
9, 10	$-\begin{bmatrix}\omega & 0\\0 & \omega^*\end{bmatrix}$	$\begin{bmatrix}0 & 1\\-1 & 0\end{bmatrix}$	$\pm\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$
11, 12	$\begin{bmatrix}i & 0\\0 & -i\end{bmatrix}$	$\begin{bmatrix}0 & 1\\-1 & 0\end{bmatrix}$	$\pm\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$

The Time-Reversal degeneracy: 3–4, 5–6, 7–8, 9–10, 11–12.

TABLE 3

	$\{C_6\|\tau\}$	$\{C_2^{(1)}\|\tau\}$	$\{I\|0\}$
1,2	$\begin{bmatrix}0 & 1\\-1 & 0\end{bmatrix}$	$\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$	$\pm\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$
3	$\begin{bmatrix}0 & \frac{1}{2} & 0 & -\frac{\sqrt{3}}{2}\\-\frac{1}{2} & 0 & \frac{\sqrt{3}}{2} & 0\\0 & \frac{\sqrt{3}}{2} & 0 & \frac{1}{2}\\-\frac{\sqrt{3}}{2} & 0 & -\frac{1}{2} & 0\end{bmatrix}$	$\begin{bmatrix}0 & 1 & 0 & 0\\1 & 0 & 0 & 0\\0 & 0 & 0 & -1\\0 & 0 & -1 & 0\end{bmatrix}$	$\begin{bmatrix}1 & 0 & 0 & 0\\0 & -1 & 0 & 0\\0 & 0 & 1 & 0\\0 & 0 & 0 & -1\end{bmatrix}$
4,5	$\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$	$\pm\begin{bmatrix}0 & i\\i & 0\end{bmatrix}$	$\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$
6	$\begin{bmatrix}0 & 0 & \omega & 0\\0 & 0 & 0 & \omega^*\\-\omega & 0 & 0 & 0\\0 & -\omega^* & 0 & 0\end{bmatrix}$	$\begin{bmatrix}0 & 0 & 0 & -1\\0 & 0 & 1 & 0\\0 & -1 & 0 & 0\\1 & 0 & 0 & 0\end{bmatrix}$	$\begin{bmatrix}1 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & -1 & 0\\0 & 0 & 0 & -1\end{bmatrix}$

The T–R degeneracy: 4–5

TABLE 4

	$\{C_6\|\tau\}$	$\{C_2^{(1)}\|0\}$	$\{I\|0\}$
1, 2	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$	$\pm\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
3	$\begin{bmatrix} 0 & 0 & \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
4, 5	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\pm\begin{bmatrix} i & 0 \\ 0 & i \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
6	$\begin{bmatrix} 0 & 0 & \omega & 0 \\ 0 & 0 & 0 & \omega^* \\ -\omega & 0 & 0 & 0 \\ 0 & -\omega^* & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$

The T–R degeneracy: 4–5.

TABLE 5

	$\{S_3^{-1}\|\}$	$\{C_2^{(1)}\|\}$
1, 2	1	± 1
3, 4	-1	± 1
5, 6	$\pm\begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
7	$\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$
8, 9	$\pm\begin{bmatrix} \omega & 0 \\ 0 & \omega^* \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$

The T–R degeneracy: 1–4, 2–3, 5–6, 7–7, 8–9.

TABLE 6

	$\{S_3^{-1}\|\}$	$\{C_2^{(1)}\|\}$
1	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
2, 3	$\pm\begin{bmatrix} \omega^2 & 0 \\ 0 & -(\omega^2)^* \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
4, 5	i	$\pm i$
6, 7	$-i$	$\pm i$
8, 9	$\pm\begin{bmatrix} \omega & 0 \\ 0 & -\omega^* \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

a) The T–R degeneracy: 2–3, 4–6, 5–7, 8–9,
b) The T–R degeneracy: 4–5, 6–7.

TABLE 7

	$\{C_2\|\}$	$\{C'^{(1)}_2\|\}$	$\{I\|0\}$
1, 2	1	1	± 1
3, 4	1	-1	± 1
5, 6	-1	1	± 1
7, 8	-1	-1	± 1
9, 10	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$	$\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}$	$\pm\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

TABLE 8

	$\{C_2\|0\}$	$\{C'^{(1)}_2\|\tau\}$	$\{I\|0\}$
1, 2	$\pm\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
3, 4	$\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$	$\pm\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

The T–R degeneracy: 3–4.

TABLE 9

	$\{C_2\|\tau\}$	$\{C'^{(1)}_2\|0\}$	$\{I\|0\}$
1, 2	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$	$\pm\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
3, 4	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\pm\begin{bmatrix} i & 0 \\ 0 & i \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

The T–R degeneracy: 3–4

TABLE 10

	$\{C_2\|\tau\}$	$\{C_2'^{(1)}\|\tau\}$	$\{I\|0\}$
1, 2	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\pm\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
3, 4	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\pm\begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

The T–R degeneracy: 3–4

TABLE 11

	$\{C_6\|\}$	$\{\sigma_1\|\}$
1, 2	ζ_1	$\pm\zeta_2$
3, 4	$-\zeta_1$	$\pm\zeta_2$
5, 6	$\pm\begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}\zeta_1$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\zeta_2$
7	$\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}\zeta_1$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}\zeta_2$
8, 9	$\pm\begin{bmatrix} \omega & 0 \\ 0 & \omega^* \end{bmatrix}\zeta_1$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}\zeta_2$

$\zeta_1 = \exp ik\tau_1$, $\zeta_2 = \exp ik\tau_2$

TABLE 12

	$\{C_3\|0\}$	$\{\sigma_1'\|\}$
1, 2	1	$\pm\zeta$
3	$\begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\zeta$
4,5	-1	$\pm i\zeta$
6	$\begin{bmatrix} \omega^2 & 0 \\ 0 & (\omega^2)^* \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}\zeta$

$\zeta = \exp\ ik\tau_3$

The T–R degeneracy: 4–5

TABLE 13

	$\{C_2'^{(1)}\|\}$	$\{\sigma_h\|\}$
1, 2	1	± 1
3, 4	—1	± 1
5	$\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$

a) No T–R degeneracy
b) The T–R degeneracy: 1–4, 2–3, 5–5

TABLE 14

	$\{C_2^{(1)}\|\}$	$\{\sigma_h\|\}$
1	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
2, 3	i	$\pm i$
4, 5	$-i$	$\pm i$

a) The T–R degeneracy: 2–3, 4–5
b) The T–R degeneracy: 2–4, 3–5.

TABLE 15

	$\{C_2'^{(1)}\|\}$	$\{\sigma_h\|\}$
1, 2	1	± 1
3, 4	-1	± 1
5	$\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$

a) No T–R degeneracy
b) The T–R degeneracy: 1–4, 2–3, 5–5

TABLE 16

	$\{C_2'^{(1)}\|\}$	$\{\sigma_h\|\}$
1	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
2, 3	i	$\pm i$
4, 5	$-i$	$\pm i$

a) The T–R degeneracy: 2–3, 4–5
b) The T–R degeneracy: 2–4, 3–5

TABLE 17

	$\{C_2^{(3)}\|\}$	$\{\sigma_h\|\}$
1, 2	1	± 1
3, 4	-1	± 1
5	$\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$

a) No T–R degeneracy
b) The T–R degeneracy: 1–4, 2–3, 5–5

TABLE 18

	$\{C_2^{(3)}\|\}$	$\{\sigma_h\|\}$
1	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
2, 3	i	$\pm i$
4, 5	$-i$	$\pm i$

a) The T–R degeneracy: 2–3, 4–5
b) The T–R degeneracy: 2–4, 3–5

TABLE 19

	$\{C_2 \mid\}$	$\{\sigma_3 \mid\}$
1, 2	ζ_1	$\pm\zeta_2$
3, 4	$-\zeta_1$	$\pm\zeta_2$
5	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}\zeta_1$	$\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}\zeta_2$

$\zeta_1 = \exp\, ik\tau_1$, $\zeta_2 = \exp\, ik\tau_2$

TABLE 20

	$\{\sigma_h \mid\}$
1, 2	± 1
3, 4	$\pm i$

a) The T–R degeneracy: 3–4
b) The T–R degeneracy: 1–2, 3–3, 4–4

TABLE 21

	$\{\sigma_2' \mid\}$
1, 2	$\pm\zeta$
3, 4	$\pm i\zeta$

$\zeta = \exp\, ik\tau_3$
The T–R degeneracy: 3–4

TABLE 22

	$\{\sigma_3 \mid\}$
1, 2	$\pm\zeta$
3, 4	$\pm i\zeta$

$\zeta = \exp\, ik\tau_2$
The T–R degeneracy: 3–4

TABLE 23

	$\{\sigma_1' \mid\}$
1, 2	$\pm\zeta$
3, 4	$\pm i\zeta$

$\zeta = \exp\, ik\tau_3$
The T–R degeneracy: 3–4

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In the Tables we use the following abbreviations:

$$\tau_1 = \begin{cases} 0 & \text{for } D_{6h}^{1,2} \\ \tau & \text{for } D_{6h}^{3,4} \end{cases}, \quad \tau_2 = \begin{cases} 0 & \text{for } D_{6h}^{1,4} \\ \tau & \text{for } D_{6h}^{2,3} \end{cases},$$

$$\tau_3 = \begin{cases} 0 & \text{for } D_{6h}^{1,3} \\ \tau & \text{for } D_{6h}^{2,4} \end{cases}, \quad \tau = \left(0, 0, \frac{c}{2}\right), \quad \omega = \exp(i\pi/6).$$

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