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The classification of surface states of topological insulators and superconductors with magnetic point group symmetry

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We present the exhaustive classification of surface states of topological insulators and superconductors protected by crystallographic magnetic point group symmetry in three spatial dimensions. Recently, Cornfeld and Chapman [Phys. Rev. B **99**, 075105 (2019)] pointed out that the topological classification of mass terms of the Dirac Hamiltonian with point group symmetry is recast as an extension problem of the Clifford algebra, and we use their results extensively. Comparing two types of Dirac Hamiltonians with and without the mass-hedgehog potential, we establish an irreducible character formula to read off which Hamiltonian in the whole K-group belongs to 4th-order topological phases in three spatial dimensions, which are equivalent to atomic insulators consisting of atoms localized at the point group center.

Subject Index I68, I90

1. Introduction

Topological insulators (TIs) and topological superconductors (TSCs) are topological classes of gapped Hamiltonians of free fermions [1,2]. Two gapped Hamiltonians are said to belong to the same topological phases if there exists a continuous path of Hamiltonians interpolating between them that preserves both symmetry and the energy gap. For TIs/TSCs protected solely by onsite symmetry, symmetry groups composed of transformations that keep the spatial position invariant, the classification problem is recast as an extension problem of the Clifford algebra [3–7], and it is shown that a nontrivial TI/TSC exhibits a robust gapless state on its boundary.

With crystalline symmetry, which involves a group element that changes its spatial position, the relationship between TIs/TSCs and gapless boundary states is more involved. This is because atomic insulators, which are occupied states of localized atomic orbitals, contribute to the topological classification while they are irrelevant to boundary gapless states. The best way to think of the structure of the bulk–boundary correspondence in the presence of crystalline symmetry is the filtration $\cdots \subset K'' \subset K' \subset K$ for the classification of TIs/TSCs with respect to the space dimension on which the TI/TSC is defined [8–10]. Precisely, for d space dimensions, let $K^{(p)}$ be the Abelian group composed of TIs/TSCs that are adiabatically connected to TIs/TSCs supported on a subspace with dimension less than or equal to $(d-p)$. The quotient group $K^{(p)}/K^{(p+1)}$ captures TIs/TSCs supported exactly on a $(d-p)$-dimensional real-space submanifold, which are called $(p+1)$th-order TIs/TSCs [11–13], and such phases host gapless boundary states if $p < d$. In particular, the group $K^{(d)}$, the $(d+1)$th-order TIs/TSCs, represents atomic insulators. Therefore, the quotient group $K/K^{(d)}$ provides the classification of TIs/TSCs with a gapless boundary state. See Refs. [14–16] for the classification of surface states of time-reversal (TR) symmetric TIs in spinful electrons with the connection to the symmetry-based indicator [17].

Recently, Cornfeld and Chapman have pointed out that for arbitrary point group symmetry (namely, a subgroup of the orthogonal group keeping a crystal structure), symmetry operators can be onsite with keeping the topological classification, resulting in the possibility that the Abelian group K of the classification of TIs/TSCs can be computed by the extension problem of the Clifford algebra as well as the classification of TIs/TSCs with onsite symmetry [18].

In this paper, for magnetic point group symmetry, we show that in addition to the group K of the entire classification, the group $K^{(d)}$ of dth-order TIs/TSCs can also be computed in a canonical way as a subgroup of K. Taking the quotient of K by $K^{(d)}$, one can get the classification of TIs/TSCs hosting a gapless boundary state.

Throughout this paper, the classification of band structures means that in the sense of the K-theory. Every classification is an Abelian group, measures the formal difference between two TIs/TSCs, and is stable under adding a common TI/TSC. Except for Section 2, we consider TIs/TSCs in three space dimensions. The same approach works for generic space dimensions.

The plan of this paper is as follows. In Section 2, we illustrate how the entire group K and the group K' of atomic insulators are computed for a simple example in 1D. Section 3 is devoted to establishing the irreducible character formulas to compute the groups K and K''' for generic magnetic point group (MPG) symmetry. In Section 3.1, we reformulate Cornfeld and Chapman's prescription so that it can be applied to generic MPG symmetry with arbitrary factor systems. In Section 4, we apply our formalism to insulators and superconductors in three space dimensions to get the complete classification of the gapless surface states. The classification tables are summarized in Tables D1–D8 in Appendix D. We summarize this paper and suggest future directions in Section 5.

2. Simple example

Before moving on to the formulation applied to any MPGs for TIs and TSCs, we give a simple example to show what we want to do in this paper. In this section, $\sigma_{\mu=0,x,y,z}$ and $\tau_{\mu=0,x,y,z}$ represent 2 by 2 Pauli matrices.

Let us consider 1D time-reversal symmetry (TRS)-broken odd-parity superconductors (SCs), i.e., SCs in which the inversion transformation keeps the normal states invariant but flips the sign of the gap functions. The topological nature of the bulk is described by the Dirac Hamiltonian

$$H(\hat{k}_x) = -i\partial_x\gamma_1 + m\Gamma_0, \qquad \gamma_1^2 = \Gamma_0^2 = 1, \qquad \{\gamma_1, \Gamma_0\} = 0, \tag{1}$$

where $\hat{k}_x = -i\partial_x$, and m is a mass parameter. The symbols γ_1 and Γ_0 are gamma matrices with the anticommutation relation. The particle–hole and inversion symmetries are written as

$$\begin{aligned} \hat{C}H(\hat{k}_x)\hat{C}^{-1} &= -H(-\hat{k}_x), \qquad \hat{C}^2 = 1, \\ \hat{I}H(\hat{k}_x)\hat{I}^{-1} &= H(-\hat{k}_x), \qquad \hat{I}^2 = 1, \\ \hat{C}\hat{I} &= -\hat{I}\hat{C}. \end{aligned} \tag{2}$$

Here, $\hat{I}$ is the unitary inversion operator, and $\hat{C}$ is the antiunitary particle–hole operator. The anticommutation relation between $\hat{C}$ and $\hat{I}$ is from the assumption of the odd parity of the superconducting gap function (see Section 4.2 for details). Note that the following algebraic relations hold:

$$\hat{C}\gamma_1\hat{C}^{-1} = \gamma_1, \qquad \hat{I}\gamma_1\hat{I}^{-1} = -\gamma_1,$$
$$\hat{C}\Gamma_0\hat{C}^{-1} = -\Gamma_0, \qquad \hat{I}\Gamma_0\hat{I}^{-1} = \Gamma_0. \tag{3}$$

To carry out the topological classification of the mass term $m\Gamma_0$, we introduce the modified operator $\tilde{I} = i\gamma_1\hat{I}$ that behaves as an onsite chiral symmetry

$$\tilde{I}H(\hat{k}_x)\tilde{I}^{-1} = -H(\hat{k}_x), \qquad \tilde{I}^2 = 1, \tag{4}$$

with the algebra among symmetry operators

$$\tilde{I}^2 = 1, \qquad \hat{C}\tilde{I} = \tilde{I}\hat{C}. \tag{5}$$

The operators $\hat{C}$ and $\tilde{I}$ compose the BDI class in the Altland–Zirnbauer (AZ) symmetry classes [19]. Thus, the mass terms $m\Gamma_0$ are classified by integers, where we denote the K-group by $K = \mathbb{Z}$ [3,4]. The generator model is given by

$$H(\hat{k}_x) = -i\partial_x\tau_y + m\tau_z, \qquad \hat{C} = \tau_x\mathcal{K}, \qquad \tilde{I} = \tau_x. \tag{6}$$

Here, $\mathcal{K}$ is the complex conjugation. Given a Dirac Hamiltonian with the modified inversion symmetry $\tilde{I}$, the $\mathbb{Z}$ index is given by the 1D winding number

$$w_{1\mathrm{D}}[H(\hat{k}_x)] = \frac{1}{2i}\mathrm{tr}\,[\gamma_1\Gamma_0\tilde{I}], \tag{7}$$

which we will use later.[1]

Not every integer of the K-group K represents a 1st-order TSC, the Kitaev chain. As is shown shortly, even integers of K are 2nd-order TSCs; i.e., they are equivalent to atomic insulators localized at the inversion center. To see this, we add a symmetry-allowed Jackiw–Rebbi kink term $M(x)\Gamma_1$ to Eq. (1) as in

$$H_{\mathrm{kink}}(\hat{k}_x, x) = -i\partial_x\gamma_1 + M(x)\Gamma_1 + m\Gamma_0,$$
$$\gamma_1^2 = \Gamma_0^2 = \Gamma_1^2 = 1,$$
$$\{\gamma_1, \Gamma_0\} = \{\gamma_1, \Gamma_1\} = \{\Gamma_0, \Gamma_1\} = 0. \tag{8}$$

We also assume the anticommutation relation $\{\Gamma_0, \tilde{I}\} = 0$ to be compatible with the sign change of the mass term $M(x)$ at $x = 0$. The particle–hole and inversion symmetries are written as

$$\hat{C}H_{\mathrm{kink}}(\hat{k}_x, x)\hat{C}^{-1} = -H_{\mathrm{kink}}(-\hat{k}_x, x), \qquad \hat{C}^2 = 1,$$
$$\hat{I}H_{\mathrm{kink}}(\hat{k}_x, x)\hat{I}^{-1} = H_{\mathrm{kink}}(-\hat{k}_x, -x), \qquad \hat{I}^2 = 1,$$
$$\hat{C}\hat{I} = -\hat{I}\hat{C}. \tag{9}$$

[1]The 1D winding number $w_{1\mathrm{D}}$ of the Hamiltonian (1) for the chiral symmetry operator $\tilde{I}$ is given by

$$w_{1\mathrm{D}} = \frac{1}{4\pi i}\int_{-\infty}^{\infty} dk_x \mathrm{tr}\,[\tilde{I}H(k_x)^{-1}\partial_{k_x}H(k_x)] = \frac{-\mathrm{sgn}(m)}{4\pi i}\mathrm{tr}\,[\gamma_1\Gamma_0\tilde{I}].$$

The formula (7) gives the difference of the winding numbers when the mass parameter m crosses the zero from the positive to the negative.

Here, $M(-x) = -M(x)$ is imposed from the inversion symmetry.[2] The key observation is the one-to-one correspondence between the Jackiw–Rebbi low-energy bound states of $H_{\mathrm{kink}}(\hat{k}_x, x)$ and atomic insulators at the inversion center. The Jackiw–Rebbi Hamiltonian $-i\partial_x\gamma_1 + M(x)\Gamma_1$ hosts zero modes localized at the inversion center $x = 0$. The uniform mass term $m\Gamma_0$ induces finite energy to those zero modes, resulting in localized modes at $x = 0$ with finite positive or negative energies, which resemble atomic states. (See footnote 3 for the quantitative details.[3])

The aforementioned one-to-one correspondence is systematically constructed by dimensional isomorphic mapping in the K-theory [20]. We denote the classification of atomic insulators at the inversion center by K_{AI}. The group K_{AI} is represented by a 0D Hamiltonian H_{0D} with the particle–hole and inversion symmetries,

$$\begin{aligned} \hat{C}_{\mathrm{0D}} H_{\mathrm{0D}} \hat{C}_{\mathrm{0D}}^{-1} &= -H_{\mathrm{0D}}, \qquad \hat{C}_{\mathrm{0D}}^2 = 1, \\ \hat{I}_{\mathrm{0D}} H_{\mathrm{0D}} \hat{I}_{\mathrm{0D}}^{-1} &= H_{\mathrm{0D}}, \qquad \hat{I}_{\mathrm{0D}}^2 = 1, \\ \hat{C}_{\mathrm{0D}} \hat{I}_{\mathrm{0D}} &= -\hat{I}_{\mathrm{0D}} \hat{C}_{\mathrm{0D}}. \end{aligned} \tag{10}$$

From $\hat{C}_{\mathrm{0D}}\hat{I}_{\mathrm{0D}} = -\hat{I}_{\mathrm{0D}}\hat{C}_{\mathrm{0D}}$, the particle–hole symmetry (PHS) operator $\hat{C}_{\mathrm{0D}}$ exchanges the positive and negative eigenvalues of $\hat{I}_{\mathrm{0D}}$, meaning that the AZ class for the Hamiltonian H_{0D} is effectively the A class. Thus, we find that the K-group K_{AI} is $K_{\mathrm{AI}} = \mathbb{Z}$ and is generated by the Hamiltonian $H_{\mathrm{0D}} = m\sigma_z$ with symmetry operators $\hat{C}_{\mathrm{0D}} = \sigma_x\mathcal{K}$ and $\hat{I}_{\mathrm{0D}} = \sigma_z$. Given a 0D Hamiltonian H_{0D} with symmetry operators $\hat{C}_{\mathrm{0D}}$ and $\hat{I}_{\mathrm{0D}}$, the dimensional raising isomorphic map to the kink Hamiltonian is given by

$$H_{\mathrm{kink}}(\hat{k}_x, x) := -i\partial_x\tau_y + M(x)\tau_x + H_{\mathrm{0D}}\tau_z, \qquad \tilde{C} = \tilde{C}_{\mathrm{0D}}\tau_z, \qquad \hat{I} = \hat{I}_{\mathrm{0D}}\tau_z. \tag{11}$$

Notice that the Hamiltonian H_{kink} and the symmetry operators $\hat{C}$ and $\hat{I}$ obtained in this way automatically satisfy the desired symmetry algebra (9). In particular, the generator model of $K_{\mathrm{AI}} = \mathbb{Z}$ is mapped as

$$H_{\mathrm{kink}}(\hat{k}_x, x) = -i\partial_x\tau_y + M(x)\tau_x + m\sigma_z\tau_z, \qquad \hat{C} = \sigma_x\tau_z\mathcal{K}, \qquad \hat{I} = \sigma_z\tau_z. \tag{12}$$

The final step is to determine which element of the K-group K admits a kink term $M(x)\Gamma_1$, which is given by the homomorphism f: $K_{\mathrm{AI}} \to K$ defined through the identification of H_{0D} and $H_{\mathrm{kink}}(\hat{k}_x, x)$. By setting the kink mass $M(x)$ to zero, the Dirac Hamiltonian (11) is regarded as one without x-dependence, which defines the homomorphism f. For the generator model (12), the modified inversion operator is $\tilde{I} = i\gamma_1\hat{I} = -\tau_x\sigma_z$, and the 1D winding number w_{1D} defined

[2] As long as we are concerned with the bound states localized at the inversion center, the configuration of $M(x)$ is assumed as $M(x) = x$ (or $M(x) = -x$). Therefore, the kink term $M(x)\,\Gamma_1$ behaves like an additional kinetic term of the Dirac Hamiltonian.

[3] The existence of the localized modes can be understood as follows. For simplicity, we set $M(x \to \infty) > 0$. For a wave function of the form $\phi(x) = \eta e^{-\int^x M(x')dx'}$, where η represents the internal degrees of freedom, the Jackiw –Rebbi Hamiltonian $-i\,\partial_x\,\gamma_1 + M(x)\,\Gamma_1$ hosts the zero modes determined by $(i\,\gamma_1 + \Gamma_1)\,\eta = 0$. Due to the chiral symmetry $\{-i\,\partial_x\,\gamma_1, +M(x)\,\Gamma_1, \Gamma_0\}$ of the Jackiw –Rebbi Hamiltonian, the zero modes can be chosen as simultaneous eigenstates of Γ_0, $\Gamma_0\,\eta = \pm\,\eta$, called chirality. The chiral index N is defined as the difference of numbers of chiral zero modes with positive and negative chiralities, which is given by

$$N = \mathrm{tr}\left[\left(\frac{1 + i\gamma_1\Gamma_1}{2}\right)\Gamma_0\right] = -\frac{1}{2i}\mathrm{tr}\left[\gamma_1\Gamma_1\Gamma_0\right] \in \mathbb{Z},$$

where $(1 + i\,\gamma_1\,\Gamma_1)/2$ is the projector onto the subspace of zero modes. We note that only the N chiral zero modes are stable under the chiral symmetry by Γ_0. The uniform mass $m\,\Gamma_0$ in Eq. (8) gives the chiral zero modes the finite energy $\pm m$ with the sign determined by the chirality $\Gamma_0 = \pm 1$.

in Eq. (7) is given by

$$w_{1\mathrm{D}}[\tilde{H}_{\mathrm{kink}}(\hat{k}_x, x)|_{M(x)\to 0}] = \frac{1}{2i}\mathrm{tr}\left[\tau_y \times \sigma_z\tau_z \times (-\tau_x\sigma_z)\right] = -2. \tag{13}$$

This means that within the K-group $K = \mathbb{Z}$, Hamiltonians admitting the kink term belong to even integers $\mathrm{Im}\, f = 2\mathbb{Z} \subset \mathbb{Z}$, resulting in 2nd-order TSCs (atomic insulators). Let us write the Abelian group of the 2nd-order TSCs by $K' := \mathrm{Im} f$. We have the subgroup structure $K' \subset K$ and conclude that the classification of 1st-order TSCs is given by the quotient $K/K' = \mathbb{Z}/2\mathbb{Z}$.

3. Formulation

In this section, generalizing the strategy illustrated in the previous section, we formulate how to compute the Abelian group K of all TIs/TSCs and the Abelian group K''' composed only of 4th-order TIs/TSCs in three space dimensions. The generalization to any space dimensions is straightforward.

3.1 *The entire K-group K for TIs/TSCs*

Let H be a 3D Dirac Hamiltonian with a uniform mass:

$$H(\boldsymbol{k}) = k_x\gamma_1 + k_2\gamma_2 + k_3\gamma_3 + m\Gamma_0,$$
$$\{\gamma_i, \gamma_j\} = 2\delta_{ij}, \qquad \Gamma_0^2 = 1, \qquad \{\gamma_i, \Gamma_0\} = 0. \tag{14}$$

Let G be an MPG equipped with the data $(O_g, \phi_g, c_g, z_{g,h})$ for $g, h \in G$. The matrix $O_g \in O(3)$ represents how the group G acts on the real-space coordinate as $\boldsymbol{x} \mapsto O_g\boldsymbol{x}$ for $g \in G$. The homomorphisms $\phi, c : G \to \mathbb{Z}_2 = \{\pm 1\}$ indicate unitary/antiunitary and symmetry/antisymmetry of the group element $g \in G$, respectively. The symmetry constraint relations are written as

$$\hat{g}H(\boldsymbol{k})\hat{g}^{-1} = c_g H(\phi_g O_g \boldsymbol{k}), \qquad \hat{g}i\hat{g}^{-1} = \phi_g i, \qquad g \in G. \tag{15}$$

The set of $U(1)$ phases $z_{g,h} \in U(1)$ for $g, h \in G$ specifies the factor system of a projective representation:

$$\hat{g}\hat{h} = z_{g,h}\widehat{gh}, \qquad g, h \in G. \tag{16}$$

For gamma matrices γ_i and Γ_0, the symmetry (15) is written as

$$\hat{g}\boldsymbol{\gamma}\hat{g}^{-1} = \phi_g c_g O_g^{-1}\boldsymbol{\gamma}, \qquad \hat{g}\Gamma_0\hat{g}^{-1} = c_g\Gamma_0. \tag{17}$$

For an $SO(3)$ rotation $R = (\boldsymbol{n}, \theta)$ with counterclockwise rotation about the $\boldsymbol{n}$-axis by the angle θ, we have the key equality

$$O_R\boldsymbol{\gamma} = q_R\boldsymbol{\gamma}q_R^{-1}, \tag{18}$$

with q_R the unitary operator canonically defined by

$$q_R = e^{\frac{\theta}{2}(n_1\gamma_2\gamma_3 + n_2\gamma_3\gamma_1 + n_3\gamma_1\gamma_2)} \tag{19}$$

irrespective of representations of the gamma matrices, where $\boldsymbol{n} = (n_1, n_2, n_3)$ is a unit vector.[4] The operator q_R can be used to make $\hat{g}$ onsite [18]. We further introduce a homomorphism $s : G \to \mathbb{Z}_2 = \{\pm 1\}$ by $s_g := \det[O_g] \in \{\pm 1\}$ specifying if $g \in G$ preserves the orientation or not. Let R_g be the $SO(3)$ part of $O_g \in O(3)$, i.e., $R_g = O_g$ for $s_g = 1$, and $R_g = IO_g$ for $s_g = -1$, where $I = \mathrm{diag}(-1, -1, -1)$ is the space inversion. We introduce the new symmetry operator $\tilde{g}$ defined

[4] In generic d space dimensions, for an $SO(d)$ rotation $R = \exp\left(\frac{i}{2}\theta_{ij}L_{ij}\right)$, in which $[L_{ij}]_{kl} = -i(\delta_{ik}\,\delta_{jl} - \delta_{jk}\,\delta_{il})$ are the generators of $SO(d)$, a Spin(d) rotation is given by $q_R = \exp\left(\frac{i}{2}\theta_{ij}\Sigma_{ij}\right)$, where $\Sigma_{ij} = \frac{-i}{4}[\gamma_i, \gamma_j]$ are the generators of Spin(d) rotations.

by

$$\tilde{g} := (\gamma_1\gamma_2\gamma_3)^{(1-s_g)/2} q_{R_g} \hat{g}. \tag{20}$$

The new operators now represent onsite symmetry:

$$\tilde{g}H(\boldsymbol{k})\tilde{g}^{-1} = c_g s_g H(\phi_g \boldsymbol{k}), \qquad \tilde{g}i\tilde{g}^{-1} = \phi_g i, \qquad g \in G. \tag{21}$$

Equivalently, for gamma matrices,

$$\tilde{g}\boldsymbol{\gamma}\tilde{g}^{-1} = c_g s_g \phi_g \boldsymbol{\gamma}, \qquad \tilde{g}\Gamma_0\tilde{g}^{-1} = c_g s_g \Gamma_0, \quad g \in G. \tag{22}$$

It is to be noted that orientation-reversing symmetry operators (i.e., for operators with $\phi_g = 1$, $s_g = -1$, and $c_g = 1$) behave as chiral symmetry. Also, we note that the new operators $\tilde{g}$ obey a different factor system from that for the $\hat{g}$: From a straightforward calculation, the factor system $\tilde{z}_{g,h}$ of the $\tilde{g}$ defined by $\tilde{g}\tilde{h} = \tilde{z}_{g,h}\widetilde{gh}$ is[5]

$$\tilde{z}_{g,h} = z'_{g,h} \times (-1)^{\frac{1-c_g\phi_g}{2}\frac{1-s_h}{2}} \times z_{g,h}, \tag{23}$$

$$z'_{g,h} := q_{R_h} q_{R_g} q^{-1}_{R_{gh}} \in \{\pm 1\}. \tag{24}$$

Here we have introduced the factor system $z'_{g,h} (= (z'_{g,h})^{-1})$ of the Spin(3)-rotation matrices q_R with the right group action, which is determined for a fixed choice of $SO(3)$-rotation parameters $(\boldsymbol{n}_g, \theta_g)$ for $g \in G$. We will use $z'_{g,h}$ frequently later.

Since the MPG G is now represented as onsite symmetry, one can apply the Wigner criteria to symmetry operators $\{\tilde{g}\}_{g\in G}$ to get the K-group K classifying the mass term $m\Gamma_0$ [21]. We decompose the group G into subsets as

$$G = G_0 \coprod aG_0 \coprod bG_0 \coprod abG_0, \tag{25}$$

where

$$G_0 = \{g \in G | \phi_g = 1, c_g s_g = 1\}, \tag{26}$$

$$^\exists a \in G, \quad -\phi_a = c_a s_a = 1, \tag{27}$$

$$^\exists b \in G, \quad -\phi_b = -c_b s_b = 1, \tag{28}$$

$$^\exists ab \in G, \quad \phi_{ab} = -c_{ab} s_{ab} = 1. \tag{29}$$

(Here, ab is not necessarily the group product of a and b, but represents a single element of G.) For an irrep α of G_0 with the factor system $\tilde{z}_{g,h}$, the Wigner criteria for the operators $\tilde{a}$ and $\tilde{b}$ are defined by

$$W^T_\alpha = \frac{1}{|G_0|}\sum_{g\in aG_0} \tilde{z}_{g,g}\tilde{\chi}_\alpha(g^2) \in \{0, \pm 1\}, \tag{30}$$

$$W^C_\alpha = \frac{1}{|G_0|}\sum_{g\in bG_0} \tilde{z}_{g,g}\tilde{\chi}_\alpha(g^2) \in \{0, \pm 1\}, \tag{31}$$

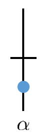
where $\tilde{\chi}_\alpha(g)$ is the irreducible character of α. We also introduce an orthogonal test for the operator $\widetilde{ab}$ by

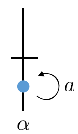
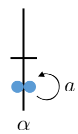
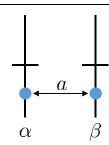
$$O^\Gamma_{\alpha\alpha} = \frac{1}{|G_0|}\sum_{g\in G_0}\left[\frac{\tilde{z}_{g,ab}}{\tilde{z}_{ab,(ab)^{-1}gab}}\tilde{\chi}_\alpha((ab)^{-1}gab)\right]^* \tilde{\chi}_\alpha(g) \in \{0, 1\}. \tag{32}$$

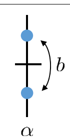
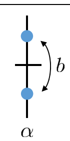
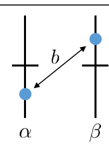
There are 19 patterns of possible combinations of W^T_α, W^C_α, $O^\Gamma_{\alpha\alpha}$, which are shown in Table 1,

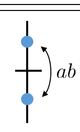
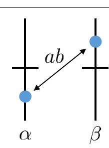
[5] Use the relations $q_{R_g}(\gamma_1\gamma_2\gamma_3) = (\gamma_1\gamma_2\gamma_3)q_{R_g}$ and $\tilde{g}q_{R_h} = q_{R_h}\tilde{g}$.

Table 1. The relationships between the Wigner criteria W^T_α, W^C_α, orthogonal test $O^\Gamma_{\alpha\alpha}$, EAZ classes, and band structures.

EAZ	Band str.
A	

W^T_α	EAZ	Band str.
1	AI	
−1	AII	
0	A_T	

W^C_α	EAZ	Band str.
1	D	
−1	C	
0	A_C	

$O^\Gamma_{\alpha\alpha}$	EAZ	Band str.
1	AIII	
0	A_Γ	

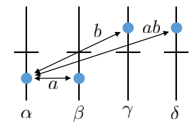
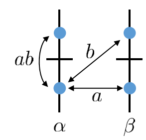
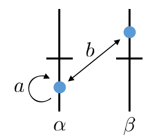
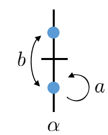
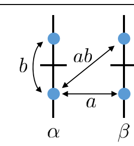
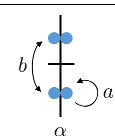
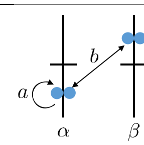
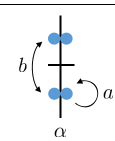
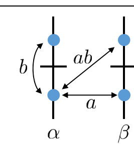
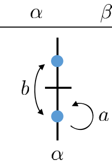
W^T_α	W^C_α	$O^\Gamma_{\alpha\alpha}$	EAZ	Band str.
0	0	0	$\mathrm{A}_{T,C}$	
0	0	1	AIII_T	
1	0	0	AI_C	
1	1	1	BDI	
0	1	0	D_T	
−1	1	1	DIII	
−1	0	0	AII_C	
−1	−1	1	CII	
0	−1	0	C_T	
1	−1	1	CI	

Table 2. The periodic table of TIs/TSCs.

EAZ class	$d=0$	$d=1$	$d=2$	$d=3$	$d=4$	$d=5$	$d=6$	$d=7$
A, A_T, A_C, A_Γ, $A_{T,C}$	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AIII, $AIII_T$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AI, AI_C	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$
D, D_T	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$
AII, AII_C	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
CII	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
C, C_T	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$

and we name them A, AI, AII, A_T, D, C, A_C, AIII, A_Γ, $A_{T,C}$, $AIII_T$, AI_C, BDI, D_T, DIII, AII_C, CII, C_T, and CI. We call them the effective AZ (EAZ) class of α. Given an EAZ class, the topological classification of the mass term $m\Gamma_0$ can be read off from the periodic table of TIs/TSCs [3,4] shown in Table 2. Summing up all the contributions from irreps of G_0, the K-group K of TIs/TSCs is determined.

3.2 *Higher-order TIs/TSCs*

Not every element of the K-group K hosts a gapless surface state since some elements of K may be compatible with spatially varying masses, which we call defect mass terms, that induce a finite energy gap to the surface state. The relationship between the K-group K and surface states is best described by the structure of subgroups [8,9]

$$0 \subset K''' \subset K'' \subset K' \subset K \tag{33}$$

for three space dimensions, where $K^{(n)}$ denotes the Abelian group composed of Dirac Hamiltonians that admit at least n additional defect mass terms [9,14] as in

$$H(\hat{\boldsymbol{k}}, \boldsymbol{r}) = -i\boldsymbol{\gamma} \cdot \partial + m\Gamma_0 + \textstyle\sum_{j=1}^{n} M_j(\boldsymbol{x})\Gamma_j, \tag{34}$$

$$\{\gamma_i, \gamma_j\} = 2\delta_{ij}, \qquad \{\Gamma_i, \Gamma_j\} = 2\delta_{ij}, \qquad \{\gamma_i, \Gamma_j\} = 0. \tag{35}$$

Here, we have introduced $\hat{\boldsymbol{k}} = -i\partial$. The additional defect mass terms $M_j(\boldsymbol{x})\Gamma_j$ decrease the dimensionality of the surface Dirac fermion. By design, the quotient group $K^{(n-1)}/K^{(n)}$ represents Dirac Hamiltonians that admit at most n defect masses, which means that the surface Dirac fermion is constrained on a $(3-n)$-dimensional subregion, and such phases are called nth-order TIs/TSCs. In particular, the group K''' of 4th-order TIs/TSCs, which are composed of Dirac Hamiltonians with 3 defect masses, represents no surface states but a bound state localized at the point group center (i.e., $\boldsymbol{r} = \boldsymbol{0}$).[6]

See Ref. [9] for explicit subgroups (33) for an additional order-two MPG symmetry for the tenfold AZ symmetry classes. For generic MPG symmetry, it is not yet known how to compute all the subgroups in Eq. (33). Nevertheless, in addition to the entire K-group K, one can compute the group K''' of 4th-order TIs/TSCs in a canonical way, as developed in the rest of this section. Therefore, we have the quotient group K/K''', the topological classification of surface states.

[6]Any point group has at least one fixed point under the action of the corresponding symmetry operation, and we call the fixed point the point group center.

3.3 *Dirac Hamiltonian with a hedgehog mass*

Let $K_{\rm AI}$ be the Abelian group generated by atomic insulators exactly at the point group center. The group $K_{\rm AI}$ is nothing but the Abelian group generated by 0D Hamiltonians with the symmetry group G with the homomorphisms ϕ_g, c_g and the factor system $z_{g,h}$. To compute the group K''', we first construct the homomorphism from the group $K_{\rm AI}$ to the group K of TIs/TSCs as follows. There is an isomorphism between the group $K_{\rm AI}$ and the group of 3D Dirac Hamiltonians with a hedgehog-mass potential,

$$H(\hat{\boldsymbol{k}}, \boldsymbol{r}) = \sum_{\mu=1}^{3} -i\partial_\mu \gamma_\mu + m\Gamma_0 + \sum_{\mu=1}^{3} M_\mu(\boldsymbol{r})\Gamma_\mu, \tag{36}$$

with a unit winding number

$$\frac{1}{8\pi}\int_{|\boldsymbol{r}|\to\infty} dS\epsilon_{ij}\epsilon_{\mu\nu\rho}\hat{M}_\mu(\boldsymbol{r})\partial_i\hat{M}_\nu(\boldsymbol{r})\partial_j\hat{M}_\rho(\boldsymbol{r}) = 1, \tag{37}$$

where $\hat{M}_\mu(\boldsymbol{r}) = M_\mu(\boldsymbol{r})/|\boldsymbol{M}(\boldsymbol{r})|$. Here, the amplitude $|\boldsymbol{M}(\boldsymbol{r})|$ of the mass vector $\boldsymbol{M}(\boldsymbol{r}) = (M_1(\boldsymbol{r}), M_2(\boldsymbol{r}), M_3(\boldsymbol{r}))$ is supposed to be finite at the infinity $|\boldsymbol{r}| \to \infty$ so that $H(\hat{\boldsymbol{k}}, \boldsymbol{r})$ hosts an exponentially localized bound state around the point group center. This relationship is, in fact, an isomorphism: As we will see shortly, given an atomic insulator $H_{\rm 0D}$ with symmetry constrained by G, one can construct the 3D Dirac Hamiltonian with a hedgehog mass in the form (36). Conversely, a 3D Dirac Hamiltonian with a hedgehog mass with a unit winding number, we have a 0D bound state that is symmetric under the group G.

Neglecting mass vectors by setting $\boldsymbol{M}(\boldsymbol{r}) \equiv \boldsymbol{0}$ defines the homomorphism f: $K_{\rm AI} \to K$. It should be noted that not every atomic insulator of $K_{\rm AI}$ is pinned at the point group center since some sets of atomic orbitals of $K_{\rm AI}$ can go far away without breaking the G symmetry, and such combinations of atomic orbitals should be zero in the target group K.[7] Thus, the group K''' representing bound states pinned at the point group center is given by the image of f, $K''' := {\rm Im}[f\colon K_{\rm AI} \to K] \subset K$.

As far as the topological classification is concerned, the hedgehog-mass vector with a unit winding number can be set as $M_\mu(\boldsymbol{r}) = r_\mu$. In doing so, the Hamiltonian becomes a Dirac Hamiltonian with six kinetic-like parameters $(\boldsymbol{k}, \boldsymbol{r})$ as

$$H_{\rm 3D}(\boldsymbol{k}, \boldsymbol{r}) = \boldsymbol{k}\cdot\boldsymbol{\gamma} + \boldsymbol{r}\cdot\boldsymbol{\Gamma} + m\Gamma_0. \tag{38}$$

The symmetry constraint is written as

$$\hat{g}H_{\rm 3D}(\boldsymbol{k}, \boldsymbol{r})\hat{g}^{-1} = c_g H_{\rm 3D}(\phi_g O_g \boldsymbol{k}, O_g \boldsymbol{r}). \qquad \hat{g}\hat{h} = z_{g,h}\widehat{gh}. \tag{39}$$

Equivalently, for gamma matrices,

$$\hat{g}\boldsymbol{\gamma}\hat{g}^{-1} = \phi_g c_g O_g^{-1}\boldsymbol{\gamma}, \qquad \hat{g}\boldsymbol{\Gamma}\hat{g}^{-1} = c_g O_g^{-1}\boldsymbol{\Gamma}, \qquad \hat{g}\Gamma_0\hat{g}^{-1} = c_g\Gamma_0. \tag{40}$$

As we did in Section 3.1, we introduce new point group operators $\check{g}$ as

$$\check{g} := (i\gamma_1\gamma_2\gamma_3\Gamma_1\Gamma_2\Gamma_3)^{\frac{1-s_g}{2}} \times q_{R_g} \times Q_{R_g} \times \hat{g}, \tag{41}$$

$$q_R = e^{\frac{\theta}{2}(n_1\gamma_2\gamma_3 + n_2\gamma_3\gamma_1 + n_3\gamma_1\gamma_2)}, \tag{42}$$

$$Q_R = e^{\frac{\theta}{2}(n_1\Gamma_2\Gamma_3 + n_2\Gamma_3\Gamma_1 + n_3\Gamma_1\Gamma_2)}, \tag{43}$$

[7]This is because nonzero elements of K represent either a surface state (i.e., a 1st, 2nd, or 3rd-order TI/TSC) of the 3D ball or a bound state (i.e., a 4th-order TI/TSC) localized and pinned at the point group center.

so that $\breve{g}$ acts on the Hamiltonian as onsite symmetry:

$$\breve{g}H_{\rm 3D}(\boldsymbol{k},\boldsymbol{r})\breve{g}^{-1} = c_g H_{\rm 3D}(\phi_g \boldsymbol{k},\boldsymbol{r}). \tag{44}$$

From a straightforward calculation, we find that $\breve{g}\breve{h} = z_{g,h}\breve{gh}$, i.e., the factor system of the $\breve{g}$ is the same as $z_{g,h}$ for the $\hat{g}$, as expected.

Since there exist the same number of "k-type" and "r-type" coordinates, the topological classification of the mass term $m\Gamma_0$ is recast as that for 0D Hamiltonians $H_{\rm 0D}$ with the same symmetry class, which is dubbed "a defect gapless state as a boundary state" [20]. The explicit construction of the dimensional raising isomorphism is as follows. Let

$$G = G_0^{\rm AI} \coprod \underline{a}G_0^{\rm AI} \coprod \underline{b}G_0^{\rm AI} \coprod \underline{ab}G_0^{\rm AI} \tag{45}$$

be the decomposition of the group G associated with the homomorphisms ϕ_g, c_g. Namely,

$$G_0^{\rm AI} = \{g \in G | \phi_g = c_g = 1\}, \tag{46}$$

$$^{\exists}\underline{a} \in G, \quad -\phi_{\underline{a}} = c_{\underline{a}} = 1, \tag{47}$$

$$^{\exists}\underline{b} \in G, \quad -\phi_{\underline{b}} = -c_{\underline{b}} = 1, \tag{48}$$

$$^{\exists}\underline{ab} \in G, \quad -\phi_{\underline{ab}} = -c_{\underline{ab}} = 1. \tag{49}$$

Let β be an irrep of $G_0^{\rm AI}$ with the factor system $z_{g,h}$. The Wigner criteria and the orthogonal test for the irrep β are defined as

$$\underline{W}_\beta^T = \frac{1}{|G_0^{\rm AI}|}\sum_{g\in \underline{a}G_0^{\rm AI}} z_{g,g}\chi_\beta(g^2) \in \{0,\pm 1\}, \tag{50}$$

$$\underline{W}_\beta^C = \frac{1}{|G_0^{\rm AI}|}\sum_{g\in \underline{b}G_0^{\rm AI}} z_{g,g}\chi_\beta(g^2) \in \{0,\pm 1\}, \tag{51}$$

$$\underline{O}_{\beta\beta}^\Gamma = \frac{1}{|G_0^{\rm AI}|}\sum_{g\in G_0^{\rm AI}} \left[\frac{z_{g,\underline{ab}}}{z_{\underline{ab},(\underline{ab})^{-1}g\underline{ab}}}\chi_\beta((\underline{ab})^{-1}g\underline{ab})\right]^* \chi_\beta(g) \in \{0,1\}. \tag{52}$$

Here, $\chi_\beta(g)$ is the irreducible character of β. The triple $(\underline{W}_\beta^T, \underline{W}_\beta^C, \underline{O}_{\beta\beta}^\Gamma)$ determines the EAZ class as β. Let $D_\beta(g)$ for $g \in G_0^{\rm AI}$ be the representation matrices of the irrep β. We introduce the mapped representation of β by $h \in G$ as

$$D_{h(\beta)}(g \in G_0^{\rm AI}) := \frac{z_{g,h}}{z_{h,h^{-1}gh}} \times \begin{cases} D_\beta(h^{-1}gh) & (\phi_h = 1), \\ D_\beta(h^{-1}gh)^* & (\phi_h = -1). \end{cases} \tag{53}$$

With this, the symmetry operators $\check{g}^{(0\mathrm{D})}$ for the 0D Hamiltonian $H_{0\mathrm{D}}$ are given as, for elements with $\phi_g = c_g = 1$,

$$\check{g}^{(0\mathrm{D})}|_{\phi_g=c_g=1} = \begin{cases} D_\beta(g) & \text{for A, AI,} \\ D_\beta(g) \oplus D_{\underline{a}(\beta)}(g) & \text{for AII, A}_T, \\ \begin{pmatrix} D_\beta(g) & \\ & D_{\underline{b}(\beta)}(g) \end{pmatrix}_\tau & \text{for D, C, A}_C,\ \text{AI}_C,\ \text{BDI, CI,} \\ \begin{pmatrix} D_\beta(g) & \\ & D_{\underline{ab}(\beta)}(g) \end{pmatrix}_\tau & \text{for AIII, A}_\Gamma, \\ \begin{pmatrix} D_\beta(g) \oplus D_{\underline{a}(\beta)}(g) & \\ & D_{\underline{b}(\beta)}(g) \oplus D_{\underline{ab}(\beta)}(g) \end{pmatrix}_\tau & \text{for A}_{T.C},\ \text{AIII}_T,\ \text{D}_T, \\ & \text{DIII, AII}_C,\ \text{CII, C}_T. \end{cases} \tag{54}$$

For other combinations of ϕ_g and c_g, there are proper expressions of the $\check{g}^{(0\mathrm{D})}$, which we do not use later. Here, the subscript τ means the matrix of the particle–hole space. A representative 0D Hamiltonian $H_{0\mathrm{D}}$ is given by $H_{0\mathrm{D}} = \mathbf{1}$ when the group G does not include an element g with $c_g = -1$, or $H_{0\mathrm{D}} = \mathbf{1} \otimes \tau_z$ when the group G includes an element g with $c_g = -1$; we denote the two cases as

$$H_{0\mathrm{D}} = \begin{cases} \mathbf{1} & (c_g = 1, {}^\forall g \in G), \\ \mathbf{1} \otimes \tau_z & (c_g = -1, {}^\exists g \in G). \end{cases} \tag{55}$$

By design, $H_{0\mathrm{D}}$ satisfies the symmetry constraints

$$\check{g}^{(0\mathrm{D})} H_{0\mathrm{D}} (\check{g}^{(0\mathrm{D})})^{-1} = c_g H_{0\mathrm{D}}, \qquad \check{g}^{(0\mathrm{D})} \check{h}^{(0\mathrm{D})} = z_{g,h} \check{gh}^{(0\mathrm{D})} \tag{56}$$

for $g, h \in G$. Starting from the 0D Hamiltonian, we have the dimensional raising isomorphisms:

$$\begin{cases} H_{1\mathrm{D}}(k_1, r_1) := k_1 \sigma_y + r_1 \sigma_x + H_{0\mathrm{D}} \sigma_z, & \check{g}^{(1\mathrm{D})} = \check{g}^{(0\mathrm{D})} \sigma_z^{\frac{1-c_g}{2}}, \\ \check{g}^{(1\mathrm{D})} H(k_1, r_1) (\check{g}^{(1\mathrm{D})})^{-1} = c_g H(\phi_g k_1, r_1), & \check{g}^{(1\mathrm{D})} \check{h}^{(1\mathrm{D})} = z_{g,h} \check{gh}^{(1\mathrm{D})}, \end{cases} \tag{57}$$

$$\begin{cases} H_{2\mathrm{D}}(k_1, k_2, r_1, r_2) := k_2 s_y + r_2 s_x + H_{1\mathrm{D}}(k_1, r_1) s_z, & \check{g}^{(2\mathrm{D})} = \check{g}^{(1\mathrm{D})} s_z^{\frac{1-c_g}{2}}, \\ \check{g}^{(2\mathrm{D})} H(k_1, k_2, r_1, r_2) (\check{g}^{(2\mathrm{D})})^{-1} = c_g H(\phi_g k_1, \phi_g k_2, r_1, r_2), & \check{g}^{(2\mathrm{D})} \check{h}^{(2\mathrm{D})} = z_{g,h} \check{gh}^{(2\mathrm{D})}, \end{cases} \tag{58}$$

$$\begin{cases} H_{3\mathrm{D}}(\boldsymbol{k}, \boldsymbol{r}) = k_3 \mu_y + r_3 \mu_x + H_{2\mathrm{D}}(k_1, k_2, r_1, r_2) \mu_z, & \check{g}^{(3\mathrm{D})} = \check{g}^{(2\mathrm{D})} \mu_z^{\frac{1-c_g}{2}}, \\ \check{g}^{(3\mathrm{D})} H(\boldsymbol{k}, \boldsymbol{r}) (\check{g}^{(3\mathrm{D})})^{-1} = c_g H(\phi_g \boldsymbol{k}, \boldsymbol{r}), & \check{g}^{(3\mathrm{D})} \check{h}^{(3\mathrm{D})} = z_{g,h} \check{gh}^{(3\mathrm{D})}. \end{cases} \tag{59}$$

Here, $\boldsymbol{\sigma}, \boldsymbol{s}, \boldsymbol{\mu}$ are Pauli matrices, and we have abbreviated $(k_1, k_2, k_3, r_1, r_2, r_3)$ by $(\boldsymbol{k}, \boldsymbol{r})$. We eventually have the mapped 3D Hamiltonian $H_{3\mathrm{D}}(\boldsymbol{k}, \boldsymbol{r})$ with the hedgehog-mass term with a unit winding number,

$$H_{3\mathrm{D}}(\boldsymbol{k}, \boldsymbol{r}) = \boldsymbol{k} \cdot \boldsymbol{\gamma} + \boldsymbol{r} \cdot \boldsymbol{\Gamma} + H_{0\mathrm{D}} \Gamma_0, \qquad \check{g}^{(3\mathrm{D})} = \Gamma_0^{\frac{1-c_g}{2}} \check{g}^{(0\mathrm{D})}, \tag{60}$$

with gamma matrices

$$(\boldsymbol{\gamma}, \boldsymbol{\Gamma}, \Gamma_0) = (\sigma_y s_z \mu_z, s_y \mu_z, \mu_y, \sigma_x s_z \mu_z, s_x \mu_z, \mu_x, \sigma_z s_z \mu_z). \tag{61}$$

To have the original MPG operators $\hat{g}$ for the symmetry (39), performing the inverse transformation of Eq. (41), we have the symmetry operators

$$\hat{g} = Q_{R_g}^{-1} \times q_{R_g}^{-1} \times (-i \Gamma_3 \Gamma_2 \Gamma_1 \gamma_3 \gamma_2 \gamma_1)^{\frac{1-s_g}{2}} \times \Gamma_0^{\frac{1-c_g}{2}} \times \check{g}^{(0\mathrm{D})}. \tag{62}$$

This establishes the isomorphism between the group $K_{\rm AI}$ of atomic insulators at the point group center and the group of 3D Dirac Hamiltonians with the hedgehog mass with a unit winding number.

3.4 *Homomorphism f: $K_{\rm AI} \to K$*

Following the previous section, we introduce the operator $\tilde{g}$ acting only on the real space by

$$\tilde{g} := Q_{R_g}^{-1} \times (-i\Gamma_3\Gamma_2\Gamma_1)^{\frac{1-s_g}{2}} \times \Gamma_0^{\frac{1-c_g}{2}} \times \check{g}^{(0{\rm D})}, \tag{63}$$

$$\tilde{g} H_{3{\rm D}}(\boldsymbol{k},\boldsymbol{r})\tilde{g}^{-1} = s_g c_g H\left(\phi_g \boldsymbol{k}, O_g^{-1}\boldsymbol{r}\right). \tag{64}$$

From a straightforward calculation, we see that the factor system of the $\tilde{g}$ matches $\tilde{z}_{g,h}$ introduced in Eq. (23). Neglecting the hedgehog-mass term $\boldsymbol{r}\cdot\boldsymbol{\Gamma}$, we have a Dirac Hamiltonian with a uniform mass

$$\begin{aligned} H'_{3{\rm D}}(\boldsymbol{k}) &:= \boldsymbol{k}\cdot\boldsymbol{\gamma} + H_{0{\rm D}}\Gamma_0, \\ \tilde{g}H'_{3{\rm D}}(\boldsymbol{k})\tilde{g}^{-1} &= s_g c_g H(\phi_g \boldsymbol{k}), \qquad \tilde{g}\tilde{h} = \tilde{z}_{g,h}\widetilde{gh}. \end{aligned} \tag{65}$$

The Hamiltonian $H'_{3{\rm D}}(\boldsymbol{k})$ belongs to the K-group K and may be reducible. Thus, $H'_{3{\rm D}}(\boldsymbol{k})$ is a direct sum of generators of K.

Computing the homomorphism f: $K_{\rm AI} \to K$ is to establish the character formula for the irreducible decomposition of the 3D Dirac Hamiltonians. Let α be an irrep of $G_0 = \{g \in G | \phi_g = c_g s_g = 1\}$ with the modified factor system $\tilde{z}_{g,h}$. When the EAZ class of α is either AIII, AIII$_T$, DIII, or CI, the irrep $\tilde{\alpha}$ contributes to the K-group K as the free Abelian group $\mathbb{Z}$ characterized by the 3D winding number $w_{3{\rm D}}$. When the EAZ class of α is either AII, AII$_C$, or CII, the irrep α contributes to the K-group K as the Abelian group $\mathbb{Z}_2$ characterized by the $\mathbb{Z}_2$ number $\nu_{3{\rm D}}$. In the rest of this subsection, we derive the character formulas to give the matrix element $f|_{\beta\to\alpha}$: $K_{\rm AI}|_\beta \to K|_\alpha$ of the homomorphism f from a given irrep β for $K_{\rm AI}$ to an irrep α for K.

The homomorphism f: $K_{\rm AI} \to K$ takes the form of $f: \mathbb{Z}^n \times \mathbb{Z}_2^m \to \mathbb{Z}^k \times \mathbb{Z}_2^l$. In Appendix C, we summarize how to compute the cokernel of f of this type.

3.4.1 *$\mathbb{Z}$ invariant $w_{3{\rm D}}$ for chiral class.*

Given an irrep α of G_0, if the chiral operator ab exists and preserves the irrep α, namely $O^\Gamma_{\alpha\alpha} = 1$, there exists an irrep $\alpha+$ of $G_0 \coprod abG_0 = \{g \in G | \phi_g = 1\}$ whose restriction on G_0 is α (see Appendix A). By using the irreducible character $\chi_{\alpha+}$ of $\alpha+$, the 3D winding number of the Dirac Hamiltonian $H(\boldsymbol{k}) = \boldsymbol{k}\cdot\boldsymbol{\gamma} + H_{0{\rm D}}\Gamma_0$ with the symmetry operators $\tilde{g}$ is given by (see Appendix B for details)

$$w_{3{\rm D}} = (-1)\times\frac{1}{4}\times\frac{1}{|G_0|}\sum_{g\in abG_0}\chi_{\alpha+}(g)^*{\rm tr}\left[\gamma_1\gamma_2\gamma_3\left\{\begin{matrix}\Gamma_0 & (c_g=1, {}^\forall g\in G)\\ \Gamma_0\tau_z & (c_g=-1, {}^\exists g\in G)\end{matrix}\right\}\tilde{g}\right]. \tag{66}$$

The prefactor (-1) was introduced to make the formula simple. Plugging the expression (63) of $\tilde{g}$ into the above formula, we see that, for $g \in abG_0$,

$$\begin{aligned} \gamma_1\gamma_2\gamma_3\Gamma_0\tilde{g} &= \gamma_1\gamma_2\gamma_3\Gamma_0 \times Q_{R_g}^{-1}\times(-i\Gamma_3\Gamma_2\Gamma_1)^{\frac{1-s_g}{2}}\times\Gamma_0^{\frac{1-c_g}{2}}\times\check{g}^{(0{\rm D})} \\ &= \begin{cases} -Q_{R_g}^{-1}\check{g}^{(0{\rm D})} & (c_g=1), \\ \gamma_1\gamma_2\gamma_3 Q_{R_g}^{-1}\check{g}^{(0{\rm D})} & (c_g=-1). \end{cases} \end{aligned} \tag{67}$$

We have used $\gamma_1\gamma_2\gamma_3\Gamma_0\Gamma_3\Gamma_2\Gamma_1 = -i$ for the gamma matrices (61). Therefore, for the Dirac Hamiltonian (65) obtained by the irrep β of $G_0^{\rm AI}$, the 3D winding number $w_{3{\rm D}}|_{\beta\to\alpha}$ of the irrep α is

$$w_{3\mathrm{D}}|_{\beta\to\alpha} = (-1)\times\frac{1}{4}\times\frac{1}{|G_0|}\sum_{g\in abG_0}\chi_{\alpha+}(g)^*\delta_{c_g,1}(-1)\times\begin{cases}\mathrm{tr}\,[Q_{R_g}^{-1}\check{g}^{(0\mathrm{D})}] & (c_g=1,\,^\forall g\in G),\\ \mathrm{tr}\,[Q_{R_g}^{-1}\tau_z\check{g}^{(0\mathrm{D})}] & (c_g=-1,\,^\exists g\in G),\end{cases}$$

$$= \frac{1}{|G_0|}\sum_{\substack{g\in G,\\ \phi_g=c_g=-s_g=1}}\chi_{\alpha+}(g)^*\times 2\cos\frac{\theta_g}{2}\times\begin{cases}\mathrm{tr}\,[\check{g}^{(0\mathrm{D})}] & (c_g=1,\,^\forall g\in G),\\ \mathrm{tr}\,[\tau_z\check{g}^{(0\mathrm{D})}] & (c_g=-1,\,^\exists g\in G),\end{cases} \tag{68}$$

where we have used $Q_{R_g}^{-1}=\cos\frac{\theta_g}{2}-\sin\frac{\theta_g}{2}\boldsymbol{n}_g\cdot\boldsymbol{\Gamma}$ and $\mathrm{tr}\,[\gamma_1\gamma_2\gamma_3Q_{R_g}]=0$. The last coefficient is given as

$$\begin{cases}\mathrm{tr}\,[\check{g}^{(0\mathrm{D})}] & (c_g=1,\,^\forall g\in G),\\ \mathrm{tr}\,[\tau_z\check{g}^{(0\mathrm{D})}] & (c_g=-1,\,^\exists g\in G),\end{cases}$$

$$=\begin{cases}\chi_\beta(g) & \text{for A, AI},\\ \chi_\beta(g)+\chi_{\underline{a}(\beta)}(g) & \text{for AII, A}_T,\\ \chi_\beta(g)-\chi_{\underline{b}(\beta)}(g) & \text{for D, C, A}_C\text{, AI}_C\text{, BDI, CI},\\ \chi_\beta(g)-\chi_{\underline{ab}(\beta)}(g) & \text{for AIII, A}_\Gamma,\\ \chi_\beta(g)+\chi_{\underline{a}(\beta)}(g)-\chi_{\underline{b}(\beta)}(g)-\chi_{\underline{ab}(\beta)}(g) & \text{for A}_{T.C}\text{, AIII}_T\text{, D}_T\text{, DIII, AII}_C\text{, CII, C}_T.\end{cases} \tag{69}$$

The matrix element $f|_{\beta\to\alpha}:\mathbb{Z}\to\mathbb{Z}$ is eventually given as

$$f|_{\beta\to\alpha}(1)=\begin{cases}w_{3\mathrm{D}}|_{\beta\to\alpha} & (\text{for AIII, DIII}),\\ \frac{1}{2}\times w_{3\mathrm{D}}|_{\beta\to\alpha} & (\text{for CII}).\end{cases} \tag{70}$$

Here, the factor $\frac{1}{2}$ for class CII is needed because the 3D winding number of class CII takes an even integer.

3.4.2 *$\mathbb{Z}_2$ invariant $\nu_{3\mathrm{D}}$ for classes AII and CII.* For an irrep of G_0 whose EAZ class is either AII, AII$_C$, or CII, the mass term is classified by $\mathbb{Z}_2$. Given a Dirac Hamiltonian $H(\boldsymbol{k})=\boldsymbol{k}\cdot\boldsymbol{\gamma}+m\Gamma_0$ with the symmetry operator $\tilde{g}$, the $\mathbb{Z}_2$ invariant $\nu_{3\mathrm{D}}$ for the irrep α is given by

$$\nu_{3\mathrm{D}}=\begin{cases}\frac{1}{4}\times\#(\alpha\text{-irreps})\ (\mathrm{mod}\ 2) & \text{for AII, AII}_C,\\ \frac{1}{8}\times\#(\alpha\text{-irreps})\ (\mathrm{mod}\ 2) & \text{for CII}.\end{cases} \tag{71}$$

Here, the number of α-irreps, denoted by $\#(\alpha\text{-irreps})$, is given by the irreducible decomposition

$$\#(\alpha\text{-irreps})=\frac{1}{|G_0|}\sum_{g\in G_0}\chi_\alpha(g)\mathrm{tr}\,[\tilde{g}]. \tag{72}$$

In particular, for the symmetry operators $\tilde{g}$ given by Eq. (63), noticing that $\phi_g=1$ and $c_gs_g=1$ for $g\in G_0$, we have

$$\#(\alpha\text{-irreps})=\frac{1}{|G_0|}\sum_{g\in G_0}\chi_\alpha(g)\mathrm{tr}\left[Q_{R_g}^{-1}\times(-i\Gamma_3\Gamma_2\Gamma_1)^{\frac{1-s_g}{2}}\times\Gamma_0^{\frac{1-c_g}{2}}\times\check{g}^{(0\mathrm{D})}\right]$$

$$=4\times\frac{1}{|G_0|}\sum_{\substack{g\in G,\\ \phi_g=c_g=s_g=1}}\chi_\alpha(g)^*\times 2\cos\frac{\theta_g}{2}\times\mathrm{tr}\,[\check{g}^{(0\mathrm{D})}]. \tag{73}$$

Here, we have used $\mathrm{tr}\,[Q_{R_g}^{-1}\Gamma_3\Gamma_2\Gamma_1\Gamma_0] = 0$. The last factor is given as

$$\mathrm{tr}\,[\check{g}^{(0\mathrm{D})}] = \begin{cases} \chi_\beta(g) & \text{for A, AI,} \\ \chi_\beta(g) + \chi_{a(\beta)}(g) & \text{for AII, A}_T, \\ \chi_\beta(g) + \chi_{b(\beta)}(g) & \text{for D, C, A}_C, \text{AI}_C, \text{BDI, CI,} \\ \chi_\beta(g) + \chi_{ab(\beta)}(g) & \text{for AIII, A}_\Gamma, \\ \chi_\beta(g) + \chi_{a(\beta)}(g) + \chi_{b(\beta)}(g) + \chi_{ab(\beta)}(g) & \text{for A}_{T.C}, \text{AIII}_T, \text{D}_T, \text{DIII, AII}_C, \\ \text{CII, C}_T. \end{cases} \tag{74}$$

This establishes the formula of the matrix element $f|_{\beta\to\alpha} : \mathbb{Z}$ or $\mathbb{Z}_2 \to \mathbb{Z}_2$:

$$\begin{aligned} f|_{\beta\to\alpha}(1) &= \nu_{3\mathrm{D}}|_{\beta\to\alpha} \\ &= \left\{ \begin{matrix} 1 & \text{for AII, AII}_C, \\ \frac{1}{2} & \text{for CII.} \end{matrix} \right\} \times \frac{1}{|G_0|} \sum_{\substack{g\in G, \\ \phi_g=c_g=p_g=1}} \chi_\alpha(g)^* \times 2\cos\frac{\theta_g}{2} \times \mathrm{tr}\,[\check{g}^{(0\mathrm{D})}] \qquad \mathrm{mod}\ 2. \end{aligned} \tag{75}$$

4. Classification of surface states of TIs and TSCs

In this section, we apply the irreducible character formulas of the homomorphism f: $K_{\mathrm{AI}} \to K$ developed in Section 3 to TIs and TSCs with crystallographic MPGs.

The factor system $z_{g,h}$ for MPGs can be arbitrary in general; however, in this paper we concern ourselves with spinless or spinful electrons, where the factor system is given by

$$z_{g,h} = \begin{cases} 1 & \text{for spinless electrons,} \\ (-1)^{\frac{1-\phi_g}{2}\frac{1-\phi_h}{2}} \times z'_{g,h} & \text{for spinful electrons,} \end{cases} \tag{76}$$

with $z'_{g,h} \in \{\pm 1\}$ being the factor system of the Spin(3) rotations introduced in Eq. (24). The sign $(-1)^{\frac{1-\phi_g}{2}\frac{1-\phi_h}{2}}$ comes from the time-reversal square $\hat{T}^2 = -1$ for spinful electrons.

4.1 *Insulators*

Let G be an MPG. The group element that is unitary or antiunitary is specified by the homomorphism ϕ: $G \to \{\pm 1\}$. For insulators, c_g are identically unity. Let $G_0 = \{g \in G | \phi_g = s_g = 1\}$ be the group of orientation-preserving unitary elements and T, P, and $P_t \in G$ be representatives such that

$$-\phi_T = s_T = 1, \qquad \phi_P = -s_P = 1, \qquad \phi_{P_t} = s_{P_t} = -1, \tag{77}$$

respectively. The group G splits as

$$G = G_0 \coprod TG_0 \coprod P_tG_0 \coprod PG_0. \tag{78}$$

For irreps α of G_0 with the modified factor system $\tilde{z}_{g,h}$ defined by Eq. (23), the Wigner criteria (30), (31) and the orthogonal test (32) determine the EAZ classes. The results are summarized in Table D1 for spinless electrons and Table D2 for spinful electrons. This extends the previous results for some point groups in spinful electrons [18,22]. From the EAZ classes, K-groups K are fixed according to the periodic table (Table 2). For example, MPG 4/m'mm for spinful electrons has the EAZ classes {DIII^2,AII$_C$}, meaning that, in three space dimensions, the K-group, the classification of uniform mass terms, is given by $K = \mathbb{Z}^{\times 2} \times \mathbb{Z}_2$.

Let $G_0^{\mathrm{AI}} = \mathrm{Ker}\,\phi = \{g \in G | \phi_g = 1\}$ be the group composed of unitary symmetries. The group G splits as

$$G = G_0^{\mathrm{AI}} \coprod \underline{a} G_0^{\mathrm{AI}}, \qquad \phi_{\underline{a}} = -1, \tag{79}$$

with $\underline{a}$ a representative of antiunitary symmetry. For an irrep β of G_0^{AI} with the factor system $z_{g,h}$, the Wigner criteria (50), (51) and the orthogonal test (52) determine the EAZ class of β and the K-group K_{AI} of atomic insulators at the point group center. The formulas (70) and (75) give us the homomorphism f: $K_{\mathrm{AI}} \to K$. The Abelian group K''' of 4th-order TIs is given by $K''' = \mathrm{Im} f$, and the classification of surface states reads as the quotient group K/K'''. The groups K/K''' are summarized in Table D3 for spinless electrons and Table D4 for spinful electrons. For example, the surface states compatible with the MPG $\bar{1}1$' composed of time-reversal and inversion symmetries are classified by $K/K''' = \mathbb{Z}_4$ in spinful electrons [17], where it is known that odd integers of $\mathbb{Z}_4 = \{0, 1, 2, 3\}$ correspond to 1st-order TIs, and $2 \in \mathbb{Z}_4$ is the 2nd-order TI that hosts a helical hinge state.

Some comments are in order. (1) No 1D building-block states exist for the classes AI and AII. Therefore, each element of the group K/K''' represents either a 1st- or 2nd-order TI. (2) For MPGs having the ordinary TRS, whose MPG name includes 1', in spinless electrons, we see that no surface states $K/K''' = 0$. This is compatible with the lack of building-block states for 1D, 2D, and 3D in class AI. (3) The 1st-order TI appears if and only if the system is in spinful electrons and the MPG includes the ordinary TRS. The "only if" part is due to the 3D TI being compatible with $O(3) \times \mathbb{Z}_2^T$ symmetry.[8] For other cases, the quotient group K/K''' represents 2nd-order TIs in spinful electrons.

4.2 *Superconductors*

Let G be an MPG equipped with the homomorphism $\phi_g \in \{\pm 1\}$ and the factor system $z_{g,h}$. We assume that the normal part $h(\boldsymbol{k})$ of the Bogoliubov–de Gennes (BdG) Hamiltonian is symmetric under the MPG G,

$$u_g h(\boldsymbol{k}) u_g^{-1} = h(\phi_g O_g \boldsymbol{k}), \qquad u_g u_h = z_{g,h} u_{gh}, \tag{80}$$

where $u_{g \in G}$ represent the transformations for internal degrees of freedom. We assume that the superconducting gap function $\Delta(\boldsymbol{k})$ obeys a 1D representation $e^{i\theta_g} \in U(1)$

[8] The 1st-order 3D TI is represented by the 3D Dirac Hamiltonian

$$\mathcal{H}(\boldsymbol{k}) = \boldsymbol{k} \cdot \boldsymbol{\sigma} \tau_z + m\tau_x,$$

where $\boldsymbol{\sigma}$ is the spin of the electron and τ_μ are the Pauli matrices for the orbital degree of freedom. On this basis, the ordinary TRS is given by $T = i\sigma_y \mathcal{K}$ ($\mathcal{K}$ is the complex conjugation), the $SO(3)$ rotation by the θ-angle around the $\boldsymbol{n}$-axis is $e^{-i\theta \boldsymbol{n}\cdot\boldsymbol{\sigma}/2}$, and the inversion is $I = \mathrm{diag}(-1, -1, -1)$, which constitutes the $O(3) \times \mathbb{Z}_2^T$ symmetry operations.

of G,[9]

$$\Delta(g\boldsymbol{k}) = e^{i\theta_g} \times \begin{cases} u_g \Delta(\boldsymbol{k}) u_g^T & (\phi_g = 1), \\ u_g \Delta(\boldsymbol{k})^* u_g^T & (\phi_g = -1), \end{cases} \tag{81}$$

with the trivial factor system $e^{i\theta_g} e^{i\phi_g \theta_h} = e^{i\theta_{gh}}$.[10] When G involves an antiunitary element possible 1D irreps can be listed in the following manner. Let $G_u = \mathrm{Ker}\phi \subset G$ be a subgroup composed only of unitary elements and $a \in G$ a representative for antiunitary symmetry such that $G = G_u \coprod a G_u$. Given a 1D irrep $\alpha_{1\mathrm{D}}$ of G_u, we have the Wigner criterion $W^T_{\alpha_{1\mathrm{D}}}$ of the irrep $\alpha_{1\mathrm{D}}$ with the trivial factor system. If $W^T_{\alpha_{1\mathrm{D}}} \neq 1$, the induced representation of G is not 1D. Thus, $W^T_{\alpha_{1\mathrm{D}}}$ must be 1. Namely, the set of 1D irreps of G is the set of irreps of G_u with the Wigner criterion $W^T_\alpha = 1$. For elements $g \in aG_u$, the induced representation of G is given by $e^{-i\theta_{a^{-1}g}}$.

For the BdG Hamiltonian

$$H(\boldsymbol{k}) = \begin{pmatrix} h(\boldsymbol{k}) & \Delta(\boldsymbol{k}) \\ \Delta(\boldsymbol{k})^\dagger & -h(-\boldsymbol{k})^T \end{pmatrix}_\tau, \tag{82}$$

the total symmetry group becomes $G \times \mathbb{Z}_2^C$, where $\mathbb{Z}_2^C$ is generated by PHS $\hat{C} = \tau_x \mathcal{K}$ with $\mathcal{K}$ the complex conjugation. It should be noted that the symmetry operators $\hat{g}$ for $g \in G$ depend on the 1D irrep of the gap function as

$$\hat{g} = \begin{cases} \begin{pmatrix} u_g & \\ & e^{i\theta_g} u_g^* \end{pmatrix} & (\phi_g = 1), \\ \begin{pmatrix} u_g & \\ & e^{i\theta_g} u_g^* \end{pmatrix} \times \mathcal{K} & (\phi_g = -1). \end{cases} \tag{83}$$

Let us fix a factor system for the total symmetry group $G \times \mathbb{Z}_2^C$. We define the operators involving $\hat{C}$ by $\widehat{Cg} = \widehat{gC} := \hat{C}\hat{g}$ for $g \in G$. With this choice, by using the equality

$$\hat{g}\hat{C} = e^{i\theta_g} \hat{C}\hat{g}, \qquad g \in G, \tag{84}$$

the factor system is determined as

$$z_{Cg,h} = z_{g,h}^{-1}, \qquad z_{g,Ch} = e^{i\theta_g} z_{g,h}^{-1}, \qquad z_{Cg,Ch} = e^{-i\theta_g} z_{g,h}, \tag{85}$$

for $g, h \in G$. In accordance with the general recipe in Section 3.1, we introduce the modified operators

$$\tilde{g} = (\gamma_1 \gamma_2 \gamma_3)^{\frac{1-s_g}{2}} q_{R_g} \hat{g}, \qquad g \in G \times \mathbb{Z}_2^C \tag{86}$$

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[9] When the gap function $\Delta(\boldsymbol{k})$ obeys an N-dimensional irrep D_α of G, there is a representation basis $\{\Delta_j(\boldsymbol{k})\}_{j=1}^N$ of the vector space in which the gap function lives satisfying

$$\Delta_i(\phi_g g\boldsymbol{k}) = [D_\alpha(g)]_{ij} \times \begin{cases} u_g \Delta_j(\boldsymbol{k}) u_g^T & (\phi_g = 1), \\ u_g \Delta_j(\boldsymbol{k})^* u_g^T & (\phi_g = -1). \end{cases}$$

The gap function $\Delta(\boldsymbol{k})$ is specified by a vector $\boldsymbol{\eta} = (\eta_1, \dots, \eta_N) \in \mathbb{C}^N$ so that $\Delta(\boldsymbol{k}) = \sum_{j=1}^N \eta_j \Delta_j(\boldsymbol{k})$. When the irrep D_α is not a trivial one (namely, an unconventional superconductor), the bare MPG symmetry G is spontaneously broken. Using the $U(1)$-phase rotation of complex fermions by the amount of $e^{-i\theta_g/2}$, we can recover the symmetry of $g \in G$ only when $D_\alpha(g)$ is a pure phase $D_\alpha(g) = e^{i\theta_g} \times \mathbf{1}$. Therefore, we focus only on gap functions obeying 1D irreps of G.

[10] The symmetry constraint (81) implies that $e^{i\theta_g} e^{i\phi_g \theta_h} (z_{g,h})^2 = e^{i\theta_{gh}}$. Therefore, for spinless electrons ($z_{g,h} \equiv 1$) and spinful electrons ($z_{g,h} \in \{\pm 1\}$), the set of $U(1)$ phases $\{e^{i\theta_g}\}_{g\in G}$ is a 1D linear representation of G.

with the modified factor system

$$\tilde{z}_{g,h} = (-1)^{\frac{1-c_g\phi_g}{2}\frac{1-s_h}{2}} \times z'_{g,h} \times z_{g,h}, \qquad g, h \in G \times \mathbb{Z}_2^C. \tag{87}$$

Note that $z'_{Cg,h} = z'_{g,Ch} = z'_{Cg,Ch} = z'_{g,h}$ for $g, h \in G$.

It is useful to introduce the the subgroup $G_* := \{g \in G | \phi_g = s_g = 1\} \subset G$ composed of orientation-preserving unitary elements and representatives T, P, $P_t \in G$ satisfying Eq. (77). The total symmetry group $G \times \mathbb{Z}_2^C$ is then decomposed as

$$G \times \mathbb{Z}_2^C = \underbrace{(G_* \coprod CP_tG_*)}_{G_0} \coprod \underbrace{(TG_* \coprod CPG_*)}_{aG_0} \coprod \underbrace{(P_tG_* \coprod CG_*)}_{bG_0} \coprod \underbrace{(PG_* \coprod CTG_*)}_{abG_0}. \tag{88}$$

Given an irrep α of the group $(G_* \coprod CP_tG_*)$ with the factor system $\tilde{z}_{g,h}$, we get the EAZ class of α from the Wigner criteria (30), (31) and the orthogonal test (32). The results are summarized in Table D5 for spinless electrons and Table D6 for spinful electrons.

The groups K_{AI}, K/K''' are given in the same way as in Section 4.1. Let $G_0^{\mathrm{AI}} = \{g \in G | \phi_g = 1\} \subset G$ be a subgroup composed of unitary symmetries and $\underline{a} \in G$ be a representative of antiunitary symmetry. The total group $G \times \mathbb{Z}_2^C$ splits as

$$G \times \mathbb{Z}_2^C = G_0^{\mathrm{AI}} \coprod \underline{a}G_0^{\mathrm{AI}} \coprod CG_0^{\mathrm{AI}} \coprod \underline{a}CG_0^{\mathrm{AI}}. \tag{89}$$

For an irrep β of G_0^{AI} with the factor system $z_{g,h}$, the Wigner criteria (50), (51) and the orthogonal test (52) determine the EAZ class of β and the K-group K_{AI}. The formulas (70) and (75) give the homomorphism f: $K_{\mathrm{AI}} \to K$. The Abelian group K''' of 4th-order TSCs is given by $K''' = \mathrm{Im} f$, and the classification of surface states is given by the quotient K/K'''. The results of the quotient groups K/K''' are summarized in Table D7 for spinless electrons and Table D8 for spinful electrons. See Table D9 for the character tables of 1D irreps of the gap functions that we used.

In spinful systems, there may exist a 1st-order TSC if the MPG G includes the ordinary TRS T. Let us write such an MPG by $G = G_{\mathrm{nm}} \times \mathbb{Z}_2^T$ with G_{nm} the point group of G. We first note that the set of 1D irreps of $G_{\mathrm{nm}} \times \mathbb{Z}_2^T$ with the trivial factor system is the set of real 1D irreps of G_{nm} since $e^{i\theta_g} = e^{i\theta_{TgT}} = e^{i\theta_T}(e^{i\theta_g}e^{i\theta_T})^* = e^{-i\theta_g}$ for $g \in G_{\mathrm{nm}}$. For the 3D Dirac Hamiltonian $H = k_1\gamma_1 + k_2\gamma_2 + k_3\gamma_3 + m\Gamma_0$, the 3D winding number detecting the 1st-order TSC is written as

$$w_{3\mathrm{D}}^{1\mathrm{st}} = -\frac{1}{4}\mathrm{tr}\,[\gamma_1\gamma_2\gamma_3\Gamma_0(i\hat{C}\hat{T})]. \tag{90}$$

From Eqs. (17), (84) and $\hat{g}\hat{T} = \hat{T}\hat{g}$, the winding number $w_{3\mathrm{D}}^{1\mathrm{st}}$ changes as

$$w_{3\mathrm{D}}^{1\mathrm{st}} \underset{g}{\to} s_g \times e^{i\theta_g} \times w_{3\mathrm{D}}^{1\mathrm{st}} \tag{91}$$

under a nonmagnetic point group $g \in G_{\mathrm{nm}}$. Recall that $s_g = \det[O_g]$ and $e^{i\theta_g} \in \{\pm 1\}$ for $G = G_{\mathrm{nm}} \times \mathbb{Z}_2^T$. We conclude that 1st-order TSCs survive if and only if the gap function $\Delta(\boldsymbol{k})$ is even under orientation-preserving symmetries and odd under orientation-reversing symmetries for $g \in G_{\mathrm{nm}}$. In Table D8, the appearance of the 1st-order TSC is highlighted by bold red characters.

5. Summary and outlook

In this paper, we have developed a way to compare the group K_{AI} of atomic insulators with the bulk K-group K in the presence of MPG symmetry in three space dimensions. As an application, we computed the quotient groups K/K''' of the bulk K-group K and the group K''' of 4th-order TIs/TSCs for all the 122 MPGs and 1D representations of the superconducting gap function, which gives an exhaustive classification of the surface states of 3D TIs and TSCs. The main results are summarized in Tables D1–D8.

Let us close by mentioning future directions.

- The formulation developed in Section 3 is applied only to TIs/TSCs without translation invariance. To apply our method to magnetic space groups that include a lattice translation, we need to properly glue local building-block Dirac Hamiltonians near high-symmetric points together in the whole real space. This can be systematically done by the Atiyah–Hirzebruch spectral sequence based on the *dual* cell decomposition of the real space, which provides an E_∞-page complementary to the Atiyah–Hirzebruch spectral sequence based on the usual cell decomposition discussed in Refs. [10,16]. We leave this problem for future work.
- Our formalism can also be applied to the classification of stable superconducting nodal structures in the Brillouin zone. For example, a point node at the wave number $\boldsymbol{k}_0$ on a high-symmetry line along the k_z-direction is written as a 3D gapless Dirac Hamiltonian $H_{\rm pn}(k_x, k_y, k_z) = (\boldsymbol{k} - \boldsymbol{k}_0) \cdot \boldsymbol{\gamma}$ in the vicinity of $\boldsymbol{k}_0$. On the one hand, any nodal structures, including point, line, and surface nodes, with the nodal point at $\boldsymbol{k}_0$, are described by a gapless 1D Dirac Hamiltonian $H_{\rm n}(k_z) = (k_z - k_{z0})\gamma_z$ on the high-symmetric line. Both types of Hamiltonians $H_{\rm pn}(\boldsymbol{k})$, $H_{\rm n}(k_z)$ are classified and constructed according to the formalism in Section 3. Comparing $H_{\rm pn}(\boldsymbol{k})$ and $H_{\rm n}(k_z)$, one can find whether a nodal point measured on the high-symmetric line is a point node or not.
- In this paper, we focus on three space dimensions. It would be interesting to generalize our character formulas (68), (75) to other space dimensions.

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Appendix A. An extension of irreducible representations

Let G be a finite group equipped with the factor system $\hat{g}\hat{h} = z_{g,h}\widehat{gh}$. Suppose that the group G sits in the short exact sequence $G_0 \to G \to \{e, ab\}$. For an irrep α of G_0, whether the mapped representation $ab(\alpha)$ is unitary equivalent to α or not is determined by the orthogonal test:

$$O^{\Gamma}_{\alpha\alpha} = \frac{1}{|G_0|} \sum_{g \in G_0} \left[\frac{z_{g,ab}}{z_{ab,(ab)^{-1}gab}} \chi_\alpha((ab)^{-1}gab) \right]^* \chi_\alpha(g) \in \{0, 1\}. \tag{A1}$$

Here $\chi_\alpha(g \in G_0)$ is the irreducible character of α. Let $D_\alpha(g)$ be a matrix representation of α. When $O^{\Gamma}_{\alpha\alpha} = 1$, there exists a unitary matrix U such that the relations

$$\frac{z_{g,ab}}{z_{ab,(ab)^{-1}gab}} D_\alpha((ab)^{-1}gab) = U^\dagger D_\alpha(g) U, \qquad g \in G_0, \tag{A2}$$

hold true. From a straightforward calculation, we find that $[U, D_\alpha((ab)^2)] = 0$ and $[D_\alpha(g), D_\alpha((ab)^2)U^{-2}] = 0$ for $g \in G_0$. The latter implies, from Schur's lemma, $U^2 = \lambda D_\alpha((ab)^2)$ with a $U(1)$ phase λ. We fix the $U(1)$ phase by demanding $U^2 = z_{ab,ab} D_\alpha((ab)^2)$, i.e., $\lambda = \pm\sqrt{z_{ab,ab}}$. Picking up a sign of the square root, we set $D_{\alpha+}(ab) := U$. For the representation matrices for other elements $g \in abG_0$, we define $D_{\alpha+}(g(ab)) := z^{-1}_{g,ab} D_\alpha(g) U = z^{-1}_{ab,(ab)^{-1}g(ab)} U D_\alpha((ab)^{-1}g(ab))$ for

$g \in G_0$. One can show that the set of matrices $\{D_{\alpha+}(g)\}_{g\in G_0 \coprod abG_0}$ obeys a projective representation of $G_0 \coprod abG_0$ with the factor system $z_{g,h}$. We note that $D_{\alpha\,+}$ should be irreducible as a representation of $G_0 \coprod abG_0$, because the restricted one D_α on G_0 of $D_{\alpha\,+}$ is irreducible.

The alternative choice $D_{\alpha\,-}(ab) := -U$ gives another inequivalent irrep of $G_0 \coprod abG_0$. In fact, using the equality

$$D_{\alpha-}(g) = \begin{cases} D_{\alpha+}(g) & (g \in G_0), \\ -D_{\alpha+}(g) & (g \in abG_0), \end{cases} \tag{A3}$$

we have

$$\begin{aligned} &\frac{1}{|G_0 \coprod abG_0|} \sum_{g\in(G_0 \coprod abG_0)} [\tilde{D}_{\alpha+}(g)^*]_{ij}[\tilde{D}_{\alpha-}(g)]_{kl} \\ &= \frac{1}{2|G_0|} \sum_{g\in G_0} [D_{\alpha+}(g)^*]_{ij}[D_{\alpha+}(g)]_{kl} - [D_{\alpha+}(gs)^*]_{ij}[D_{\alpha+}(gs)]_{kl}] \\ &= \frac{1}{2|G_0|} \sum_{g\in G_0} \Big[[D_\alpha(g)^*]_{ij}[D_\alpha(g)]_{kl} - [D_\alpha(g)^*]_{im}U^*_{mj}[D_\alpha(g)]_{kn}U_{nl}\Big] \\ &= 0. \end{aligned} \tag{A4}$$

Here, we have used the orthogonality relation between irreps:

$$\frac{1}{|G_0|} \sum_{g\in G_0} [D_\alpha(g)^*]_{ij}[D_\beta(g)]_{kl} = \frac{1}{\dim(\alpha)} \delta_{\alpha\beta}\delta_{ik}\delta_{jl}. \tag{A5}$$

Appendix B. The 3D winding number for Dirac Hamiltonians

Before going on to construct the 3D winding number w_{3D} for generic cases, we first consider the cases where the chiral symmetry Γ is the only symmetry of the system, i.e., AIII of the AZ class. For the Dirac Hamiltonian $H(\boldsymbol{k}) = \boldsymbol{k} \cdot \boldsymbol{\gamma} + m\Gamma_0$ with chiral symmetry $\Gamma H(\boldsymbol{k})\Gamma^{-1} = -H(\boldsymbol{k})$, the 3D winding number w_{3D} is given by

$$w_{3D} = -\frac{1}{4}\mathrm{tr}\,[\gamma_1\gamma_2\gamma_3\Gamma_0\Gamma]. \tag{B1}$$

Actually, the minimal 4 by 4 model $H(\boldsymbol{k}) = \boldsymbol{k} \cdot \boldsymbol{\sigma}\mu_x + m\mu_y$, $\Gamma = \mu_z$ has $w_{3D} = 1$. We should suitably generalize this formula to generic cases.

Let us consider a 3D Dirac Hamiltonian $H(\boldsymbol{k}) = \boldsymbol{k} \cdot \boldsymbol{\gamma} + m\Gamma_0$ with unitary antisymmetry:

$$\tilde{g}H(\boldsymbol{k})\tilde{g}^{-1} = c_g s_g H(\boldsymbol{k}), \qquad g \in G_0 \coprod abG_0. \tag{B2}$$

Let α be an irrep with the orthogonal test $O^\Gamma_{\alpha\alpha} = 1$ so that the 3D winding number w_{3D} is well defined. The integer w_{3D} counts how many times the "irreducible" 3D Dirac Hamiltonians made from the irrep α occur in $H(\boldsymbol{k})$. A subtle point is that the $\tilde{g}$ square for $g \in abG_0$ is not proportional to the identity operator in general, which spoils the formula (B1). Instead, we employ the extended irreps $D_{\alpha+}$ and $D_{\alpha-}$ introduced in Appendix A. The irreps $D_{\alpha+}$ and $D_{\alpha-}$ play the roles of the positive and negative chiralities. To apply the orthogonality relation of the irreducible character, we introduce new operators $\rho(g)$ for $g \in G_0 \coprod abG_0$ with the same factor system $\tilde{z}_{g,h}$ as

$$\rho(g) := (-\gamma_1\gamma_2\gamma_3\Gamma_0)^{\frac{1-c_g s_g}{2}}\tilde{g}, \qquad g \in G_0 \coprod abG_0, \qquad \rho(g)\rho(h) = \tilde{z}_{g,h}\rho(gh), \tag{B3}$$

so that $\rho(g)$ displays unitary symmetry:

$$\rho(g)H(\boldsymbol{k})\rho(g)^{-1} = H(\boldsymbol{k}), \qquad g \in G_0 \coprod abG_0. \tag{B4}$$

Then, given a 3D Dirac Hamiltonian $H(\boldsymbol{k})$ and symmetry operators $\tilde{g}$, $w_{3\mathrm{D}}$ is given as

$$\begin{aligned} w_{3\mathrm{D}} &= \frac{1}{4}\left[\#(\alpha + \text{-irreps in } \rho) - \#(\alpha\text{-irreps in } \rho)\right] \\ &= \frac{1}{4} \times \frac{1}{|G_0 \coprod abG_0|} \sum_{g \in G_0 \coprod abG_0} \{\chi_{\alpha+}(g) - \chi_{\alpha-}(g)\}^* \times \mathrm{tr}\,[\rho(g)] \\ &= -\frac{1}{4} \times \frac{1}{|G_0|} \sum_{g \in abG_0} \chi_{\alpha+}(g)^* \times \mathrm{tr}\,[\gamma_1\gamma_2\gamma_3\Gamma_0\tilde{g}]. \end{aligned} \tag{B5}$$

Appendix C. The cokernel of *f*: $K_{\mathrm{AI}} \to K$

In this appendix, we formulate how to compute the cokernel of the homomorphism between Abelian groups involving $\mathbb{Z}$ and $\mathbb{Z}_2$. Let us consider a homomorphism

$$f : \mathbb{Z}^{\oplus n} \oplus \mathbb{Z}_2^{\oplus m} \to \mathbb{Z}^{\oplus k} \oplus \mathbb{Z}_2^{\oplus l}. \tag{C1}$$

Let $\{x_j\}_{j=1}^n$, $\{y_j\}_{j=1}^m$, $\{z_j\}_{j=1}^k$, $\{w_j\}_{j=1}^l$ be bases of $\mathbb{Z}^{\oplus n}$, $\mathbb{Z}_2^{\oplus m}$, $\mathbb{Z}^{\oplus k}$, $\mathbb{Z}_2^{\oplus l}$, respectively. The representative matrix M, which is defined by

$$f(x_1, \dots, x_n; y_1, \dots, y_m) = (z_1, \dots, z_k; w_1, \dots, w_l)M, \tag{C2}$$

is written as

$$M = \left[\begin{array}{c|c} A & O \\ \hline B & C \end{array}\right], \qquad A \in \mathrm{Mat}_{k\times n}(\mathbb{Z}), \qquad B \in \mathrm{Mat}_{l\times n}(\mathbb{Z}_2), \qquad C \in \mathrm{Mat}_{l\times m}(\mathbb{Z}_2). \tag{C3}$$

Applying the Smith decomposition to C, we have

$$uCv = \left[\begin{array}{c|c} \mathbf{1_p} & O \\ \hline O & O \end{array}\right] \tag{C4}$$

with u, v unimodular matrices. Then, M is written as

$$\begin{aligned} M &= \left[\begin{array}{c|c} \mathbf{1_n} & O \\ \hline O & u^{-1} \end{array}\right] \left[\begin{array}{c|c} A & O \\ \hline uB & \begin{array}{c|c} \mathbf{1_p} & O \\ \hline O & O \end{array} \end{array}\right] \left[\begin{array}{c|c} \mathbf{1_n} & O \\ \hline O & v^{-1} \end{array}\right] \\ &= \left[\begin{array}{c|c} \mathbf{1_n} & O \\ \hline O & u^{-1} \end{array}\right] \left[\begin{array}{c|c} A & O \\ \hline \begin{array}{c} O \\ \hline [uB]_{\mathrm{even}} \end{array} & \begin{array}{c|c} \mathbf{1_p} & O \\ \hline O & O \end{array} \end{array}\right] \left[\begin{array}{c|c} \mathbf{1_n} & O \\ \hline \begin{array}{c} [uB]_{\mathrm{odd}} \\ \hline O \end{array} & v^{-1} \end{array}\right]. \end{aligned} \tag{C5}$$

Here, we have introduced the notation of submatrices:

$$uB = \left[\begin{array}{ccc} [uB]_{1,1} & \cdots & [uB]_{1,n} \\ \vdots & & \vdots \\ [uB]_{p,1} & \cdots & [uB]_{p,n} \\ \hline [uB]_{p+1,1} & \cdots & [uB]_{p+1,n} \\ \vdots & & \vdots \\ [uB]_{l,1} & \cdots & [uB]_{l,n} \end{array}\right] =: \left[\begin{array}{c} [uB]_{\mathrm{odd}} \\ \hline [uB]_{\mathrm{even}} \end{array}\right]. \tag{C6}$$

The problem to compute the cokernel of f is recast as that of the restricted homomorphism

$$f' : \mathbb{Z}^{\oplus n} \to \mathbb{Z}^{\oplus m} \oplus \mathbb{Z}_2^{\oplus(l-p)} \tag{C7}$$

with the representation matrix

$$M' = \begin{bmatrix} A \\ [uB]_{\text{even}} \end{bmatrix}. \tag{C8}$$

This can be done by embedding $\mathbb{Z}_2$ into $\mathbb{Z}$, and taking the quotient of the homomorphism $\mathbb{Z} \xrightarrow{2} \mathbb{Z}$. The cokernel of f' is the same as that of the homomorphism $f'' : \mathbb{Z}^{\oplus(n+l-p)} \to \mathbb{Z}^{\oplus(m+l-p)}$ with the representation matrix

$$M'' = \begin{bmatrix} A & O \\ [uB]_{\text{even}} & \mathbf{2}_{l-p} \end{bmatrix}. \tag{C9}$$

Applying the Smith decomposition to M'', we have

$$u'M''v' = \left[\begin{array}{cccc|c} d_1 & & & & \\ & d_2 & & & \\ & & \ddots & & O \\ & & & d_q & \\ \hline & & O_{m+l-p-q,q} & & O \end{array}\right] \tag{C10}$$

with $d_j (j = 1, \ldots, q)$ nonnegative integers. The cokernel of f is eventually given by

$$\operatorname{coker} f \cong \mathbb{Z}^{\oplus(m+l-p-q)} \oplus \bigoplus_{j=1}^{q} \mathbb{Z}_{d_j}. \tag{C11}$$

Appendix D. Classification tables

This appendix summarizes the classification tables. Tables D1 and D2 show EAZ classes for spinless and spinful electrons, respectively. Tables D3 and D4 show the classification of surface states of 3D TIs for spinless and spinful electrons, respectively. Tables D5 and D6 show EAZ classes for superconductors of spinless and spinful electrons, respectively. Tables D7 and D8 show the classification of surface states of 3D TSCs of spinless and spinful electrons, respectively. In Tables D3, D4, D7, and D8, "Free" and "Tor" stand for the free and torsion parts of the quotient group K/K''', respectively. Table D9 is the character tables for one-dimensional representations of 3D crystallographic point groups which are used to specify the symmetry of the gap function in Tables D5, D6, D7, and D8.

Table D1. EAZ classes for spinless electrons with crystallographic MPG symmetry.

MPG	EAZ	MPG	EAZ	MPG	EAZ
1	{A}	4’22’	{AII}	6/m1’	$\{\mathrm{AIII}_T{}^3\}$
11’	{AI}	42’2’	$\{\mathrm{AII}^4\}$	6’/m	$\{\mathrm{AIII}_T$, CII}
$\bar{1}$	{AIII}	4mm	$\{\mathrm{A}_\Gamma{}^2\}$	6/m’	$\{\mathrm{A}_C{}^3\}$
$\bar{1}$1’	{CI}	4mm1’	$\{\mathrm{D}_T{}^2\}$	6’/m’	$\{\mathrm{AIII}_T$, DIII}
$\bar{1}'$	{C}	4’m’m	$\{\mathrm{D}_T\}$	622	$\{\mathrm{A}^3\}$
2	$\{\mathrm{A}^2\}$	4m’m’	$\{\mathrm{D}^4\}$	6221’	$\{\mathrm{AII}^3\}$
21’	$\{\mathrm{A}_T\}$	$\bar{4}$2m	{AIII}	6’22’	$\{\mathrm{AII}^3\}$
2’	{AII}	$\bar{4}$2m1’	{DIII}	62’2’	$\{\mathrm{AII}^6\}$
m	{AIII}	$\bar{4}$’2’m	$\{\mathrm{AII}_C\}$	6mm	$\{\mathrm{A}_\Gamma{}^3\}$
m1’	{BDI}	$\bar{4}$’2m’	{D}	6mm1’	$\{\mathrm{D}_T{}^3\}$
m’	{D}	$\bar{4}$2’m’	$\{\mathrm{DIII}^2\}$	6’mm’	$\{\mathrm{D}_T$, DIII}
2/m	$\{\mathrm{AIII}^2\}$	4/mmm	$\{\mathrm{AIII}^2\}$	6m’m’	$\{\mathrm{D}^6\}$
2/m1’	$\{\mathrm{AIII}_T\}$	4/mmm1’	$\{\mathrm{DIII}^2\}$	$\bar{6}$m2	{AIII, $\mathrm{A}_\Gamma\}$
2’/m	{CII}	4/m’mm	$\{\mathrm{AII}_C{}^2\}$	$\bar{6}$m21’	$\{\mathrm{D}_T$, DIII}
2/m’	$\{\mathrm{A}_C\}$	4’/mm’m	{DIII}	$\bar{6}$’m’2	$\{\mathrm{D}^3\}$
2’/m’	{DIII}	4’/m’m’m	{DIII}	$\bar{6}$’m2’	{DIII, $\mathrm{AII}_C\}$
222	{A}	4/mm’m’	$\{\mathrm{DIII}^4\}$	$\bar{6}$m’2’	$\{\mathrm{DIII}^3\}$
2221’	{AII}	4/m’m’m’	$\{\mathrm{D}^2\}$	6/mmm	$\{\mathrm{AIII}^3\}$
2’2’2	$\{\mathrm{AII}^2\}$	3	$\{\mathrm{A}^3\}$	6/mmm1’	$\{\mathrm{DIII}^3\}$
mm2	$\{\mathrm{A}_\Gamma\}$	31’	{AI, $\mathrm{A}_T\}$	6/m’mm	$\{\mathrm{AII}_C{}^3\}$
mm21’	$\{\mathrm{D}_T\}$	$\bar{3}$	$\{\mathrm{AIII}^3\}$	6’/mmm’	{DIII, $\mathrm{AII}_C\}$
m’m2’	{DIII}	$\bar{3}$1’	$\{\mathrm{AIII}_T$, CI}	6’/m’mm’	$\{\mathrm{DIII}^3\}$
m’m’2	$\{\mathrm{D}^2\}$	$\bar{3}'$	{C, $\mathrm{A}_C\}$	6/mm’m’	$\{\mathrm{DIII}^6\}$
mmm	{AIII}	32	$\{\mathrm{A}^3\}$	6/m’m’m’	$\{\mathrm{D}^3\}$
mmm1’	{DIII}	321’	{AII, $\mathrm{A}_T\}$	23	$\{\mathrm{A}^3\}$
m’mm	$\{\mathrm{AII}_C\}$	32’	$\{\mathrm{AII}^3\}$	231’	{AII, $\mathrm{A}_T\}$
m’m’m	$\{\mathrm{DIII}^2\}$	3m	{AIII, $\mathrm{A}_\Gamma\}$	m$\bar{3}$	$\{\mathrm{AIII}^3\}$
m’m’m’	{D}	3m1’	{BDI, $\mathrm{D}_T\}$	m$\bar{3}$1’	$\{\mathrm{AIII}_T$, DIII}
4	$\{\mathrm{A}^4\}$	3m’	$\{\mathrm{D}^3\}$	m’$\bar{3}'$	{D, $\mathrm{A}_C\}$
41’	$\{\mathrm{A}_T{}^2\}$	$\bar{3}$m	$\{\mathrm{AIII}^3\}$	432	$\{\mathrm{A}^3\}$
4’	$\{\mathrm{A}_T\}$	$\bar{3}$m1’	$\{\mathrm{AIII}_T$, DIII}	4321’	$\{\mathrm{AII}^3\}$
$\bar{4}$	$\{\mathrm{AIII}^2\}$	$\bar{3}$’m	$\{\mathrm{AII}_C$, CII}	4’32’	$\{\mathrm{AII}^3\}$
$\bar{4}$1’	$\{\mathrm{AIII}_T\}$	$\bar{3}$’m’	{D, $\mathrm{A}_C\}$	$\bar{4}$3m	{AIII, $\mathrm{A}_\Gamma\}$
$\bar{4}'$	$\{\mathrm{A}_C\}$	$\bar{3}$m’	$\{\mathrm{DIII}^3\}$	$\bar{4}$3m1’	$\{\mathrm{D}_T$, DIII}
4/m	$\{\mathrm{AIII}^4\}$	6	$\{\mathrm{A}^6\}$	$\bar{4}$’3m’	$\{\mathrm{D}^3\}$
4/m1’	$\{\mathrm{AIII}_T{}^2\}$	61’	$\{\mathrm{A}_T{}^3\}$	m$\bar{3}$m	$\{\mathrm{AIII}^3\}$
4’/m	$\{\mathrm{AIII}_T\}$	6’	{AII, $\mathrm{A}_T\}$	m$\bar{3}$m1’	$\{\mathrm{DIII}^3\}$
4/m’	$\{\mathrm{A}_C{}^2\}$	$\bar{6}$	$\{\mathrm{AIII}^3\}$	m’$\bar{3}$’m	{DIII, $\mathrm{AII}_C\}$
4’/m’	$\{\mathrm{AIII}_T\}$	$\bar{6}$1’	$\{\mathrm{AIII}_T$, BDI}	m$\bar{3}$m’	$\{\mathrm{DIII}^3\}$
422	$\{\mathrm{A}^2\}$	$\bar{6}'$	{D, $\mathrm{A}_C\}$	m’$\bar{3}$’m’	$\{\mathrm{D}^3\}$
4221’	$\{\mathrm{AII}^2\}$	6/m	$\{\mathrm{AIII}^6\}$		

Table D2. EAZ classes for spinful electrons with crystallographic MPG symmetry.

MPG	EAZ	MPG	EAZ	MPG	EAZ
1	{A}	4’22’	{AII^2, A$_T$}	6/m1’	{AIII$_T{}^2$, DIII^2}
11’	{AII}	42’2’	{AII^4}	6’/m	{AIII$_T$, DIII}
$\bar{1}$	{AIII}	4mm	{AIII^2, A$_\Gamma$}	6/m’	{D^2, A$_C{}^2$}
$\bar{1}$1’	{DIII}	4mm1’	{D$_T$, DIII^2}	6’/m’	{AIII$_T$, DIII}
$\bar{1}'$	{D}	4’m’m	{BDI, DIII}	622	{A^6}
2	{A^2}	4m’m’	{D^4}	6221’	{AII^6}
21’	{AII^2}	$\bar{4}$2m	{AIII^2, A$_\Gamma$}	6’22’	{AII^3}
2’	{AII}	$\bar{4}$2m1’	{DIII^2, AII$_C$}	62’2’	{AII^6}
m	{AIII}	$\bar{4}$’2’m	{DIII, CII}	6mm	{AIII^2, A$_\Gamma{}^2$}
m1’	{DIII}	$\bar{4}$’2m’	{D^2, A$_C$}	6mm1’	{D$_T{}^2$, DIII^2}
m’	{D}	$\bar{4}$2’m’	{DIII^2}	6’mm’	{D$_T$, DIII}
2/m	{AIII^2}	4/mmm	{AIII^5}	6m’m’	{D^6}
2/m1’	{DIII^2}	4/mmm1’	{DIII^5}	$\bar{6}$m2	{AIII^3}
2’/m	{DIII}	4/m’mm	{DIII^2, AII$_C$}	$\bar{6}$m21’	{DIII^3}
2/m’	{D^2}	4’/mm’m	{AIII$_T$, DIII^2}	$\bar{6}$’m’2	{D^3}
2’/m’	{DIII}	4’/m’m’m	{D$_T$, DIII^2}	$\bar{6}$’m2’	{DIII, AII$_C$}
222	{A^4}	4/mm’m’	{DIII^4}	$\bar{6}$m’2’	{DIII^3}
2221’	{AII^4}	4/m’m’m’	{D^5}	6/mmm	{AIII^6}
2’2’2	{AII^2}	3	{A^3}	6/mmm1’	{DIII^6}
mm2	{AIII^2}	31’	{AII, A$_T$}	6/m’mm	{DIII^2, AII$_C{}^2$}
mm21’	{DIII^2}	$\bar{3}$	{AIII^3}	6’/mmm’	{DIII^3}
m’m2’	{DIII}	$\bar{3}$1’	{AIII$_T$, DIII}	6’/m’mm’	{DIII^3}
m’m’2	{D^2}	$\bar{3}'$	{D, A$_C$}	6/mm’m’	{DIII^6}
mmm	{AIII^4}	32	{A^3}	6/m’m’m’	{D^6}
mmm1’	{DIII^4}	321’	{AII^3}	23	{A^4}
m’mm	{DIII^2}	32’	{AII^3}	231’	{AII^2, A$_T$}
m’m’m	{DIII^2}	3m	{AIII, A$_\Gamma$}	m$\bar{3}$	{AIII^4}
m’m’m’	{D^4}	3m1’	{D$_T$, DIII}	m$\bar{3}$1’	{AIII$_T$, DIII^2}
4	{A^4}	3m’	{D^3}	m’$\bar{3}'$	{D^2, A$_C$}
41’	{AII^2, A$_T$}	$\bar{3}$m	{AIII^3}	432	{A^5}
4’	{AI, AII}	$\bar{3}$m1’	{DIII^3}	4321’	{AII^5}
$\bar{4}$	{AIII^2}	$\bar{3}$’m	{DIII, AII$_C$}	4’32’	{AII^4}
$\bar{4}$1’	{DIII, CII}	$\bar{3}$’m’	{D^3}	$\bar{4}$3m	{AIII^2, A$_\Gamma$}
$\bar{4}'$	{D, C}	$\bar{3}$m’	{DIII^3}	$\bar{4}$3m1’	{D$_T$, DIII^2}
4/m	{AIII^4}	6	{A^6}	$\bar{4}$’3m’	{D^4}
4/m1’	{AIII$_T$, DIII^2}	61’	{AII^2, A$_T{}^2$}	m$\bar{3}$m	{AIII^5}
4’/m	{DIII, CI}	6’	{AII, A$_T$}	m$\bar{3}$m1’	{DIII^5}
4/m’	{D^2, A$_C$}	$\bar{6}$	{AIII^3}	m’$\bar{3}$’m	{DIII^2, AII$_C$}
4’/m’	{BDI, DIII}	$\bar{6}$1’	{AIII$_T$, DIII}	m$\bar{3}$m’	{DIII^4}
422	{A^5}	$\bar{6}'$	{D, A$_C$}	m’$\bar{3}$’m’	{D^5}
4221’	{AII^5}	6/m	{AIII^6}		

Table D3. The classification of surface states of 3D TIs of spinless electrons with crystallographic MPG symmetry.

MPG	Free	Tor	MPG	Free	Tor	MPG	Free	Tor
1	0	{}	4’22’	0	{}	6/m1’	0	{}
11’	0	{}	42’2’	0	{2}	6’/m	0	{}
$\bar{1}$	0	{2}	4mm	0	{}	6/m’	0	{}
$\bar{1}$1’	0	{}	4mm1’	0	{}	6’/m’	0	{2}
$\bar{1}'$	0	{}	4’m’m	0	{}	622	0	{}
2	0	{}	4m’m’	0	{}	6221’	0	{}
21’	0	{}	$\bar{4}$2m	0	{}	6’22’	0	{2}
2’	0	{2}	$\bar{4}$2m1’	0	{}	62’2’	0	{2}
m	1	{}	$\bar{4}$’2’m	0	{}	6mm	0	{}
m1’	0	{}	$\bar{4}$’2m’	0	{}	6mm1’	0	{}
m’	0	{}	$\bar{4}$2’m’	0	{2}	6’mm’	1	{}
2/m	1	{}	4/mmm	0	{}	6m’m’	0	{}
2/m1’	0	{}	4/mmm1’	0	{}	$\bar{6}$m2	0	{}
2’/m	0	{}	4/m’mm	0	{}	$\bar{6}$m21’	0	{}
2/m’	0	{}	4’/mm’m	0	{}	$\bar{6}$’m’2	0	{}
2’/m’	0	{2}	4’/m’m’m	0	{}	$\bar{6}$’m2’	1	{}
222	0	{}	4/mm’m’	1	{}	$\bar{6}$m’2’	1	{}
2221’	0	{}	4/m’m’m’	0	{}	6/mmm	0	{}
2’2’2	0	{2}	3	0	{}	6/mmm1’	0	{}
mm2	0	{}	31’	0	{}	6/m’mm	0	{}
mm21’	0	{}	$\bar{3}$	0	{2}	6’/mmm’	0	{}
m’m2’	1	{}	$\bar{3}$1’	0	{}	6’/m’mm’	1	{}
m’m’2	0	{}	$\bar{3}'$	0	{}	6/mm’m’	1	{}
mmm	0	{}	32	0	{}	6/m’m’m’	0	{}
mmm1’	0	{}	321’	0	{}	23	0	{}
m’mm	0	{}	32’	0	{2}	231’	0	{}
m’m’m	1	{}	3m	1	{}	m$\bar{3}$	0	{}
m’m’m’	0	{}	3m1’	0	{}	m$\bar{3}$1’	0	{}
4	0	{}	3m’	0	{}	m’$\bar{3}'$	0	{}
41’	0	{}	$\bar{3}$m	1	{}	432	0	{}
4’	0	{}	$\bar{3}$m1’	0	{}	4321’	0	{}
$\bar{4}$	0	{2}	$\bar{3}$’m	0	{}	4’32’	0	{}
$\bar{4}$1’	0	{}	$\bar{3}$’m’	0	{}	$\bar{4}$3m	0	{}
$\bar{4}'$	0	{}	$\bar{3}$m’	0	{2}	$\bar{4}$3m1’	0	{}
4/m	1	{}	6	0	{}	$\bar{4}$’3m’	0	{}
4/m1’	0	{}	61’	0	{}	m$\bar{3}$m	0	{}
4’/m	0	{}	6’	0	{2}	m$\bar{3}$m1’	0	{}
4/m’	0	{}	$\bar{6}$	1	{}	m’$\bar{3}$’m	0	{}
4’/m’	0	{}	$\bar{6}$1’	0	{}	m$\bar{3}$m’	0	{}
422	0	{}	$\bar{6}'$	0	{}	m’$\bar{3}$’m’	0	{}
4221’	0	{}	6/m	1	{}			

Table D4. The classification of surface states of 3D TIs of spinful electrons with crystallographic MPG symmetry.

MPG	Free	Tor	MPG	Free	Tor	MPG	Free	Tor
1	0	{}	4’22’	0	{2}	6/m1’	1	{2}
11’	0	{2}	42’2’	0	{2}	6’/m	1	{}
$\bar{1}$	0	{2}	4mm	2	{}	6/m’	0	{}
$\bar{1}$1’	0	{4}	4mm1’	2	{}	6’/m’	0	{2}
$\bar{1}'$	0	{}	4’m’m	1	{}	622	0	{}
2	0	{}	4m’m’	0	{}	6221’	0	{2, 2, 2}
21’	0	{2, 2}	$\bar{4}$2m	1	{}	6’22’	0	{2}
2’	0	{2}	$\bar{4}$2m1’	1	{2}	62’2’	0	{2}
m	1	{}	$\bar{4}$’2’m	1	{}	6mm	2	{}
m1’	1	{}	$\bar{4}$’2m’	0	{}	6mm1’	2	{}
m’	0	{}	$\bar{4}$2’m’	0	{2}	6’mm’	1	{}
2/m	1	{}	4/mmm	3	{}	6m’m’	0	{}
2/m1’	1	{2}	4/mmm1’	3	{}	$\bar{6}$m2	2	{}
2’/m	1	{}	4/m’mm	2	{}	$\bar{6}$m21’	2	{}
2/m’	0	{}	4’/mm’m	2	{}	$\bar{6}$’m’2	0	{}
2’/m’	0	{2}	4’/m’m’m	1	{}	$\bar{6}$’m2’	1	{}
222	0	{}	4/mm’m’	1	{}	$\bar{6}$m’2’	1	{}
2221’	0	{2, 2, 2}	4/m’m’m’	0	{}	6/mmm	3	{}
2’2’2	0	{2}	3	0	{}	6/mmm1’	3	{}
mm2	2	{}	31’	0	{2}	6/m’mm	2	{}
mm21’	2	{}	$\bar{3}$	0	{2}	6’/mmm’	2	{}
m’m2’	1	{}	$\bar{3}$1’	0	{4}	6’/m’mm’	1	{}
m’m’2	0	{}	$\bar{3}'$	0	{}	6/mm’m’	1	{}
mmm	3	{}	32	0	{}	6/m’m’m’	0	{}
mmm1’	3	{}	321’	0	{2, 2}	23	0	{}
m’mm	2	{}	32’	0	{2}	231’	0	{2}
m’m’m	1	{}	3m	1	{}	m$\bar{3}$	1	{}
m’m’m’	0	{}	3m1’	1	{}	m$\bar{3}$1’	1	{}
4	0	{}	3m’	0	{}	m’$\bar{3}'$	0	{}
41’	0	{2, 2}	$\bar{3}$m	1	{}	432	0	{}
4’	0	{2}	$\bar{3}$m1’	1	{2}	4321’	0	{2, 2}
$\bar{4}$	0	{2}	$\bar{3}$’m	1	{}	4’32’	0	{2}
$\bar{4}$1’	0	{4}	$\bar{3}$’m’	0	{}	$\bar{4}$3m	1	{}
$\bar{4}'$	0	{}	$\bar{3}$m’	0	{2}	$\bar{4}$3m1’	1	{}
4/m	1	{}	6	0	{}	$\bar{4}$’3m’	0	{}
4/m1’	1	{2}	61’	0	{2, 2}	m$\bar{3}$m	2	{}
4’/m	1	{}	6’	0	{2}	m$\bar{3}$m1’	2	{}
4/m’	0	{}	$\bar{6}$	1	{}	m’$\bar{3}$’m	1	{}
4’/m’	0	{2}	$\bar{6}$1’	1	{}	m$\bar{3}$m’	1	{}
422	0	{}	$\bar{6}'$	0	{}	m’$\bar{3}$’m’	0	{}
4221’	0	{2, 2, 2}	6/m	1	{}			

Table D5. EAZ classes of superconductors of spinless electrons with crystallographic MPG symmetry.

MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ
1	1	A	{D}	m'mm	2mm	A_2	$\{A_{T,C}\}$	4m'm'	4	^1E	$\{D^5\}$
11'	1	A	{BDI}	m'mm	2mm	B_2	{DIII}	$\bar{4}2m$	$\bar{4}2m_{110}$	A_1	{CII}
$\bar{1}$	$\bar{1}$	A_g	{BDI}	m'mm	2mm	B_1	{DIII}	$\bar{4}2m$	$\bar{4}2m_{110}$	B_1	{CI}
$\bar{1}$	$\bar{1}$	A_u	{DIII}	m'm'm	112/m	A_g	{DIII}	$\bar{4}2m$	$\bar{4}2m_{110}$	B_2	{DIII}
$\bar{1}1'$	$\bar{1}$	A_g	$\{AI_C\}$	m'm'm	112/m	A_u	{DIII}	$\bar{4}2m$	$\bar{4}2m_{110}$	A_2	{BDI}
$\bar{1}1'$	$\bar{1}$	A_u	$\{AIII_T\}$	m'm'm	112/m	B_g	$\{D_T{}^2\}$	$\bar{4}2m1'$	$\bar{4}2m_{110}$	A_1	$\{AII_C\}$
$\bar{1}'$	1	A	$\{A_C\}$	m'm'm	112/m	B_u	$\{DIII^4\}$	$\bar{4}2m1'$	$\bar{4}2m_{110}$	B_1	$\{AIII_T\}$
2	121	A	$\{A_C\}$	m'm'm'	222	A_1	$\{A_C\}$	$\bar{4}2m1'$	$\bar{4}2m_{110}$	B_2	$\{DIII^2\}$
2	121	B	$\{D^2\}$	m'm'm'	222	B_3	$\{D^2\}$	$\bar{4}2m1'$	$\bar{4}2m_{110}$	A_2	$\{D_T\}$
21'	121	A	$\{AIII_T\}$	m'm'm'	222	B_2	$\{D^2\}$	$\bar{4}'2'm$	$m_{110}m_{1\bar{1}0}2$	A_1	$\{AII_C{}^2\}$
21'	121	B	$\{D_T\}$	m'm'm'	222	B_1	$\{D^2\}$	$\bar{4}'2'm$	$m_{110}m_{1\bar{1}0}2$	A_2	$\{A_{T,C}\}$
2'	1	A	{DIII}	4	4	A	$\{A_C{}^2\}$	$\bar{4}'2m'$	222	A_1	$\{A_C\}$
m	1m1	A'	{DIII}	4	4	B	$\{A_C{}^2\}$	$\bar{4}'2m'$	222	B_1	$\{D^2\}$
m	1m1	A"	{BDI}	4	4	^2E	$\{D^2, A_C\}$	$\bar{4}2'm'$	$\bar{4}$	A	{DIII}
m1'	1m1	A'	$\{D_T\}$	4	4	^1E	$\{D^2, A_C\}$	$\bar{4}2'm'$	$\bar{4}$	B	{DIII}
m1'	1m1	A"	$\{BDI^2\}$	41'	4	A	$\{AIII_T{}^2\}$	$\bar{4}2'm'$	$\bar{4}$	^2E	$\{D_T, DIII^2\}$
m'	1	A	$\{D^2\}$	41'	4	B	$\{A_{T,C}\}$	$\bar{4}2'm'$	$\bar{4}$	^1E	$\{D_T, DIII^2\}$
2/m	12/m1	A_g	$\{AIII_T\}$	4'	112	A	$\{AIII_T\}$	4/mmm	4/mmm	A_{1g}	$\{CII^2\}$
2/m	12/m1	A_u	$\{AIII_T\}$	$\bar{4}$	$\bar{4}$	A	$\{AIII_T\}$	4/mmm	4/mmm	A_{1u}	$\{CI^2\}$
2/m	12/m1	B_g	$\{BDI^2\}$	$\bar{4}$	$\bar{4}$	B	$\{AIII_T\}$	4/mmm	4/mmm	B_{1g}	$\{AIII_T\}$
2/m	12/m1	B_u	$\{DIII^2\}$	$\bar{4}$	$\bar{4}$	^2E	{BDI, DIII}	4/mmm	4/mmm	B_{1u}	$\{AIII_T\}$
2/m1'	12/m1	A_g	$\{A_{T,C}\}$	$\bar{4}$	$\bar{4}$	^1E	{BDI, DIII}	4/mmm	4/mmm	B_{2g}	$\{AIII_T\}$
2/m1'	12/m1	A_u	$\{AIII_T{}^2\}$	$\bar{4}1'$	$\bar{4}$	A	$\{A_{T,C}\}$	4/mmm	4/mmm	B_{2u}	$\{AIII_T\}$
2/m1'	12/m1	B_g	{BDI}	$\bar{4}1'$	$\bar{4}$	B	$\{AIII_T{}^2\}$	4/mmm	4/mmm	A_{2g}	$\{BDI^2\}$
2/m1'	12/m1	B_u	{DIII}	$\bar{4}'$	112	A	$\{A_C{}^2\}$	4/mmm	4/mmm	A_{2u}	$\{DIII^2\}$
2'/m	1m1	A'	$\{AII_C\}$	4/m	4/m	A_g	$\{AIII_T{}^2\}$	4/mmm1'	4/mmm	A_{1g}	$\{AII_C{}^2\}$
2'/m	1m1	A"	$\{AIII_T\}$	4/m	4/m	A_u	$\{AIII_T{}^2\}$	4/mmm1'	4/mmm	A_{1u}	$\{AIII_T{}^2\}$
2/m'	121	A	$\{A_C{}^2\}$	4/m	4/m	B_g	$\{AIII_T{}^2\}$	4/mmm1'	4/mmm	B_{1g}	{DIII}
2/m'	121	B	{D}	4/m	4/m	B_u	$\{AIII_T{}^2\}$	4/mmm1'	4/mmm	B_{1u}	{DIII}
2'/m'	$\bar{1}$	A_g	$\{D_T\}$	4/m	4/m	^2E_g	$\{AIII_T, BDI^2\}$	4/mmm1'	4/mmm	B_{2g}	{DIII}
2'/m'	$\bar{1}$	A_u	$\{DIII^2\}$	4/m	4/m	^2E_u	$\{AIII_T, DIII^2\}$	4/mmm1'	4/mmm	B_{2u}	{DIII}

Table D5. Continued

MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ
222	222	A_1	{C}	4/m	4/m	^1E_g	$\{AIII_T, BDI^2\}$	4/mmm1’	4/mmm	A_{2g}	$\{D_T{}^2\}$
222	222	B_3	{D}	4/m	4/m	^1E_u	$\{AIII_T, DIII^2\}$	4/mmm1’	4/mmm	A_{2u}	$\{DIII^4\}$
222	222	B_2	{D}	4/m1’	4/m	A_g	$\{A_{T,C}{}^2\}$	4/m’mm	4mm	A_1	$\{AII_C{}^4\}$
222	222	B_1	{D}	4/m1’	4/m	A_u	$\{AIII_T{}^4\}$	4/m’mm	4mm	A_2	$\{A_{T,C}{}^2\}$
2221’	222	A_1	{CII}	4/m1’	4/m	B_g	$\{AIII_T\}$	4/m’mm	4mm	B_1	$\{AII_C\}$
2221’	222	B_3	{DIII}	4/m1’	4/m	B_u	$\{AIII_T\}$	4/m’mm	4mm	B_2	$\{AII_C\}$
2221’	222	B_2	{DIII}	4’/m	112/m	A_g	$\{A_{T,C}\}$	4’/mm’m	$m_{110}m_{1\bar{1}0}m$	A_g	$\{AII_C\}$
2221’	222	B_1	{DIII}	4’/m	112/m	A_u	$\{AIII_T{}^2\}$	4’/mm’m	$m_{110}m_{1\bar{1}0}m$	A_u	$\{AIII_T\}$
2’2’2	112	A	$\{AII_C\}$	4/m’	4	A	$\{A_C{}^4\}$	4’/mm’m	$m_{110}m_{1\bar{1}0}m$	B_{1g}	$\{D_T\}$
2’2’2	112	B	$\{DIII^2\}$	4/m’	4	B	$\{A_C\}$	4’/mm’m	$m_{110}m_{1\bar{1}0}m$	B_{1u}	$\{DIII^2\}$
mm2	mm2	A_1	$\{AII_C\}$	4’/m’	$\bar{4}$	A	$\{A_{T,C}\}$	4’/m’m’m	$\bar{4}2m_{110}$	A_1	$\{AII_C\}$
mm2	mm2	A_2	$\{AI_C\}$	4’/m’	$\bar{4}$	B	$\{AIII_T{}^2\}$	4’/m’m’m	$\bar{4}2m_{110}$	B_1	$\{AIII_T\}$
mm2	mm2	B_2	$\{D_T\}$	422	422	A_1	$\{C^2\}$	4’/m’m’m	$\bar{4}2m_{110}$	B_2	$\{DIII^2\}$
mm2	mm2	B_1	$\{D_T\}$	422	422	B_1	$\{A_C\}$	4’/m’m’m	$\bar{4}2m_{110}$	A_2	$\{D_T\}$
mm21’	mm2	A_1	{DIII}	422	422	B_2	$\{A_C\}$	4/mm’m’	4/m	A_g	$\{DIII^2\}$
mm21’	mm2	A_2	{BDI}	422	422	A_2	$\{D^2\}$	4/mm’m’	4/m	A_u	$\{DIII^2\}$
mm21’	mm2	B_2	$\{D_T{}^2\}$	4221’	422	A_1	$\{CII^2\}$	4/mm’m’	4/m	B_g	$\{DIII^2\}$
mm21’	mm2	B_1	$\{D_T{}^2\}$	4221’	422	B_1	$\{AII_C\}$	4/mm’m’	4/m	B_u	$\{DIII^2\}$
m’m2’	1m1	A’	$\{DIII^2\}$	4221’	422	B_2	$\{AII_C\}$	4/mm’m’	4/m	^2E_g	$\{D_T{}^2, DIII\}$
m’m2’	1m1	A”	$\{D_T\}$	4221’	422	A_2	$\{DIII^2\}$	4/mm’m’	4/m	^2E_u	$\{DIII^5\}$
m’m’2	112	A	{D}	4’22’	222	A_1	{CII}	4/mm’m’	4/m	^1E_g	$\{D_T{}^2, DIII\}$
m’m’2	112	B	$\{D^4\}$	4’22’	222	B_1	{DIII}	4/mm’m’	4/m	^1E_u	$\{DIII^5\}$
mmm	mmm	A_g	{CII}	42’2’	4	A	$\{AII_C{}^2\}$	4/m’m’m’	422	A_1	$\{A_C{}^2\}$
mmm	mmm	A_u	{CI}	42’2’	4	B	$\{AII_C{}^2\}$	4/m’m’m’	422	B_1	{D}
mmm	mmm	B_{3g}	{BDI}	42’2’	4	^2E	$\{DIII^2, AII_C\}$	4/m’m’m’	422	B_2	{D}
mmm	mmm	B_{3u}	{DIII}	42’2’	4	^2E	$\{DIII^2, AII_C\}$	4/m’m’m’	422	A_2	$\{D^4\}$
mmm	mmm	B_{2g}	{BDI}	4mm	4mm	A_1	$\{AII_C{}^2\}$	3	3	A	$\{D, A_C\}$
mmm	mmm	B_{2u}	{DIII}	4mm	4mm	A_2	$\{AI_C{}^2\}$	3	3	^2E	$\{D, A_C\}$
mmm	mmm	B_{1g}	{BDI}	4mm	4mm	B_1	$\{A_{T,C}\}$	3	3	^1E	$\{D, A_C\}$
mmm	mmm	B_{1u}	{DIII}	4mm	4mm	B_2	$\{A_{T,C}\}$	31’	3	A	$\{AIII_T, BDI\}$
mmm1’	mmm	A_g	$\{AII_C\}$	4mm1’	4mm	A_1	$\{DIII^2\}$	$\bar{3}$	$\bar{3}$	A_g	$\{AIII_T, BDI\}$

Table D5. Continued

MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ
mmm1’	mmm	A_u	{AIII$_T$}	4mm1’	4mm	A_2	{BDI^2}	$\bar{3}$	$\bar{3}$	^2E_g	{AIII$_T$, BDI}
mmm1’	mmm	B_{3g}	{D$_T$}	4mm1’	4mm	B_1	{D$_T$}	$\bar{3}$	$\bar{3}$	^1E_g	{AIII$_T$, BDI}
mmm1’	mmm	B_{3u}	{DIII^2}	4mm1’	4mm	B_2	{D$_T$}	$\bar{3}$	$\bar{3}$	A_u	{AIII$_T$, DIII}
mmm1’	mmm	B_{2g}	{D$_T$}	4’m’m	$m_{110}m_{1\bar{1}0}2$	A_1	{DIII}	$\bar{3}$	$\bar{3}$	^2E_u	{AIII$_T$, DIII}
mmm1’	mmm	B_{2u}	{DIII^2}	4’m’m	$m_{110}m_{1\bar{1}0}2$	A_2	{BDI}	$\bar{3}$	$\bar{3}$	^1E_u	{AIII$_T$, DIII}
mmm1’	mmm	B_{1g}	{D$_T$}	4m’m’	4	A	{D^2}	$\bar{3}$1’	$\bar{3}$	A_g	{A$_{T,C}$, AI$_C$}
mmm1’	mmm	B_{1u}	{DIII^2}	4m’m’	4	B	{D^2}	$\bar{3}$1’	$\bar{3}$	A_u	{AIII$_T{}^3$}
m’mm	2mm	A_1	{AII$_C{}^2$}	4m’m’	4	^{2}E	{D^5}	$\bar{3}'$	3	A	{A$_C{}^3$}
32	$32_{100}1$	A_1	{C, A$_C$}	6’/m’	$\bar{3}$	A_g	{A$_{T,C}$, D$_T$}	6/m’mm	6mm	B_1	{DIII, AII$_C$}
32	$32_{100}1$	A_2	{D^3}	6’/m’	$\bar{3}$	A_u	{AIII$_T{}^2$, DIII^2}	6/m’mm	6mm	B_2	{DIII, AII$_C$}
321’	$32_{100}1$	A_1	{AIII$_T$, CII}	622	622	A_1	{C^3}	6’/mmm’	$\bar{6}2_{210}m_{100}$	A’$_1$	{AII$_C{}^3$}
321’	$32_{100}1$	A_2	{D$_T$, DIII}	622	622	B_2	{D, A$_C$}	6’/mmm’	$\bar{6}2_{210}m_{100}$	A”$_1$	{A$_{T,C}$, AIII$_T$}
32’	3	A	{DIII, AII$_C$}	622	622	B_1	{D, A$_C$}	6’/mmm’	$\bar{6}2_{210}m_{100}$	A”$_2$	{DIII^3}
32’	3	^{2}E	{DIII, AII$_C$}	622	622	A_2	{D^3}	6’/mmm’	$\bar{6}2_{210}m_{100}$	A’$_2$	{D$_T$, DIII}
32’	3	^{1}E	{DIII, AII$_C$}	6221’	622	A_1	{CII^3}	6’/m’mm’	$\bar{3}m_{100}$	A_{1g}	{DIII, AII$_C$}
3m	$31m_{100}$	A_1	{DIII, AII$_C$}	6221’	622	B_2	{DIII, AII$_C$}	6’/m’mm’	$\bar{3}m_{100}$	A_{1u}	{AIII$_T$, DIII}
3m	$31m_{100}$	A_2	{AI$_C$, BDI}	6221’	622	B_1	{DIII, AII$_C$}	6’/m’mm’	$\bar{3}m_{100}$	A_{2g}	{D$_T{}^3$}
3m1’	$31m_{100}$	A_1	{D$_T$, DIII}	6221’	622	A_2	{DIII^3}	6’/m’mm’	$\bar{3}m_{100}$	A_{2u}	{DIII^6}
3m1’	$31m_{100}$	A_2	{BDI^3}	6’22’	$32_{100}1$	A_1	{AII$_C$, CII}	6/mm’m’	6/m	A_g	{DIII^3}
3m’	3	A	{D^3}	6’22’	$32_{100}1$	A_2	{DIII^3}	6/mm’m’	6/m	$^1E_{2g}$	{DIII^3}
3m’	3	^{2}E	{D^3}	62’2’	6	A	{AII$_C{}^3$}	6/mm’m’	6/m	$^2E_{2g}$	{DIII^3}
3m’	3	^{1}E	{D^3}	62’2’	6	$^1E_2$	{AII$_C{}^3$}	6/mm’m’	6/m	A_u	{DIII^3}
$\bar{3}$m	$\bar{3}m_{100}$	A_{1g}	{AIII$_T$, CII}	62’2’	6	$^2E_2$	{AII$_C{}^3$}	6/mm’m’	6/m	$^1E_{2u}$	{DIII^3}
$\bar{3}$m	$\bar{3}m_{100}$	A_{1u}	{AIII$_T$, CI}	62’2’	6	$^2E_1$	{DIII^2, AII$_C{}^2$}	6/mm’m’	6/m	$^2E_{2u}$	{DIII^3}
$\bar{3}$m	$\bar{3}m_{100}$	A_{2g}	{BDI^3}	62’2’	6	$^1E_1$	{DIII^2, AII$_C{}^2$}	6/mm’m’	6/m	$^2E_{1g}$	{D$_T{}^2$, DIII^2}
$\bar{3}$m	$\bar{3}m_{100}$	A_{2u}	{DIII^3}	62’2’	6	B	{DIII^2, AII$_C{}^2$}	6/mm’m’	6/m	$^1E_{1g}$	{D$_T{}^2$, DIII^2}
$\bar{3}$m1’	$\bar{3}m_{100}$	A_{1g}	{A$_{T,C}$, AII$_C$}	6mm	6mm	A_1	{AII$_C{}^3$}	6/mm’m’	6/m	B_g	{D$_T{}^2$, DIII^2}
$\bar{3}$m1’	$\bar{3}m_{100}$	A_{1u}	{AIII$_T{}^3$}	6mm	6mm	A_2	{AI$_C{}^3$}	6/mm’m’	6/m	$^2E_{1u}$	{DIII^6}
$\bar{3}$m1’	$\bar{3}m_{100}$	A_{2g}	{BDI, D$_T$}	6mm	6mm	B_1	{A$_{T,C}$, D$_T$}	6/mm’m’	6/m	$^1E_{1u}$	{DIII^6}
$\bar{3}$m1’	$\bar{3}m_{100}$	A_{2u}	{DIII^3}	6mm	6mm	B_2	{A$_{T,C}$, D$_T$}	6/mm’m’	6/m	B_u	{DIII^6}

Table D5. Continued

MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ
$\bar{3}$’m	$31\mathrm{m}_{100}$	A_1	$\{\mathrm{AII}_C{}^3\}$	6mm1’	6mm	A_1	$\{\mathrm{DIII}^3\}$	6/m’m’m’	622	A_1	$\{\mathrm{A}_C{}^3\}$
$\bar{3}$’m	$31\mathrm{m}_{100}$	A_2	$\{\mathrm{A}_{T,C}, \mathrm{AIII}_T\}$	6mm1’	6mm	A_2	$\{\mathrm{BDI}^3\}$	6/m’m’m’	622	B_2	$\{\mathrm{D}^3\}$
$\bar{3}$’m’	$32_{100}1$	A_1	$\{\mathrm{A}_C{}^3\}$	6mm1’	6mm	B_1	$\{\mathrm{D}_T{}^3\}$	6/m’m’m’	622	B_1	$\{\mathrm{D}^3\}$
$\bar{3}$’m’	$32_{100}1$	A_2	$\{\mathrm{D}^3\}$	6mm1’	6mm	B_2	$\{\mathrm{D}_T{}^3\}$	6/m’m’m’	622	A_2	$\{\mathrm{D}^6\}$
$\bar{3}$m’	$\bar{3}$	A_g	$\{\mathrm{D}_T, \mathrm{DIII}\}$	6’mm’	$31\mathrm{m}_{100}$	A_1	$\{\mathrm{DIII}^3\}$	23	23	A	$\{\mathrm{C}, \mathrm{A}_C\}$
$\bar{3}$m’	$\bar{3}$	$^2\mathrm{E}_\mathrm{g}$	$\{\mathrm{D}_T, \mathrm{DIII}\}$	6’mm’	$31\mathrm{m}_{100}$	A_2	$\{\mathrm{BDI}, \mathrm{D}_T\}$	23	23	$^2\mathrm{E}$	$\{\mathrm{C}, \mathrm{A}_C\}$
$\bar{3}$m’	$\bar{3}$	$^1\mathrm{E}_\mathrm{g}$	$\{\mathrm{D}_T, \mathrm{DIII}\}$	6m’m’	6	A	$\{\mathrm{D}^3\}$	23	23	$^1\mathrm{E}$	$\{\mathrm{C}, \mathrm{A}_C\}$
$\bar{3}$m’	$\bar{3}$	A_u	$\{\mathrm{DIII}^3\}$	6m’m’	6	$^1\mathrm{E}_2$	$\{\mathrm{D}^3\}$	231’	23	A	$\{\mathrm{AIII}_T, \mathrm{CII}\}$
$\bar{3}$m’	$\bar{3}$	$^2\mathrm{E}_\mathrm{u}$	$\{\mathrm{DIII}^3\}$	6m’m’	6	$^2\mathrm{E}_2$	$\{\mathrm{D}^3\}$	m$\bar{3}$	m$\bar{3}$	A_g	$\{\mathrm{AIII}_T, \mathrm{CII}\}$
$\bar{3}$m’	$\bar{3}$	$^1\mathrm{E}_\mathrm{u}$	$\{\mathrm{DIII}^3\}$	6m’m’	6	$^2\mathrm{E}_1$	$\{\mathrm{D}^6\}$	m$\bar{3}$	m$\bar{3}$	A_u	$\{\mathrm{AIII}_T, \mathrm{CI}\}$
6	6	A	$\{\mathrm{A}_C{}^3\}$	6m’m’	6	$^1\mathrm{E}_1$	$\{\mathrm{D}^6\}$	m$\bar{3}$	m$\bar{3}$	$^2\mathrm{E}_\mathrm{g}$	$\{\mathrm{AIII}_T, \mathrm{CII}\}$
6	6	$^1\mathrm{E}_2$	$\{\mathrm{A}_C{}^3\}$	6m’m’	6	B	$\{\mathrm{D}^6\}$	m$\bar{3}$	m$\bar{3}$	$^2\mathrm{E}_\mathrm{u}$	$\{\mathrm{AIII}_T, \mathrm{CI}\}$
6	6	$^2\mathrm{E}_2$	$\{\mathrm{A}_C{}^3\}$	$\bar{6}$m2	$\bar{6}2_{210}\mathrm{m}_{100}$	A’$_1$	$\{\mathrm{AII}_C, \mathrm{CII}\}$	m$\bar{3}$	m$\bar{3}$	$^1\mathrm{E}_\mathrm{g}$	$\{\mathrm{AIII}_T, \mathrm{CII}\}$
6	6	$^2\mathrm{E}_1$	$\{\mathrm{D}^2, \mathrm{A}_C{}^2\}$	$\bar{6}$m2	$\bar{6}2_{210}\mathrm{m}_{100}$	A”$_1$	$\{\mathrm{AI}_C, \mathrm{CI}\}$	m$\bar{3}$	m$\bar{3}$	$^1\mathrm{E}_\mathrm{u}$	$\{\mathrm{AIII}_T, \mathrm{CI}\}$
6	6	$^1\mathrm{E}_1$	$\{\mathrm{D}^2, \mathrm{A}_C{}^2\}$	$\bar{6}$m2	$\bar{6}2_{210}\mathrm{m}_{100}$	A”$_2$	$\{\mathrm{D}_T, \mathrm{DIII}\}$	m$\bar{3}$1’	m$\bar{3}$	A_g	$\{\mathrm{A}_{T,C}, \mathrm{AII}_C\}$
6	6	B	$\{\mathrm{D}^2, \mathrm{A}_C{}^2\}$	$\bar{6}$m2	$\bar{6}2_{210}\mathrm{m}_{100}$	A’$_2$	$\{\mathrm{BDI}, \mathrm{D}_T\}$	m$\bar{3}$1’	m$\bar{3}$	A_u	$\{\mathrm{AIII}_T{}^3\}$
61’	6	A	$\{\mathrm{AIII}_T{}^3\}$	$\bar{6}$m21’	$\bar{6}2_{210}\mathrm{m}_{100}$	A’$_1$	$\{\mathrm{DIII}, \mathrm{AII}_C\}$	m’$\bar{3}$’	23	A	$\{\mathrm{A}_C{}^3\}$
61’	6	B	$\{\mathrm{A}_{T,C}, \mathrm{D}_T\}$	$\bar{6}$m21’	$\bar{6}2_{210}\mathrm{m}_{100}$	A”$_1$	$\{\mathrm{AIII}_T, \mathrm{BDI}\}$	432	432	A_1	$\{\mathrm{C}^3\}$
6’	3	A	$\{\mathrm{AIII}_T, \mathrm{DIII}\}$	$\bar{6}$m21’	$\bar{6}2_{210}\mathrm{m}_{100}$	A”$_2$	$\{\mathrm{D}_T{}^2, \mathrm{DIII}^2\}$	432	432	A_2	$\{\mathrm{D}, \mathrm{A}_C\}$
$\bar{6}$	$\bar{6}$	A’	$\{\mathrm{AIII}_T, \mathrm{DIII}\}$	$\bar{6}$m21’	$\bar{6}2_{210}\mathrm{m}_{100}$	A’$_2$	$\{\mathrm{D}_T{}^3\}$	4321’	432	A_1	$\{\mathrm{CII}^3\}$
$\bar{6}$	$\bar{6}$	^{2}E’	$\{\mathrm{AIII}_T, \mathrm{DIII}\}$	$\bar{6}$’m’2	312_{120}	A_1	$\{\mathrm{D}, \mathrm{A}_C\}$	4321’	432	A_2	$\{\mathrm{DIII}, \mathrm{AII}_C\}$
$\bar{6}$	$\bar{6}$	^{1}E’	$\{\mathrm{AIII}_T, \mathrm{DIII}\}$	$\bar{6}$’m’2	312_{120}	A_2	$\{\mathrm{D}^6\}$	4’32’	23	A	$\{\mathrm{AII}_C, \mathrm{CII}\}$
$\bar{6}$	$\bar{6}$	A”	$\{\mathrm{AIII}_T, \mathrm{BDI}\}$	$\bar{6}$’m2’	$31\mathrm{m}_{100}$	A_1	$\{\mathrm{DIII}^2, \mathrm{AII}_C{}^2\}$	4’32’	23	$^2\mathrm{E}$	$\{\mathrm{AII}_C, \mathrm{CII}\}$
$\bar{6}$	$\bar{6}$	^{2}E”	$\{\mathrm{AIII}_T, \mathrm{BDI}\}$	$\bar{6}$’m2’	$31\mathrm{m}_{100}$	A_2	$\{\mathrm{A}_{T,C}, \mathrm{D}_T\}$	4’32’	23	$^1\mathrm{E}$	$\{\mathrm{AII}_C, \mathrm{CII}\}$
$\bar{6}$	$\bar{6}$	^{1}E”	$\{\mathrm{AIII}_T, \mathrm{BDI}\}$	$\bar{6}$m’2’	$\bar{6}$	A’	$\{\mathrm{DIII}^3\}$	$\bar{4}$3m	$\bar{4}$3m	A_1	$\{\mathrm{AII}_C, \mathrm{CII}\}$
$\bar{6}$1’	$\bar{6}$	A’	$\{\mathrm{A}_{T,C}, \mathrm{D}_T\}$	$\bar{6}$m’2’	$\bar{6}$	^{2}E’	$\{\mathrm{DIII}^3\}$	$\bar{4}$3m	$\bar{4}$3m	A_2	$\{\mathrm{AI}_C, \mathrm{CI}\}$
$\bar{6}$1’	$\bar{6}$	A”	$\{\mathrm{AIII}_T{}^2, \mathrm{BDI}^2\}$	$\bar{6}$m’2’	$\bar{6}$	^{1}E’	$\{\mathrm{DIII}^3\}$	$\bar{4}$3m1’	$\bar{4}$3m	A_1	$\{\mathrm{DIII}, \mathrm{AII}_C\}$
$\bar{6}$’	3	A	$\{\mathrm{D}^2, \mathrm{A}_C{}^2\}$	$\bar{6}$m’2’	$\bar{6}$	A”	$\{\mathrm{D}_T, \mathrm{DIII}\}$	$\bar{4}$3m1’	$\bar{4}$3m	A_2	$\{\mathrm{AIII}_T, \mathrm{BDI}\}$
6/m	6/m	A_g	$\{\mathrm{AIII}_T{}^3\}$	$\bar{6}$m’2’	$\bar{6}$	^{2}E”	$\{\mathrm{D}_T, \mathrm{DIII}\}$	$\bar{4}$’3m’	23	A	$\{\mathrm{D}, \mathrm{A}_C\}$
6/m	6/m	$^1\mathrm{E}_{2\mathrm{g}}$	$\{\mathrm{AIII}_T{}^3\}$	$\bar{6}$m’2’	$\bar{6}$	^{1}E”	$\{\mathrm{D}_T, \mathrm{DIII}\}$	$\bar{4}$’3m’	23	$^2\mathrm{E}$	$\{\mathrm{D}, \mathrm{A}_C\}$

Table D5. Continued

MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ
6/m	6/m	${}^2E_{2g}$	$\{AIII_T{}^3\}$	6/mmm	6/mmm	A_{1g}	$\{CII^3\}$	$\bar{4}$'3m'	23	${}^1E$	$\{D, A_C\}$
6/m	6/m	A_u	$\{AIII_T{}^3\}$	6/mmm	6/mmm	A_{1u}	$\{CI^3\}$	m$\bar{3}$m	m$\bar{3}$m	A_{1g}	$\{CII^3\}$
6/m	6/m	${}^1E_{2u}$	$\{AIII_T{}^3\}$	6/mmm	6/mmm	B_{2g}	$\{AIII_T, BDI\}$	m$\bar{3}$m	m$\bar{3}$m	A_{1u}	$\{CI^3\}$
6/m	6/m	${}^2E_{2u}$	$\{AIII_T{}^3\}$	6/mmm	6/mmm	B_{2u}	$\{AIII_T, DIII\}$	m$\bar{3}$m	m$\bar{3}$m	A_{2g}	$\{AIII_T, BDI\}$
6/m	6/m	${}^2E_{1g}$	$\{AIII_T{}^2, BDI^2\}$	6/mmm	6/mmm	B_{1g}	$\{AIII_T, BDI\}$	m$\bar{3}$m	m$\bar{3}$m	A_{2u}	$\{AIII_T, DIII\}$
6/m	6/m	${}^1E_{1g}$	$\{AIII_T{}^2, BDI^2\}$	6/mmm	6/mmm	B_{1u}	$\{AIII_T, DIII\}$	m$\bar{3}$m1'	m$\bar{3}$m	A_{1g}	$\{AII_C{}^3\}$
6/m	6/m	B_g	$\{AIII_T{}^2, BDI^2\}$	6/mmm	6/mmm	A_{2g}	$\{BDI^3\}$	m$\bar{3}$m1'	m$\bar{3}$m	A_{1u}	$\{AIII_T{}^3\}$
6/m	6/m	${}^2E_{1u}$	$\{AIII_T{}^2, DIII^2\}$	6/mmm	6/mmm	A_{2u}	$\{DIII^3\}$	m$\bar{3}$m1'	m$\bar{3}$m	A_{2g}	$\{D_T, DIII\}$
6/m	6/m	${}^1E_{1u}$	$\{AIII_T{}^2, DIII^2\}$	6/mmm1'	6/mmm	A_{1g}	$\{AII_C{}^3\}$	m$\bar{3}$m1'	m$\bar{3}$m	A_{2u}	$\{DIII^3\}$
6/m	6/m	B_u	$\{AIII_T{}^2, DIII^2\}$	6/mmm1'	6/mmm	A_{1u}	$\{AIII_T{}^3\}$	m'$\bar{3}$'m	$\bar{4}$3m	A_1	$\{AII_C{}^3\}$
6/m1'	6/m	A_g	$\{A_{T,C}{}^3\}$	6/mmm1'	6/mmm	B_{2g}	$\{D_T, DIII\}$	m'$\bar{3}$'m	$\bar{4}$3m	A_2	$\{A_{T,C}, AIII_T\}$
6/m1'	6/m	A_u	$\{AIII_T{}^6\}$	6/mmm1'	6/mmm	B_{2u}	$\{DIII^3\}$	m$\bar{3}$m'	m$\bar{3}$	A_g	$\{DIII, AII_C\}$
6/m1'	6/m	B_g	$\{AIII_T, BDI\}$	6/mmm1'	6/mmm	B_{1g}	$\{D_T, DIII\}$	m$\bar{3}$m'	m$\bar{3}$	A_u	$\{AIII_T, DIII\}$
6/m1'	6/m	B_u	$\{AIII_T, DIII\}$	6/mmm1'	6/mmm	B_{1u}	$\{DIII^3\}$	m$\bar{3}$m'	m$\bar{3}$	${}^2E_g$	$\{DIII, AII_C\}$
6'/m	$\bar{6}$	A'	$\{A_{T,C}, AII_C\}$	6/mmm1'	6/mmm	A_{2g}	$\{D_T{}^3\}$	m$\bar{3}$m'	m$\bar{3}$	${}^2E_u$	$\{AIII_T, DIII\}$
6'/m	$\bar{6}$	A"	$\{AIII_T{}^3\}$	6/mmm1'	6/mmm	A_{2u}	$\{DIII^6\}$	m$\bar{3}$m'	m$\bar{3}$	${}^1E_g$	$\{DIII, AII_C\}$
6/m'	6	A	$\{A_C{}^6\}$	6/m'mm	6mm	A_1	$\{AII_C{}^6\}$	m$\bar{3}$m'	m$\bar{3}$	${}^1E_u$	$\{AIII_T, DIII\}$
6/m'	6	B	$\{D, A_C\}$	6/m'mm	6mm	A_2	$\{A_{T,C}{}^3\}$	m'$\bar{3}$'m'	432	A_1	$\{A_C{}^3\}$
								m'$\bar{3}$'m'	432	A_2	$\{D^3\}$

Table D6. EAZ classes of superconductors of spinful electrons with crystallographic MPG symmetry.

MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ
1	1	A	{D}	m’mm	2mm	A_2	$\{DIII^4\}$	4m’m’	4	^1E	$\{D^2\}$
11’	1	A	{DIII}	m’mm	2mm	B_2	{DIII}	$\bar{4}2m$	$\bar{4}2m_{110}$	A_1	$\{BDI^2, D_T\}$
$\bar{1}$	$\bar{1}$	A_g	{BDI}	m’mm	2mm	B_1	{DIII}	$\bar{4}2m$	$\bar{4}2m_{110}$	B_1	$\{D_T, DIII^2\}$
$\bar{1}$	$\bar{1}$	A_u	{DIII}	m’m’m	112/m	A_g	$\{D_T^2\}$	$\bar{4}2m$	$\bar{4}2m_{110}$	B_2	$\{AIII_T, AI_C\}$
$\bar{1}1’$	$\bar{1}$	A_g	$\{D_T\}$	m’m’m	112/m	A_u	$\{DIII^4\}$	$\bar{4}2m$	$\bar{4}2m_{110}$	A_2	$\{AIII_T, AII_C\}$
$\bar{1}1’$	$\bar{1}$	A_u	$\{DIII^2\}$	m’m’m	112/m	B_g	{DIII}	$\bar{4}2m1’$	$\bar{4}2m_{110}$	A_1	$\{D_T^2, DIII\}$
$\bar{1}'$	1	A	$\{D^2\}$	m’m’m	112/m	B_u	{DIII}	$\bar{4}2m1’$	$\bar{4}2m_{110}$	B_1	$\{DIII^5\}$
2	121	A	$\{D^2\}$	m’m’m’	222	A_1	$\{D^8\}$	$\bar{4}2m1’$	$\bar{4}2m_{110}$	B_2	$\{A_{T,C}, DIII\}$
2	121	B	$\{A_C\}$	m’m’m’	222	B_3	$\{D^2\}$	$\bar{4}2m1’$	$\bar{4}2m_{110}$	A_2	$\{DIII, AII_C^2\}$
21’	121	A	$\{DIII^2\}$	m’m’m’	222	B_2	$\{D^2\}$	$\bar{4}’2’m$	$m_{110}m_{1\bar{1}0}2$	A_1	$\{AIII_T, D_T\}$
21’	121	B	$\{AII_C\}$	m’m’m’	222	B_1	$\{D^2\}$	$\bar{4}’2’m$	$m_{110}m_{1\bar{1}0}2$	A_2	$\{DIII^2, AII_C\}$
2’	1	A	{DIII}	4	4	A	$\{D^2, A_C\}$	$\bar{4}’2m’$	222	A_1	$\{D^5\}$
m	1m1	A’	{BDI}	4	4	B	$\{D^2, A_C\}$	$\bar{4}’2m’$	222	B_1	$\{D, A_C^2\}$
m	1m1	A”	{DIII}	4	4	^2E	$\{A_C^2\}$	$\bar{4}2’m’$	$\bar{4}$	A	$\{D_T, DIII^2\}$
m1’	1m1	A’	$\{D_T\}$	4	4	^1E	$\{A_C^2\}$	$\bar{4}2’m’$	$\bar{4}$	B	$\{D_T, DIII^2\}$
m1’	1m1	A”	$\{DIII^2\}$	41’	4	A	$\{AIII_T, DIII^2\}$	$\bar{4}2’m’$	$\bar{4}$	^2E	{DIII}
m’	1	A	$\{D^2\}$	41’	4	B	$\{D_T, AII_C\}$	$\bar{4}2’m’$	$\bar{4}$	^1E	{DIII}
2/m	12/m1	A_g	$\{BDI^2\}$	4’	112	A	{BDI, DIII}	4/mmm	4/mmm	A_{1g}	$\{BDI^5\}$
2/m	12/m1	A_u	$\{DIII^2\}$	$\bar{4}$	$\bar{4}$	A	{BDI, DIII}	4/mmm	4/mmm	A_{1u}	$\{DIII^5\}$
2/m	12/m1	B_g	$\{AIII_T\}$	$\bar{4}$	$\bar{4}$	B	{BDI, DIII}	4/mmm	4/mmm	B_{1g}	$\{AIII_T^2, BDI\}$
2/m	12/m1	B_u	$\{AIII_T\}$	$\bar{4}$	$\bar{4}$	^2E	$\{AIII_T\}$	4/mmm	4/mmm	B_{1u}	$\{AIII_T^2, DIII\}$
2/m1’	12/m1	A_g	$\{D_T^2\}$	$\bar{4}$	$\bar{4}$	^1E	$\{AIII_T\}$	4/mmm	4/mmm	B_{2g}	$\{AIII_T^2, BDI\}$
2/m1’	12/m1	A_u	$\{DIII^4\}$	$\bar{4}1’$	$\bar{4}$	A	$\{D_T, AII_C\}$	4/mmm	4/mmm	B_{2u}	$\{AIII_T^2, DIII\}$
2/m1’	12/m1	B_g	{DIII}	$\bar{4}1’$	$\bar{4}$	B	$\{AIII_T, DIII^2\}$	4/mmm	4/mmm	A_{2g}	$\{AIII_T^2, CII\}$
2/m1’	12/m1	B_u	{DIII}	$\bar{4}'$	112	A	$\{D^2, A_C\}$	4/mmm	4/mmm	A_{2u}	$\{AIII_T^2, CI\}$
2’/m	1m1	A’	$\{D_T\}$	4/m	4/m	A_g	$\{AIII_T, BDI^2\}$	4/mmm1’	4/mmm	A_{1g}	$\{D_T^5\}$
2’/m	1m1	A”	$\{DIII^2\}$	4/m	4/m	A_u	$\{AIII_T, DIII^2\}$	4/mmm1’	4/mmm	A_{1u}	$\{DIII^{10}\}$
2/m’	121	A	$\{D^4\}$	4/m	4/m	B_g	$\{AIII_T, BDI^2\}$	4/mmm1’	4/mmm	B_{1g}	$\{D_T, DIII^2\}$
2/m’	121	B	{D}	4/m	4/m	B_u	$\{AIII_T, DIII^2\}$	4/mmm1’	4/mmm	B_{1u}	$\{DIII^4\}$
2’/m’	$\bar{1}$	A_g	$\{D_T\}$	4/m	4/m	^2E_g	$\{AIII_T^2\}$	4/mmm1’	4/mmm	B_{2g}	$\{D_T, DIII^2\}$
2’/m’	$\bar{1}$	A_u	$\{DIII^2\}$	4/m	4/m	^2E_u	$\{AIII_T^2\}$	4/mmm1’	4/mmm	B_{2u}	$\{DIII^4\}$

Table D6. Continued

MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ
222	222	A_1	$\{D^4\}$	4/m	4/m	^1E_g	$\{AIII_T^2\}$	4/mmm1’	4/mmm	A_{2g}	$\{DIII^2, AII_C\}$
222	222	B_3	$\{A_C^2\}$	4/m	4/m	^1E_u	$\{AIII_T^2\}$	4/mmm1’	4/mmm	A_{2u}	$\{AIII_T, DIII^2\}$
222	222	B_2	$\{A_C^2\}$	4/m1’	4/m	A_g	$\{A_{T,C}, D_T^2\}$	4/m’mm	4mm	A_1	$\{A_{T,C}, D_T^2\}$
222	222	B_1	$\{A_C^2\}$	4/m1’	4/m	A_u	$\{AIII_T^2, DIII^4\}$	4/m’mm	4mm	A_2	$\{DIII^4, AII_C^2\}$
2221’	222	A_1	$\{DIII^4\}$	4/m1’	4/m	B_g	$\{BDI, DIII\}$	4/m’mm	4mm	B_1	$\{DIII^2\}$
2221’	222	B_3	$\{AII_C^2\}$	4/m1’	4/m	B_u	$\{DIII^2\}$	4/m’mm	4mm	B_2	$\{DIII^2\}$
2221’	222	B_2	$\{AII_C^2\}$	4’/m	112/m	A_g	$\{AI_C, D_T\}$	4’/mm’m	$m_{110}m_{1\bar{1}0}m$	A_g	$\{BDI, D_T^2\}$
2221’	222	B_1	$\{AII_C^2\}$	4’/m	112/m	A_u	$\{AIII_T, DIII^2\}$	4’/mm’m	$m_{110}m_{1\bar{1}0}m$	A_u	$\{DIII^5\}$
2’2’2	112	A	$\{DIII^2\}$	4/m’	4	A	$\{D^4, A_C^2\}$	4’/mm’m	$m_{110}m_{1\bar{1}0}m$	B_{1g}	$\{A_{T,C}, DIII\}$
2’2’2	112	B	$\{AII_C\}$	4/m’	4	B	$\{D^2\}$	4’/mm’m	$m_{110}m_{1\bar{1}0}m$	B_{1u}	$\{AIII_T^2, DIII\}$
mm2	mm2	A_1	$\{BDI^2\}$	4’/m’	$\bar{4}$	A	$\{D_T^2\}$	4’/m’m’m	$\bar{4}2m_{110}$	A_1	$\{D_T^4\}$
mm2	mm2	A_2	$\{DIII^2\}$	4’/m’	$\bar{4}$	B	$\{BDI^2, DIII^2\}$	4’/m’m’m	$\bar{4}2m_{110}$	B_1	$\{D_T^2, DIII^4\}$
mm2	mm2	B_2	$\{AIII_T\}$	422	422	A_1	$\{D^5\}$	4’/m’m’m	$\bar{4}2m_{110}$	B_2	$\{BDI, DIII\}$
mm2	mm2	B_1	$\{AIII_T\}$	422	422	B_1	$\{D, A_C^2\}$	4’/m’m’m	$\bar{4}2m_{110}$	A_2	$\{DIII^2\}$
mm21’	mm2	A_1	$\{D_T^2\}$	422	422	B_2	$\{D, A_C^2\}$	4/mm’m’	4/m	A_g	$\{D_T^2, DIII\}$
mm21’	mm2	A_2	$\{DIII^4\}$	422	422	A_2	$\{C, A_C^2\}$	4/mm’m’	4/m	A_u	$\{DIII^5\}$
mm21’	mm2	B_2	$\{DIII\}$	4221’	422	A_1	$\{DIII^5\}$	4/mm’m’	4/m	B_g	$\{D_T^2, DIII\}$
mm21’	mm2	B_1	$\{DIII\}$	4221’	422	B_1	$\{DIII, AII_C^2\}$	4/mm’m’	4/m	B_u	$\{DIII^5\}$
m’m2’	1m1	A’	$\{D_T\}$	4221’	422	B_2	$\{DIII, AII_C^2\}$	4/mm’m’	4/m	^2E_g	$\{DIII^2\}$
m’m2’	1m1	A”	$\{DIII^2\}$	4221’	422	A_2	$\{AII_C^2, CII\}$	4/mm’m’	4/m	^2E_u	$\{DIII^2\}$
m’m’2	112	A	$\{D^4\}$	4’22’	222	A_1	$\{D_T, DIII^2\}$	4/mm’m’	4/m	^1E_g	$\{DIII^2\}$
m’m’2	112	B	$\{D\}$	4’22’	222	B_1	$\{AIII_T, AII_C\}$	4/mm’m’	4/m	^1E_u	$\{DIII^2\}$
mmm	mmm	A_g	$\{BDI^4\}$	42’2’	4	A	$\{DIII^2, AII_C\}$	4/m’m’m’	422	A_1	$\{D^{10}\}$
mmm	mmm	A_u	$\{DIII^4\}$	42’2’	4	B	$\{DIII^2, AII_C\}$	4/m’m’m’	422	B_1	$\{D^4\}$
mmm	mmm	B_{3g}	$\{AIII_T^2\}$	42’2’	4	^2E	$\{AII_C^2\}$	4/m’m’m’	422	B_2	$\{D^4\}$
mmm	mmm	B_{3u}	$\{AIII_T^2\}$	42’2’	4	^1E	$\{AII_C^2\}$	4/m’m’m’	422	A_2	$\{D^2, A_C\}$
mmm	mmm	B_{2g}	$\{AIII_T^2\}$	4mm	4mm	A_1	$\{AI_C, BDI^2\}$	3	3	A	$\{D, A_C\}$
mmm	mmm	B_{2u}	$\{AIII_T^2\}$	4mm	4mm	A_2	$\{DIII^2, AII_C\}$	3	3	^2E	$\{D, A_C\}$
mmm	mmm	B_{1g}	$\{AIII_T^2\}$	4mm	4mm	B_1	$\{AIII_T, D_T\}$	3	3	^1E	$\{D, A_C\}$
mmm	mmm	B_{1u}	$\{AIII_T^2\}$	4mm	4mm	B_2	$\{AIII_T, D_T\}$	31’	3	A	$\{AIII_T, DIII\}$
mmm1’	mmm	A_g	$\{D_T^4\}$	4mm1’	4mm	A_1	$\{BDI, D_T^2\}$	$\bar{3}$	$\bar{3}$	A_g	$\{AIII_T, BDI\}$

Table D6. Continued

MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ
mmm1'	mmm	A_u	$\{DIII^8\}$	4mm1'	4mm	A_2	$\{DIII^5\}$	$\bar{3}$	$\bar{3}$	^2E_g	$\{AIII_T, BDI\}$
mmm1'	mmm	B_{3g}	$\{DIII^2\}$	4mm1'	4mm	B_1	$\{D_T^2, DIII\}$	$\bar{3}$	$\bar{3}$	^1E_g	$\{AIII_T, BDI\}$
mmm1'	mmm	B_{3u}	$\{DIII^2\}$	4mm1'	4mm	B_2	$\{D_T^2, DIII\}$	$\bar{3}$	$\bar{3}$	A_u	$\{AIII_T, DIII\}$
mmm1'	mmm	B_{2g}	$\{DIII^2\}$	4'm'm	$m_{110}m_{1\bar{1}0}2$	A_1	$\{BDI^2, D_T\}$	$\bar{3}$	$\bar{3}$	^2E_u	$\{AIII_T, DIII\}$
mmm1'	mmm	B_{2u}	$\{DIII^2\}$	4'm'm	$m_{110}m_{1\bar{1}0}2$	A_2	$\{D_T, DIII^2\}$	$\bar{3}$	$\bar{3}$	^1E_u	$\{AIII_T, DIII\}$
mmm1'	mmm	B_{1g}	$\{DIII^2\}$	4m'm'	4	A	$\{D^5\}$	$\bar{3}$1'	$\bar{3}$	A_g	$\{A_{T,C}, D_T\}$
mmm1'	mmm	B_{1u}	$\{DIII^2\}$	4m'm'	4	B	$\{D^5\}$	$\bar{3}$1'	$\bar{3}$	A_u	$\{AIII_T^2, DIII^2\}$
m'mm	2mm	A_1	$\{D_T^2\}$	4m'm'	4	^2E	$\{D^2\}$	$\bar{3}'$	3	A	$\{D^2, A_C^2\}$
32	$32_{100}1$	A_1	$\{D^3\}$	6'/m'	$\bar{3}$	A_g	$\{A_{T,C}, D_T\}$	6/m'mm	6mm	B_1	$\{DIII, AII_C\}$
32	$32_{100}1$	A_2	$\{C, A_C\}$	6'/m'	$\bar{3}$	A_u	$\{AIII_T^2, DIII^2\}$	6/m'mm	6mm	B_2	$\{DIII, AII_C\}$
321'	$32_{100}1$	A_1	$\{DIII^3\}$	622	622	A_1	$\{D^6\}$	6'/mmm'	$\bar{6}2_{210}m_{100}$	A'_1	$\{D_T^3\}$
321'	$32_{100}1$	A_2	$\{AII_C, CII\}$	622	622	B_2	$\{A_C^3\}$	6'/mmm'	$\bar{6}2_{210}m_{100}$	A''_1	$\{DIII^6\}$
32'	3	A	$\{DIII, AII_C\}$	622	622	B_1	$\{A_C^3\}$	6'/mmm'	$\bar{6}2_{210}m_{100}$	A''_2	$\{AIII_T, DIII\}$
32'	3	^2E	$\{DIII, AII_C\}$	622	622	A_2	$\{C^2, A_C^2\}$	6'/mmm'	$\bar{6}2_{210}m_{100}$	A'_2	$\{DIII, AII_C\}$
32'	3	^1E	$\{DIII, AII_C\}$	6221'	622	A_1	$\{DIII^6\}$	6'/m'mm'	$\bar{3}m_{100}$	A_{1g}	$\{D_T^3\}$
3m	$31m_{100}$	A_1	$\{AI_C, BDI\}$	6221'	622	B_2	$\{AII_C^3\}$	6'/m'mm'	$\bar{3}m_{100}$	A_{1u}	$\{DIII^6\}$
3m	$31m_{100}$	A_2	$\{DIII, AII_C\}$	6221'	622	B_1	$\{AII_C^3\}$	6'/m'mm'	$\bar{3}m_{100}$	A_{2g}	$\{DIII, AII_C\}$
3m1'	$31m_{100}$	A_1	$\{BDI, D_T\}$	6221'	622	A_2	$\{AII_C^2, CII^2\}$	6'/m'mm'	$\bar{3}m_{100}$	A_{2u}	$\{AIII_T, DIII\}$
3m1'	$31m_{100}$	A_2	$\{DIII^3\}$	6'22'	$32_{100}1$	A_1	$\{DIII^3\}$	6/mm'm'	6/m	A_g	$\{D_T^2, DIII^2\}$
3m'	3	A	$\{D^3\}$	6'22'	$32_{100}1$	A_2	$\{AII_C, CII\}$	6/mm'm'	6/m	$^1E_{2g}$	$\{D_T^2, DIII^2\}$
3m'	3	^2E	$\{D^3\}$	62'2'	6	A	$\{DIII^2, AII_C^2\}$	6/mm'm'	6/m	$^2E_{2g}$	$\{D_T^2, DIII^2\}$
3m'	3	^1E	$\{D^3\}$	62'2'	6	$^1E_2$	$\{DIII^2, AII_C^2\}$	6/mm'm'	6/m	A_u	$\{DIII^6\}$
$\bar{3}$m	$\bar{3}m_{100}$	A_{1g}	$\{BDI^3\}$	62'2'	6	$^2E_2$	$\{DIII^2, AII_C^2\}$	6/mm'm'	6/m	$^1E_{2u}$	$\{DIII^6\}$
$\bar{3}$m	$\bar{3}m_{100}$	A_{1u}	$\{DIII^3\}$	62'2'	6	$^2E_1$	$\{AII_C^3\}$	6/mm'm'	6/m	$^2E_{2u}$	$\{DIII^6\}$
$\bar{3}$m	$\bar{3}m_{100}$	A_{2g}	$\{AIII_T, CII\}$	62'2'	6	$^1E_1$	$\{AII_C^3\}$	6/mm'm'	6/m	$^2E_{1g}$	$\{DIII^3\}$
$\bar{3}$m	$\bar{3}m_{100}$	A_{2u}	$\{AIII_T, CI\}$	62'2'	6	B	$\{AII_C^3\}$	6/mm'm'	6/m	$^1E_{1g}$	$\{DIII^3\}$
$\bar{3}$m1'	$\bar{3}m_{100}$	A_{1g}	$\{D_T^3\}$	6mm	6mm	A_1	$\{AI_C^2, BDI^2\}$	6/mm'm'	6/m	B_g	$\{DIII^3\}$
$\bar{3}$m1'	$\bar{3}m_{100}$	A_{1u}	$\{DIII^6\}$	6mm	6mm	A_2	$\{DIII^2, AII_C^2\}$	6/mm'm'	6/m	$^2E_{1u}$	$\{DIII^3\}$
$\bar{3}$m1'	$\bar{3}m_{100}$	A_{2g}	$\{DIII, AII_C\}$	6mm	6mm	B_1	$\{A_{T,C}, AIII_T\}$	6/mm'm'	6/m	$^1E_{1u}$	$\{DIII^3\}$
$\bar{3}$m1'	$\bar{3}m_{100}$	A_{2u}	$\{AIII_T, DIII\}$	6mm	6mm	B_2	$\{A_{T,C}, AIII_T\}$	6/mm'm'	6/m	B_u	$\{DIII^3\}$

Table D6. Continued

MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ
$\bar{3}$’m	31m$_{100}$	A$_1$	{A$_{T,C}$, D$_T$}	6mm1’	6mm	A$_1$	{BDI^2, D$_T{}^2$}	6/m’m’m’	622	A$_1$	{D^{12}}
$\bar{3}$’m	31m$_{100}$	A$_2$	{DIII^2, AII$_C{}^2$}	6mm1’	6mm	A$_2$	{DIII^6}	6/m’m’m’	622	B$_2$	{D^3}
$\bar{3}$’m’	32$_{100}$1	A$_1$	{D^6}	6mm1’	6mm	B$_1$	{D$_T$, DIII}	6/m’m’m’	622	B$_1$	{D^3}
$\bar{3}$’m’	32$_{100}$1	A$_2$	{D, A$_C$}	6mm1’	6mm	B$_2$	{D$_T$, DIII}	6/m’m’m’	622	A$_2$	{D^2, A$_C{}^2$}
$\bar{3}$m’	$\bar{3}$	A$_g$	{D$_T$, DIII}	6’mm’	31m$_{100}$	A$_1$	{BDI, D$_T$}	23	23	A	{D^2, A$_C$}
$\bar{3}$m’	$\bar{3}$	^{2}E$_g$	{D$_T$, DIII}	6’mm’	31m$_{100}$	A$_2$	{DIII^3}	23	23	^{2}E	{D^2, A$_C$}
$\bar{3}$m’	$\bar{3}$	^{1}E$_g$	{D$_T$, DIII}	6m’m’	6	A	{D^6}	23	23	^{1}E	{D^2, A$_C$}
$\bar{3}$m’	$\bar{3}$	A$_u$	{DIII^3}	6m’m’	6	^{1}E$_2$	{D^6}	231’	23	A	{AIII$_T$, DIII^2}
$\bar{3}$m’	$\bar{3}$	^{2}E$_u$	{DIII^3}	6m’m’	6	^{2}E$_2$	{D^6}	m$\bar{3}$	m$\bar{3}$	A$_g$	{AIII$_T$, BDI^2}
$\bar{3}$m’	$\bar{3}$	^{1}E$_u$	{DIII^3}	6m’m’	6	^{2}E$_1$	{D^3}	m$\bar{3}$	m$\bar{3}$	A$_u$	{AIII$_T$, DIII^2}
6	6	A	{D^2, A$_C{}^2$}	6m’m’	6	^{1}E$_1$	{D^3}	m$\bar{3}$	m$\bar{3}$	^{2}E$_g$	{AIII$_T$, BDI^2}
6	6	^{1}E$_2$	{D^2, A$_C{}^2$}	6m’m’	6	B	{D^3}	m$\bar{3}$	m$\bar{3}$	^{2}E$_u$	{AIII$_T$, DIII^2}
6	6	^{2}E$_2$	{D^2, A$_C{}^2$}	$\bar{6}$m2	$\bar{6}$2$_{210}$m$_{100}$	A’$_1$	{BDI^3}	m$\bar{3}$	m$\bar{3}$	^{1}E$_g$	{AIII$_T$, BDI^2}
6	6	^{2}E$_1$	{A$_C{}^3$}	$\bar{6}$m2	$\bar{6}$2$_{210}$m$_{100}$	A”$_1$	{DIII^3}	m$\bar{3}$	m$\bar{3}$	^{1}E$_u$	{AIII$_T$, DIII^2}
6	6	^{1}E$_1$	{A$_C{}^3$}	$\bar{6}$m2	$\bar{6}$2$_{210}$m$_{100}$	A”$_2$	{AIII$_T$, CI}	m$\bar{3}$1’	m$\bar{3}$	A$_g$	{A$_{T,C}$, D$_T{}^2$}
6	6	B	{A$_C{}^3$}	$\bar{6}$m2	$\bar{6}$2$_{210}$m$_{100}$	A’$_2$	{AIII$_T$, CII}	m$\bar{3}$1’	m$\bar{3}$	A$_u$	{AIII$_T{}^2$, DIII^4}
61’	6	A	{AIII$_T{}^2$, DIII^2}	$\bar{6}$m21’	$\bar{6}$2$_{210}$m$_{100}$	A’$_1$	{D$_T{}^3$}	m’$\bar{3}$’	23	A	{D^4, A$_C{}^2$}
61’	6	B	{A$_{T,C}$, AII$_C$}	$\bar{6}$m21’	$\bar{6}$2$_{210}$m$_{100}$	A”$_1$	{DIII^6}	432	432	A$_1$	{D^5}
6’	3	A	{AIII$_T$, DIII}	$\bar{6}$m21’	$\bar{6}$2$_{210}$m$_{100}$	A”$_2$	{AIII$_T$, DIII}	432	432	A$_2$	{C, A$_C{}^2$}
$\bar{6}$	$\bar{6}$	A’	{AIII$_T$, BDI}	$\bar{6}$m21’	$\bar{6}$2$_{210}$m$_{100}$	A’$_2$	{DIII, AII$_C$}	4321’	432	A$_1$	{DIII^5}
$\bar{6}$	$\bar{6}$	^{2}E’	{AIII$_T$, BDI}	$\bar{6}$’m’2	312$_{120}$	A$_1$	{D^6}	4321’	432	A$_2$	{AII$_C{}^2$, CII}
$\bar{6}$	$\bar{6}$	^{1}E’	{AIII$_T$, BDI}	$\bar{6}$’m’2	312$_{120}$	A$_2$	{D, A$_C$}	4’32’	23	A	{DIII^2, AII$_C$}
$\bar{6}$	$\bar{6}$	A”	{AIII$_T$, DIII}	$\bar{6}$’m2’	31m$_{100}$	A$_1$	{A$_{T,C}$, D$_T$}	4’32’	23	^{2}E	{DIII^2, AII$_C$}
$\bar{6}$	$\bar{6}$	^{2}E”	{AIII$_T$, DIII}	$\bar{6}$’m2’	31m$_{100}$	A$_2$	{DIII^2, AII$_C{}^2$}	4’32’	23	^{1}E	{DIII^2, AII$_C$}
$\bar{6}$	$\bar{6}$	^{1}E”	{AIII$_T$, DIII}	$\bar{6}$m’2’	$\bar{6}$	A’	{D$_T$, DIII}	$\bar{4}$3m	$\bar{4}$3m	A$_1$	{AI$_C$, BDI^2}
$\bar{6}$1’	$\bar{6}$	A’	{A$_{T,C}$, D$_T$}	$\bar{6}$m’2’	$\bar{6}$	^{2}E’	{D$_T$, DIII}	$\bar{4}$3m	$\bar{4}$3m	A$_2$	{DIII^2, AII$_C$}
$\bar{6}$1’	$\bar{6}$	A”	{AIII$_T{}^2$, DIII^2}	$\bar{6}$m’2’	$\bar{6}$	^{1}E’	{D$_T$, DIII}	$\bar{4}$3m1’	$\bar{4}$3m	A$_1$	{BDI, D$_T{}^2$}
$\bar{6}$’	3	A	{D^2, A$_C{}^2$}	$\bar{6}$m’2’	$\bar{6}$	A”	{DIII^3}	$\bar{4}$3m1’	$\bar{4}$3m	A$_2$	{DIII^5}
6/m	6/m	A$_g$	{AIII$_T{}^2$, BDI^2}	$\bar{6}$m’2’	$\bar{6}$	^{2}E”	{DIII^3}	$\bar{4}$’3m’	23	A	{D^5}

Table D6. Continued

MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ	MPG	G_u	Irrep	EAZ
6/m	6/m	$^1E_{2g}$	$\{AIII_T^2, BDI^2\}$	$\bar{6}m'2'$	$\bar{6}$	$^1E''$	$\{DIII^3\}$	$\bar{4}'3m'$	23	^2E	$\{D^5\}$
6/m	6/m	$^2E_{2g}$	$\{AIII_T^2, BDI^2\}$	6/mmm	6/mmm	A_{1g}	$\{BDI^6\}$	$\bar{4}'3m'$	23	^1E	$\{D^5\}$
6/m	6/m	A_u	$\{AIII_T^2, DIII^2\}$	6/mmm	6/mmm	A_{1u}	$\{DIII^6\}$	$m\bar{3}m$	$m\bar{3}m$	A_{1g}	$\{BDI^5\}$
6/m	6/m	$^1E_{2u}$	$\{AIII_T^2, DIII^2\}$	6/mmm	6/mmm	B_{2g}	$\{AIII_T^3\}$	$m\bar{3}m$	$m\bar{3}m$	A_{1u}	$\{DIII^5\}$
6/m	6/m	$^2E_{2u}$	$\{AIII_T^2, DIII^2\}$	6/mmm	6/mmm	B_{2u}	$\{AIII_T^3\}$	$m\bar{3}m$	$m\bar{3}m$	A_{2g}	$\{AIII_T^2, CII\}$
6/m	6/m	$^2E_{1g}$	$\{AIII_T^3\}$	6/mmm	6/mmm	B_{1g}	$\{AIII_T^3\}$	$m\bar{3}m$	$m\bar{3}m$	A_{2u}	$\{AIII_T^2, CI\}$
6/m	6/m	$^1E_{1g}$	$\{AIII_T^3\}$	6/mmm	6/mmm	B_{1u}	$\{AIII_T^3\}$	$m\bar{3}m1'$	$m\bar{3}m$	A_{1g}	$\{D_T^5\}$
6/m	6/m	B_g	$\{AIII_T^3\}$	6/mmm	6/mmm	A_{2g}	$\{AIII_T^2, CII^2\}$	$m\bar{3}m1'$	$m\bar{3}m$	A_{1u}	$\{DIII^{10}\}$
6/m	6/m	$^2E_{1u}$	$\{AIII_T^3\}$	6/mmm	6/mmm	A_{2u}	$\{AIII_T^2, CI^2\}$	$m\bar{3}m1'$	$m\bar{3}m$	A_{2g}	$\{DIII^2, AII_C\}$
6/m	6/m	$^1E_{1u}$	$\{AIII_T^3\}$	6/mmm1'	6/mmm	A_{1g}	$\{D_T^6\}$	$m\bar{3}m1'$	$m\bar{3}m$	A_{2u}	$\{AIII_T, DIII^2\}$
6/m	6/m	B_u	$\{AIII_T^3\}$	6/mmm1'	6/mmm	A_{1u}	$\{DIII^{12}\}$	$m'\bar{3}'m$	$\bar{4}3m$	A_1	$\{A_{T,C}, D_T^2\}$
6/m1'	6/m	A_g	$\{A_{T,C}^2, D_T^2\}$	6/mmm1'	6/mmm	B_{2g}	$\{DIII^3\}$	$m'\bar{3}'m$	$\bar{4}3m$	A_2	$\{DIII^4, AII_C^2\}$
6/m1'	6/m	A_u	$\{AIII_T^4, DIII^4\}$	6/mmm1'	6/mmm	B_{2u}	$\{DIII^3\}$	$m\bar{3}m'$	$m\bar{3}$	A_g	$\{D_T^2, DIII\}$
6/m1'	6/m	B_g	$\{AIII_T, DIII\}$	6/mmm1'	6/mmm	B_{1g}	$\{DIII^3\}$	$m\bar{3}m'$	$m\bar{3}$	A_u	$\{DIII^5\}$
6/m1'	6/m	B_u	$\{AIII_T, DIII\}$	6/mmm1'	6/mmm	B_{1u}	$\{DIII^3\}$	$m\bar{3}m'$	$m\bar{3}$	^2E_g	$\{D_T^2, DIII\}$
6'/m	$\bar{6}$	A'	$\{A_{T,C}, D_T\}$	6/mmm1'	6/mmm	A_{2g}	$\{DIII^2, AII_C^2\}$	$m\bar{3}m'$	$m\bar{3}$	^2E_u	$\{DIII^5\}$
6'/m	$\bar{6}$	A''	$\{AIII_T^2, DIII^2\}$	6/mmm1'	6/mmm	A_{2u}	$\{AIII_T^2, DIII^2\}$	$m\bar{3}m'$	$m\bar{3}$	^1E_g	$\{D_T^2, DIII\}$
6/m'	6	A	$\{D^4, A_C^4\}$	6/m'mm	6mm	A_1	$\{A_{T,C}^2, D_T^2\}$	$m\bar{3}m'$	$m\bar{3}$	^1E_u	$\{DIII^5\}$
6/m'	6	B	$\{D, A_C\}$	6/m'mm	6mm	A_2	$\{DIII^4, AII_C^4\}$	$m'\bar{3}'m'$	432	A_1	$\{D^{10}\}$
								$m'\bar{3}'m'$	432	A_2	$\{D^2, A_C\}$

Table D7. The classification of surface states of 3D TSCs of spinless electrons with crystallographic MPG symmetry.

MPG	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor
1	1	A	0	{}	m’mm	2mm	A_2	0	{}	4m’m’	4	^1E	0	{}
11’	1	A	0	{}	m’mm	2mm	B_2	1	{}	$\bar{4}2m$	$\bar{4}2m_{110}$	A_1	0	{}
$\bar{1}$	$\bar{1}$	A_g	0	{}	m’mm	2mm	B_1	1	{}	$\bar{4}2m$	$\bar{4}2m_{110}$	B_1	0	{}
$\bar{1}$	$\bar{1}$	A_u	0	{4}	m’m’m	112/m	A_g	1	{}	$\bar{4}2m$	$\bar{4}2m_{110}$	B_2	0	{2}
$\bar{1}$1’	$\bar{1}$	A_g	0	{}	m’m’m	112/m	A_u	0	{2}	$\bar{4}2m$	$\bar{4}2m_{110}$	A_2	0	{}
$\bar{1}$1’	$\bar{1}$	A_u	0	{2}	m’m’m	112/m	B_g	0	{}	$\bar{4}$2m1’	$\bar{4}2m_{110}$	A_1	0	{}
$\bar{1}'$	1	A	0	{}	m’m’m	112/m	B_u	3	{}	$\bar{4}$2m1’	$\bar{4}2m_{110}$	B_1	0	{}
2	121	A	0	{}	m’m’m’	222	A_1	0	{}	$\bar{4}$2m1’	$\bar{4}2m_{110}$	B_2	1	{}
2	121	B	0	{}	m’m’m’	222	B_3	0	{}	$\bar{4}$2m1’	$\bar{4}2m_{110}$	A_2	0	{}
21’	121	A	1	{}	m’m’m’	222	B_2	0	{}	$\bar{4}$’2’m	$m_{110}m_{1\bar{1}0}2$	A_1	0	{2}
21’	121	B	0	{}	m’m’m’	222	B_1	0	{}	$\bar{4}$’2’m	$m_{110}m_{1\bar{1}0}2$	A_2	0	{}
2’	1	A	1	{}	4	4	A	0	{}	$\bar{4}$’2m’	222	A_1	0	{}
m	1m1	A’	1	{}	4	4	B	0	{}	$\bar{4}$’2m’	222	B_1	0	{}
m	1m1	A”	0	{}	4	4	^2E	0	{}	$\bar{4}$2’m’	$\bar{4}$	A	0	{2}
m1’	1m1	A’	0	{}	4	4	^1E	0	{}	$\bar{4}$2’m’	$\bar{4}$	B	0	{2}
m1’	1m1	A”	0	{}	41’	4	A	2	{}	$\bar{4}$2’m’	$\bar{4}$	^2E	1	{}
m’	1	A	0	{}	41’	4	B	0	{}	$\bar{4}$2’m’	$\bar{4}$	^1E	1	{}
2/m	12/m1	A_g	1	{}	4’	112	A	1	{}	4/mmm	4/mmm	A_{1g}	0	{}
2/m	12/m1	A_u	0	{2}	$\bar{4}$	$\bar{4}$	A	0	{2}	4/mmm	4/mmm	A_{1u}	0	{}
2/m	12/m1	B_g	0	{}	$\bar{4}$	$\bar{4}$	B	0	{2}	4/mmm	4/mmm	B_{1g}	0	{}
2/m	12/m1	B_u	1	{2}	$\bar{4}$	$\bar{4}$	^2E	0	{2}	4/mmm	4/mmm	B_{1u}	0	{}
2/m1’	12/m1	A_g	0	{}	$\bar{4}$	$\bar{4}$	^1E	0	{2}	4/mmm	4/mmm	B_{2g}	0	{}
2/m1’	12/m1	A_u	1	{}	$\bar{4}$1’	$\bar{4}$	A	0	{}	4/mmm	4/mmm	B_{2u}	0	{}
2/m1’	12/m1	B_g	0	{}	$\bar{4}$1’	$\bar{4}$	B	1	{}	4/mmm	4/mmm	A_{2g}	0	{}
2/m1’	12/m1	B_u	0	{2}	$\bar{4}'$	112	A	0	{}	4/mmm	4/mmm	A_{2u}	0	{2, 2}
2’/m	1m1	A’	0	{2}	4/m	4/m	A_g	1	{}	4/mmm1’	4/mmm	A_{1g}	0	{}
2’/m	1m1	A”	1	{}	4/m	4/m	A_u	0	{2}	4/mmm1’	4/mmm	A_{1u}	0	{}
2/m’	121	A	0	{}	4/m	4/m	B_g	1	{}	4/mmm1’	4/mmm	B_{1g}	0	{}
2/m’	121	B	0	{}	4/m	4/m	B_u	0	{2}	4/mmm1’	4/mmm	B_{1u}	0	{}

Table D7. Continued

MPG	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor
2’/m’	$\bar{1}$	A_g	0	{}	4/m	4/m	^2E_g	0	{}	4/mmm1’	4/mmm	B_{2g}	0	{}
2’/m’	$\bar{1}$	A_u	1	{2}	4/m	4/m	^2E_u	1	{2}	4/mmm1’	4/mmm	B_{2u}	0	{}
222	222	A_1	0	{}	4/m	4/m	^1E_g	0	{}	4/mmm1’	4/mmm	A_{2g}	0	{}
222	222	B_3	0	{}	4/m	4/m	^1E_u	1	{2}	4/mmm1’	4/mmm	A_{2u}	2	{}
222	222	B_2	0	{}	4/m1’	4/m	A_g	0	{}	4/m’mm	4mm	A_1	0	{2, 2}
222	222	B_1	0	{}	4/m1’	4/m	A_u	2	{}	4/m’mm	4mm	A_2	0	{}
2221’	222	A_1	0	{}	4/m1’	4/m	B_g	0	{}	4/m’mm	4mm	B_1	0	{}
2221’	222	B_3	1	{}	4/m1’	4/m	B_u	0	{}	4/m’mm	4mm	B_2	0	{}
2221’	222	B_2	1	{}	4’/m	112/m	A_g	0	{}	4’/mm’m	$m_{110}m_{1\bar{1}0}m$	A_g	0	{}
2221’	222	B_1	1	{}	4’/m	112/m	A_u	1	{}	4’/mm’m	$m_{110}m_{1\bar{1}0}m$	A_u	0	{}
2’2’2	112	A	0	{2}	4/m’	4	A	0	{}	4’/mm’m	$m_{110}m_{1\bar{1}0}m$	B_{1g}	0	{}
2’2’2	112	B	2	{}	4/m’	4	B	0	{}	4’/mm’m	$m_{110}m_{1\bar{1}0}m$	B_{1u}	1	{}
mm2	mm2	A_1	0	{2}	4’/m’	$\bar{4}$	A	0	{}	4’/m’m’m	$\bar{4}2m_{110}$	A_1	0	{}
mm2	mm2	A_2	0	{}	4’/m’	$\bar{4}$	B	1	{}	4’/m’m’m	$\bar{4}2m_{110}$	B_1	0	{}
mm2	mm2	B_2	0	{}	422	422	A_1	0	{}	4’/m’m’m	$\bar{4}2m_{110}$	B_2	1	{}
mm2	mm2	B_1	0	{}	422	422	B_1	0	{}	4’/m’m’m	$\bar{4}2m_{110}$	A_2	0	{}
mm21’	mm2	A_1	1	{}	422	422	B_2	0	{}	4/mm’m’	4/m	A_g	1	{}
mm21’	mm2	A_2	0	{}	422	422	A_2	0	{}	4/mm’m’	4/m	A_u	0	{2}
mm21’	mm2	B_2	0	{}	4221’	422	A_1	0	{}	4/mm’m’	4/m	B_g	1	{}
mm21’	mm2	B_1	0	{}	4221’	422	B_1	0	{}	4/mm’m’	4/m	B_u	0	{2}
m’m2’	1m1	A’	2	{}	4221’	422	B_2	0	{}	4/mm’m’	4/m	^2E_g	0	{}
m’m2’	1m1	A”	0	{}	4221’	422	A_2	2	{}	4/mm’m’	4/m	^2E_u	3	{}
m’m’2	112	A	0	{}	4’22’	222	A_1	0	{}	4/mm’m’	4/m	^1E_g	0	{}
m’m’2	112	B	0	{}	4’22’	222	B_1	1	{}	4/mm’m’	4/m	^1E_u	3	{}
mmm	mmm	A_g	0	{}	42’2’	4	A	0	{2}	4/m’m’m’	422	A_1	0	{}
mmm	mmm	A_u	0	{}	42’2’	4	B	0	{2}	4/m’m’m’	422	B_1	0	{}
mmm	mmm	B_{3g}	0	{}	42’2’	4	^2E	2	{}	4/m’m’m’	422	B_2	0	{}
mmm	mmm	B_{3u}	0	{2}	42’2’	4	^1E	2	{}	4/m’m’m’	422	A_2	0	{}
mmm	mmm	B_{2g}	0	{}	4mm	4mm	A_1	0	{2, 2}	3	3	A	0	{}

Table D7. Continued

MPG	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor
mmm	mmm	B_{2u}	0	{2}	4mm	4mm	A_2	0	{}	3	3	^2E	0	{}
mmm	mmm	B_{1g}	0	{}	4mm	4mm	B_1	0	{}	3	3	^1E	0	{}
mmm	mmm	B_{1u}	0	{2}	4mm	4mm	B_2	0	{}	31’	3	A	1	{}
mmm1’	mmm	A_g	0	{}	4mm1’	4mm	A_1	2	{}	$\bar{3}$	$\bar{3}$	A_g	0	{}
mmm1’	mmm	A_u	0	{}	4mm1’	4mm	A_2	0	{}	$\bar{3}$	$\bar{3}$	^2E_g	0	{}
mmm1’	mmm	B_{3g}	0	{}	4mm1’	4mm	B_1	0	{}	$\bar{3}$	$\bar{3}$	^1E_g	0	{}
mmm1’	mmm	B_{3u}	1	{}	4mm1’	4mm	B_2	0	{}	$\bar{3}$	$\bar{3}$	A_u	0	{4}
mmm1’	mmm	B_{2g}	0	{}	4’m’m	$m_{110}m_{1\bar{1}0}2$	A_1	1	{}	$\bar{3}$	$\bar{3}$	^2E_u	0	{4}
mmm1’	mmm	B_{2u}	1	{}	4’m’m	$m_{110}m_{1\bar{1}0}2$	A_2	0	{}	$\bar{3}$	$\bar{3}$	^1E_u	0	{4}
mmm1’	mmm	B_{1g}	0	{}	4m’m’	4	A	0	{}	$\bar{3}$1’	$\bar{3}$	A_g	0	{}
mmm1’	mmm	B_{1u}	1	{}	4m’m’	4	B	0	{}	$\bar{3}$1’	$\bar{3}$	A_u	1	{2}
m’mm	2mm	A_1	0	{2}	4m’m’	4	^2E	0	{}	$\bar{3}'$	3	A	0	{}
32	$32_{100}1$	A_1	0	{}	6’/m’	$\bar{3}$	A_g	0	{}	6/m’mm	6mm	B_1	1	{}
32	$32_{100}1$	A_2	0	{}	6’/m’	$\bar{3}$	A_u	2	{2}	6/m’mm	6mm	B_2	1	{}
321’	$32_{100}1$	A_1	1	{}	622	622	A_1	0	{}	6’/mmm’	$\bar{6}2_{210}m_{100}$	A'_1	0	{2}
321’	$32_{100}1$	A_2	1	{}	622	622	B_2	0	{}	6’/mmm’	$\bar{6}2_{210}m_{100}$	A''_1	0	{}
32’	3	A	1	{}	622	622	B_1	0	{}	6’/mmm’	$\bar{6}2_{210}m_{100}$	A''_2	2	{}
32’	3	^2E	1	{}	622	622	A_2	0	{}	6’/mmm’	$\bar{6}2_{210}m_{100}$	A'_2	1	{}
32’	3	^1E	1	{}	6221’	622	A_1	0	{}	6’/m’mm’	$\bar{3}m_{100}$	A_{1g}	1	{}
3m	$31m_{100}$	A_1	1	{2}	6221’	622	B_2	1	{}	6’/m’mm’	$\bar{3}m_{100}$	A_{1u}	0	{2}
3m	$31m_{100}$	A_2	0	{}	6221’	622	B_1	1	{}	6’/m’mm’	$\bar{3}m_{100}$	A_{2g}	0	{}
3m1’	$31m_{100}$	A_1	1	{}	6221’	622	A_2	3	{}	6’/m’mm’	$\bar{3}m_{100}$	A_{2u}	4	{}
3m1’	$31m_{100}$	A_2	0	{}	6’22’	$32_{100}1$	A_1	0	{2}	6/mm’m’	6/m	A_g	1	{}
3m’	3	A	0	{}	6’22’	$32_{100}1$	A_2	3	{}	6/mm’m’	6/m	$^1E_{2g}$	1	{}
3m’	3	^2E	0	{}	62’2’	6	A	0	{2}	6/mm’m’	6/m	$^2E_{2g}$	1	{}
3m’	3	^1E	0	{}	62’2’	6	$^1E_2$	0	{2}	6/mm’m’	6/m	A_u	0	{2}
$\bar{3}$m	$\bar{3}m_{100}$	A_{1g}	1	{}	62’2’	6	$^2E_2$	0	{2}	6/mm’m’	6/m	$^1E_{2u}$	0	{2}
$\bar{3}$m	$\bar{3}m_{100}$	A_{1u}	0	{2}	62’2’	6	$^2E_1$	2	{}	6/mm’m’	6/m	$^2E_{2u}$	0	{2}
$\bar{3}$m	$\bar{3}m_{100}$	A_{2g}	0	{}	62’2’	6	$^1E_1$	2	{}	6/mm’m’	6/m	$^2E_{1g}$	0	{}

Table D7. Continued

MPG	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor
$\bar{3}m$	$\bar{3}m_{100}$	A_{2u}	1	{2, 2}	62’2’	6	B	2	{}	6/mm’m’	6/m	$^1E_{1g}$	0	{}
$\bar{3}m1'$	$\bar{3}m_{100}$	A_{1g}	0	{}	6mm	6mm	A_1	0	{2, 2, 2}	6/mm’m’	6/m	B_g	0	{}
$\bar{3}m1'$	$\bar{3}m_{100}$	A_{1u}	1	{}	6mm	6mm	A_2	0	{}	6/mm’m’	6/m	$^2E_{1u}$	3	{}
$\bar{3}m1'$	$\bar{3}m_{100}$	A_{2g}	0	{}	6mm	6mm	B_1	0	{}	6/mm’m’	6/m	$^1E_{1u}$	3	{}
$\bar{3}m1'$	$\bar{3}m_{100}$	A_{2u}	1	{2}	6mm	6mm	B_2	0	{}	6/mm’m’	6/m	B_u	3	{}
$\bar{3}'m$	$31m_{100}$	A_1	0	{2, 2}	6mm1’	6mm	A_1	3	{}	6/m’m’m’	622	A_1	0	{}
$\bar{3}'m$	$31m_{100}$	A_2	1	{}	6mm1’	6mm	A_2	0	{}	6/m’m’m’	622	B_2	0	{}
$\bar{3}'m'$	$32_{100}1$	A_1	0	{}	6mm1’	6mm	B_1	0	{}	6/m’m’m’	622	B_1	0	{}
$\bar{3}'m'$	$32_{100}1$	A_2	0	{}	6mm1’	6mm	B_2	0	{}	6/m’m’m’	622	A_2	0	{}
$\bar{3}m'$	$\bar{3}$	A_g	0	{}	6’mm’	$31m_{100}$	A_1	3	{}	23	23	A	0	{}
$\bar{3}m'$	$\bar{3}$	^2E_g	0	{}	6’mm’	$31m_{100}$	A_2	0	{}	23	23	^2E	0	{}
$\bar{3}m'$	$\bar{3}$	^1E_g	0	{}	6m’m’	6	A	0	{}	23	23	^1E	0	{}
$\bar{3}m'$	$\bar{3}$	A_u	1	{2}	6m’m’	6	$^1E_2$	0	{}	231’	23	A	1	{}
$\bar{3}m'$	$\bar{3}$	^2E_u	1	{2}	6m’m’	6	$^2E_2$	0	{}	$m\bar{3}$	$m\bar{3}$	A_g	0	{}
$\bar{3}m'$	$\bar{3}$	^1E_u	1	{2}	6m’m’	6	$^2E_1$	0	{}	$m\bar{3}$	$m\bar{3}$	A_u	0	{}
6	6	A	0	{}	6m’m’	6	$^1E_1$	0	{}	$m\bar{3}$	$m\bar{3}$	^2E_g	0	{}
6	6	$^1E_2$	0	{}	6m’m’	6	B	0	{}	$m\bar{3}$	$m\bar{3}$	^2E_u	0	{}
6	6	$^2E_2$	0	{}	$\bar{6}m2$	$\bar{6}2_{210}m_{100}$	A'_1	0	{2}	$m\bar{3}$	$m\bar{3}$	^1E_g	0	{}
6	6	$^2E_1$	0	{}	$\bar{6}m2$	$\bar{6}2_{210}m_{100}$	A''_1	0	{}	$m\bar{3}$	$m\bar{3}$	^1E_u	0	{}
6	6	$^1E_1$	0	{}	$\bar{6}m2$	$\bar{6}2_{210}m_{100}$	A''_2	0	{2}	$m\bar{3}1'$	$m\bar{3}$	A_g	0	{}
6	6	B	0	{}	$\bar{6}m2$	$\bar{6}2_{210}m_{100}$	A'_2	0	{}	$m\bar{3}1'$	$m\bar{3}$	A_u	1	{}
61’	6	A	3	{}	$\bar{6}m21'$	$\bar{6}2_{210}m_{100}$	A'_1	1	{}	$m'\bar{3}'$	23	A	0	{}
61’	6	B	0	{}	$\bar{6}m21'$	$\bar{6}2_{210}m_{100}$	A''_1	0	{}	432	432	A_1	0	{}
6’	3	A	2	{}	$\bar{6}m21'$	$\bar{6}2_{210}m_{100}$	A''_2	1	{}	432	432	A_2	0	{}
$\bar{6}$	$\bar{6}$	A’	1	{}	$\bar{6}m21'$	$\bar{6}2_{210}m_{100}$	A'_2	0	{}	4321’	432	A_1	0	{}
$\bar{6}$	$\bar{6}$	$^2E'$	1	{}	$\bar{6}'m'2$	312_{120}	A_1	0	{}	4321’	432	A_2	1	{}
$\bar{6}$	$\bar{6}$	$^1E'$	1	{}	$\bar{6}'m'2$	312_{120}	A_2	0	{}	4’32’	23	A	0	{}
$\bar{6}$	$\bar{6}$	A”	0	{}	$\bar{6}'m2'$	$31m_{100}$	A_1	2	{2}	4’32’	23	^2E	0	{}
$\bar{6}$	$\bar{6}$	$^2E''$	0	{}	$\bar{6}'m2'$	$31m_{100}$	A_2	0	{}	4’32’	23	^1E	0	{}

Table D7. Continued

MPG	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor
$\bar{6}$	$\bar{6}$	^{1}E”	0	{}	$\bar{6}$m’2’	$\bar{6}$	A’	2	{}	$\bar{4}$3m	$\bar{4}$3m	A_1	0	{2}
$\bar{6}$1’	$\bar{6}$	A’	0	{}	$\bar{6}$m’2’	$\bar{6}$	^{2}E’	2	{}	$\bar{4}$3m	$\bar{4}$3m	A_2	0	{}
$\bar{6}$1’	$\bar{6}$	A”	1	{}	$\bar{6}$m’2’	$\bar{6}$	^{1}E’	2	{}	$\bar{4}$3m1’	$\bar{4}$3m	A_1	1	{}
$\bar{6}'$	3	A	0	{}	$\bar{6}$m’2’	$\bar{6}$	A”	0	{}	$\bar{4}$3m1’	$\bar{4}$3m	A_2	0	{}
6/m	6/m	A_g	1	{}	$\bar{6}$m’2’	$\bar{6}$	^{2}E”	0	{}	$\bar{4}$’3m’	23	A	0	{}
6/m	6/m	$^1E_{2g}$	1	{}	$\bar{6}$m’2’	$\bar{6}$	^{1}E”	0	{}	$\bar{4}$’3m’	23	^{2}E	0	{}
6/m	6/m	$^2E_{2g}$	1	{}	6/mmm	6/mmm	A_{1g}	0	{}	$\bar{4}$’3m’	23	^{1}E	0	{}
6/m	6/m	A_u	0	{2}	6/mmm	6/mmm	A_{1u}	0	{}	m$\bar{3}$m	m$\bar{3}$m	A_{1g}	0	{}
6/m	6/m	$^1E_{2u}$	0	{2}	6/mmm	6/mmm	B_{2g}	0	{}	m$\bar{3}$m	m$\bar{3}$m	A_{1u}	0	{}
6/m	6/m	$^2E_{2u}$	0	{2}	6/mmm	6/mmm	B_{2u}	0	{2}	m$\bar{3}$m	m$\bar{3}$m	A_{2g}	0	{}
6/m	6/m	$^2E_{1g}$	0	{}	6/mmm	6/mmm	B_{1g}	0	{}	m$\bar{3}$m	m$\bar{3}$m	A_{2u}	0	{2}
6/m	6/m	$^1E_{1g}$	0	{}	6/mmm	6/mmm	B_{1u}	0	{2}	m$\bar{3}$m1’	m$\bar{3}$m	A_{1g}	0	{}
6/m	6/m	B_g	0	{}	6/mmm	6/mmm	A_{2g}	0	{}	m$\bar{3}$m1’	m$\bar{3}$m	A_{1u}	0	{}
6/m	6/m	$^2E_{1u}$	1	{2}	6/mmm	6/mmm	A_{2u}	0	{2, 2, 2}	m$\bar{3}$m1’	m$\bar{3}$m	A_{2g}	0	{}
6/m	6/m	$^1E_{1u}$	1	{2}	6/mmm1’	6/mmm	A_{1g}	0	{}	m$\bar{3}$m1’	m$\bar{3}$m	A_{2u}	1	{}
6/m	6/m	B_u	1	{2}	6/mmm1’	6/mmm	A_{1u}	0	{}	m’$\bar{3}$’m	$\bar{4}$3m	A_1	0	{2}
6/m1’	6/m	A_g	0	{}	6/mmm1’	6/mmm	B_{2g}	0	{}	m’$\bar{3}$’m	$\bar{4}$3m	A_2	0	{}
6/m1’	6/m	A_u	3	{}	6/mmm1’	6/mmm	B_{2u}	1	{}	m$\bar{3}$m’	m$\bar{3}$	A_g	0	{}
6/m1’	6/m	B_g	0	{}	6/mmm1’	6/mmm	B_{1g}	0	{}	m$\bar{3}$m’	m$\bar{3}$	A_u	0	{}
6/m1’	6/m	B_u	0	{2}	6/mmm1’	6/mmm	B_{1u}	1	{}	m$\bar{3}$m’	m$\bar{3}$	^2E_g	0	{}
6’/m	$\bar{6}$	A’	0	{2}	6/mmm1’	6/mmm	A_{2g}	0	{}	m$\bar{3}$m’	m$\bar{3}$	^2E_u	0	{}
6’/m	$\bar{6}$	A”	2	{}	6/mmm1’	6/mmm	A_{2u}	3	{}	m$\bar{3}$m’	m$\bar{3}$	^1E_g	0	{}
6/m’	6	A	0	{}	6/m’mm	6mm	A_1	0	{2, 2, 2}	m$\bar{3}$m’	m$\bar{3}$	^1E_u	0	{}
6/m’	6	B	0	{}	6/m’mm	6mm	A_2	0	{}	m’$\bar{3}$’m’	432	A_1	0	{}
										m’$\bar{3}$’m’	432	A_2	0	{}

Table D8. The classification of surface states of 3*D* TSCs of spinful electrons with crystallographic MPG symmetry. The bold red characters **1** represent the 1st-order TSC.

MPG	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor
1	1	A	0	{}	m’mm	2mm	A_2	4	{}	4m’m’	4	^{1}E	0	{}
11’	1	A	**1**	{}	m’mm	2mm	B_2	1	{}	$\bar{4}$2m	$\bar{4}2m_{110}$	A_1	0	{}
$\bar{1}$	$\bar{1}$	A_g	0	{}	m’mm	2mm	B_1	1	{}	$\bar{4}$2m	$\bar{4}2m_{110}$	B_1	1	{2}
$\bar{1}$	$\bar{1}$	A_u	0	{4}	m’m’m	112/m	A_g	0	{}	$\bar{4}$2m	$\bar{4}2m_{110}$	B_2	0	{2}
$\bar{1}$1’	$\bar{1}$	A_g	0	{}	m’m’m	112/m	A_u	3	{}	$\bar{4}$2m	$\bar{4}2m_{110}$	A_2	1	{2}
$\bar{1}$1’	$\bar{1}$	A_u	**1**	{4}	m’m’m	112/m	B_g	1	{}	$\bar{4}$2m1’	$\bar{4}2m_{110}$	A_1	1	{}
$\bar{1}$′	1	A	0	{}	m’m’m	112/m	B_u	0	{2}	$\bar{4}$2m1’	$\bar{4}2m_{110}$	B_1	**1+3**	{}
2	121	A	0	{}	m’m’m’	222	A_1	0	{}	$\bar{4}$2m1’	$\bar{4}2m_{110}$	B_2	0	{2}
2	121	B	0	{}	m’m’m’	222	B_3	0	{}	$\bar{4}$2m1’	$\bar{4}2m_{110}$	A_2	1	{2}
21’	121	A	**1+1**	{}	m’m’m’	222	B_2	0	{}	$\bar{4}$’2’m	$m_{110}m_{1\bar{1}0}2$	A_1	1	{}
21’	121	B	0	{2}	m’m’m’	222	B_1	0	{}	$\bar{4}$’2’m	$m_{110}m_{1\bar{1}0}2$	A_2	2	{2}
2’	1	A	1	{}	4	4	A	0	{}	$\bar{4}$’2m’	222	A_1	0	{}
m	1m1	A’	0	{}	4	4	B	0	{}	$\bar{4}$’2m’	222	B_1	0	{}
m	1m1	A”	1	{}	4	4	^{2}E	0	{}	$\bar{4}$2’m’	$\bar{4}$	A	1	{}
m1’	1m1	A’	0	{}	4	4	^{1}E	0	{}	$\bar{4}$2’m’	$\bar{4}$	B	1	{}
m1’	1m1	A”	**1+1**	{}	41’	4	A	**1+2**	{}	$\bar{4}$2’m’	$\bar{4}$	^{2}E	0	{2}
m’	1	A	0	{}	41’	4	B	0	{2}	$\bar{4}$2’m’	$\bar{4}$	^{1}E	0	{2}
2/m	12/m1	A_g	0	{}	4’	112	A	1	{}	4/mmm	4/mmm	A_{1g}	0	{}
2/m	12/m1	A_u	1	{2}	$\bar{4}$	$\bar{4}$	A	0	{2}	4/mmm	4/mmm	A_{1u}	3	{2, 2}
2/m	12/m1	B_g	1	{}	$\bar{4}$	$\bar{4}$	B	0	{2}	4/mmm	4/mmm	B_{1g}	1	{}
2/m	12/m1	B_u	0	{2}	$\bar{4}$	$\bar{4}$	^{2}E	0	{2}	4/mmm	4/mmm	B_{1u}	2	{}
2/m1’	12/m1	A_g	0	{}	$\bar{4}$	$\bar{4}$	^{1}E	0	{2}	4/mmm	4/mmm	B_{2g}	1	{}
2/m1’	12/m1	A_u	**1+2**	{2}	$\bar{4}$1’	$\bar{4}$	A	0	{2}	4/mmm	4/mmm	B_{2u}	2	{}
2/m1’	12/m1	B_g	1	{}	$\bar{4}$1’	$\bar{4}$	B	**1+1**	{2}	4/mmm	4/mmm	A_{2g}	2	{}
2/m1’	12/m1	B_u	0	{4}	$\bar{4}$′	112	A	0	{}	4/mmm	4/mmm	A_{2u}	1	{2}
2’/m	1m1	A’	0	{}	4/m	4/m	A_g	0	{}	4/mmm1’	4/mmm	A_{1g}	0	{}
2’/m	1m1	A”	2	{}	4/m	4/m	A_u	1	{2}	4/mmm1’	4/mmm	A_{1u}	**1+7**	{}
2/m’	121	A	0	{}	4/m	4/m	B_g	0	{}	4/mmm1’	4/mmm	B_{1g}	1	{}
2/m’	121	B	0	{}	4/m	4/m	B_u	1	{2}	4/mmm1’	4/mmm	B_{1u}	3	{}

Table D8. Continued

MPG	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor
2'/m'	$\bar{1}$	A_g	0	{}	4/m	4/m	^2E_g	1	{}	4/mmm1'	4/mmm	B_{2g}	1	{}
2'/m'	$\bar{1}$	A_u	1	{2}	4/m	4/m	^2E_u	0	{2}	4/mmm1'	4/mmm	B_{2u}	3	{}
222	222	A_1	0	{}	4/m	4/m	^1E_g	1	{}	4/mmm1'	4/mmm	A_{2g}	2	{}
222	222	B_3	0	{}	4/m	4/m	^1E_u	0	{2}	4/mmm1'	4/mmm	A_{2u}	1	{2}
222	222	B_2	0	{}	4/m1'	4/m	A_g	0	{}	4/m'mm	4mm	A_1	0	{}
222	222	B_1	0	{}	4/m1'	4/m	A_u	**1+3**	{2}	4/m'mm	4mm	A_2	4	{2}
2221'	222	A_1	**1+3**	{}	4/m1'	4/m	B_g	0	{2}	4/m'mm	4mm	B_1	2	{}
2221'	222	B_3	0	{2, 2}	4/m1'	4/m	B_u	1	{2}	4/m'mm	4mm	B_2	2	{}
2221'	222	B_2	0	{2, 2}	4'/m	112/m	A_g	0	{}	4'/mm'm	$m_{110}m_{1\bar{1}0}m$	A_g	0	{}
2221'	222	B_1	0	{2, 2}	4'/m	112/m	A_u	2	{2}	4'/mm'm	$m_{110}m_{1\bar{1}0}m$	A_u	4	{}
2'2'2	112	A	2	{}	4/m'	4	A	0	{}	4'/mm'm	$m_{110}m_{1\bar{1}0}m$	B_{1g}	1	{}
2'2'2	112	B	0	{2}	4/m'	4	B	0	{}	4'/mm'm	$m_{110}m_{1\bar{1}0}m$	B_{1u}	2	{}
mm2	mm2	A_1	0	{}	4'/m'	$\bar{4}$	A	0	{}	4'/m'm'm	$\bar{4}2m_{110}$	A_1	0	{}
mm2	mm2	A_2	2	{}	4'/m'	$\bar{4}$	B	1	{2}	4'/m'm'm	$\bar{4}2m_{110}$	B_1	3	{}
mm2	mm2	B_2	1	{}	422	422	A_1	0	{}	4'/m'm'm	$\bar{4}2m_{110}$	B_2	0	{2}
mm2	mm2	B_1	1	{}	422	422	B_1	0	{}	4'/m'm'm	$\bar{4}2m_{110}$	A_2	2	{}
mm21'	mm2	A_1	0	{}	422	422	B_2	0	{}	4/mm'm'	4/m	A_g	0	{}
mm21'	mm2	A_2	**1+3**	{}	422	422	A_2	0	{}	4/mm'm'	4/m	A_u	3	{}
mm21'	mm2	B_2	1	{}	4221'	422	A_1	**1+4**	{}	4/mm'm'	4/m	B_g	0	{}
mm21'	mm2	B_1	1	{}	4221'	422	B_1	1	{2}	4/mm'm'	4/m	B_u	3	{}
m'm2'	1m1	A'	0	{}	4221'	422	B_2	1	{2}	4/mm'm'	4/m	^2E_g	1	{}
m'm2'	1m1	A"	2	{}	4221'	422	A_2	0	{2, 2}	4/mm'm'	4/m	^2E_u	0	{2}
m'm'2	112	A	0	{}	4'22'	222	A_1	2	{}	4/mm'm'	4/m	^1E_g	1	{}
m'm'2	112	B	0	{}	4'22'	222	B_1	1	{2}	4/mm'm'	4/m	^1E_u	0	{2}
mmm	mmm	A_g	0	{}	42'2'	4	A	2	{}	4/m'm'm'	422	A_1	0	{}
mmm	mmm	A_u	3	{2}	42'2'	4	B	2	{}	4/m'm'm'	422	B_1	0	{}
mmm	mmm	B_{3g}	2	{}	42'2'	4	^2E	0	{2}	4/m'm'm'	422	B_2	0	{}
mmm	mmm	B_{3u}	1	{2}	42'2'	4	^1E	0	{2}	4/m'm'm'	422	A_2	0	{}
mmm	mmm	B_{2g}	2	{}	4mm	4mm	A_1	0	{}	3	3	A	0	{}
mmm	mmm	B_{2u}	1	{2}	4mm	4mm	A_2	2	{2}	3	3	^2E	0	{}
mmm	mmm	B_{1g}	2	{}	4mm	4mm	B_1	1	{}	3	3	^1E	0	{}

Table D8. Continued

MPG	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor
mmm	mmm	B_{1u}	1	{2}	4mm	4mm	B_2	1	{}	31’	3	A	**1+1**	{}
mmm1’	mmm	A_g	0	{}	4mm1’	4mm	A_1	0	{}	$\bar{3}$	$\bar{3}$	A_g	0	{}
mmm1’	mmm	A_u	**1+6**	{}	4mm1’	4mm	A_2	**1+4**	{}	$\bar{3}$	$\bar{3}$	^2E_g	0	{}
mmm1’	mmm	B_{3g}	2	{}	4mm1’	4mm	B_1	1	{}	$\bar{3}$	$\bar{3}$	^1E_g	0	{}
mmm1’	mmm	B_{3u}	1	{2}	4mm1’	4mm	B_2	1	{}	$\bar{3}$	$\bar{3}$	A_u	0	{4}
mmm1’	mmm	B_{2g}	2	{}	4’m’m	$m_{110}m_{1\bar{1}0}2$	A_1	0	{}	$\bar{3}$	$\bar{3}$	^2E_u	0	{4}
mmm1’	mmm	B_{2u}	1	{2}	4’m’m	$m_{110}m_{1\bar{1}0}2$	A_2	2	{}	$\bar{3}$	$\bar{3}$	^1E_u	0	{4}
mmm1’	mmm	B_{1g}	2	{}	4m’m’	4	A	0	{}	$\bar{3}$1’	$\bar{3}$	A_g	0	{}
mmm1’	mmm	B_{1u}	1	{2}	4m’m’	4	B	0	{}	$\bar{3}$1’	$\bar{3}$	A_u	**1+1**	{4}
m’mm	2mm	A_1	0	{}	4m’m’	4	^2E	0	{}	$\bar{3}'$	3	A	0	{}
32	$32_{100}1$	A_1	0	{}	6’/m’	$\bar{3}$	A_g	0	{}	6/m’mm	6mm	B_1	1	{}
32	$32_{100}1$	A_2	0	{}	6’/m’	$\bar{3}$	A_u	2	{2}	6/m’mm	6mm	B_2	1	{}
321’	$32_{100}1$	A_1	**1+2**	{}	622	622	A_1	0	{}	6’/mmm’	$\bar{6}2_{210}m_{100}$	A'_1	0	{}
321’	$32_{100}1$	A_2	0	{2}	622	622	B_2	0	{}	6’/mmm’	$\bar{6}2_{210}m_{100}$	A''_1	5	{}
32’	3	A	1	{}	622	622	B_1	0	{}	6’/mmm’	$\bar{6}2_{210}m_{100}$	A''_2	1	{}
32’	3	^2E	1	{}	622	622	A_2	0	{}	6’/mmm’	$\bar{6}2_{210}m_{100}$	A'_2	1	{}
32’	3	^1E	1	{}	6221’	622	A_1	**1+5**	{}	6’/m’mm’	$\bar{3}m_{100}$	A_{1g}	0	{}
3m	$31m_{100}$	A_1	0	{}	6221’	622	B_2	0	{2, 2}	6’/m’mm’	$\bar{3}m_{100}$	A_{1u}	4	{}
3m	$31m_{100}$	A_2	1	{2}	6221’	622	B_1	0	{2, 2}	6’/m’mm’	$\bar{3}m_{100}$	A_{2g}	1	{}
3m1’	$31m_{100}$	A_1	0	{}	6221’	622	A_2	0	{2, 2}	6’/m’mm’	$\bar{3}m_{100}$	A_{2u}	0	{2}
3m1’	$31m_{100}$	A_2	**1+2**	{}	6’22’	$32_{100}1$	A_1	3	{}	6/mm’m’	6/m	A_g	0	{}
3m’	3	A	0	{}	6’22’	$32_{100}1$	A_2	0	{2}	6/mm’m’	6/m	$^1E_{2g}$	0	{}
3m’	3	^2E	0	{}	62’2’	6	A	2	{}	6/mm’m’	6/m	$^2E_{2g}$	0	{}
3m’	3	^1E	0	{}	62’2’	6	$^1E_2$	2	{}	6/mm’m’	6/m	A_u	3	{}
$\bar{3}$m	$\bar{3}m_{100}$	A_{1g}	0	{}	62’2’	6	$^2E_2$	2	{}	6/mm’m’	6/m	$^1E_{2u}$	3	{}
$\bar{3}$m	$\bar{3}m_{100}$	A_{1u}	1	{2, 2}	62’2’	6	$^2E_1$	0	{2}	6/mm’m’	6/m	$^2E_{2u}$	3	{}
$\bar{3}$m	$\bar{3}m_{100}$	A_{2g}	1	{}	62’2’	6	$^1E_1$	0	{2}	6/mm’m’	6/m	$^2E_{1g}$	1	{}
$\bar{3}$m	$\bar{3}m_{100}$	A_{2u}	0	{2}	62’2’	6	B	0	{2}	6/mm’m’	6/m	$^1E_{1g}$	1	{}
$\bar{3}$m1’	$\bar{3}m_{100}$	A_{1g}	0	{}	6mm	6mm	A_1	0	{}	6/mm’m’	6/m	B_g	1	{}
$\bar{3}$m1’	$\bar{3}m_{100}$	A_{1u}	**1+3**	{2}	6mm	6mm	A_2	2	{2, 2}	6/mm’m’	6/m	$^2E_{1u}$	0	{2}

Table D8. Continued

MPG	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor
$\bar{3}$m1’	$\bar{3}$m$_{100}$	A$_{2g}$	1	{}	6mm	6mm	B$_1$	1	{}	6/mm’m’	6/m	^{1}E$_{1u}$	0	{2}
$\bar{3}$m1’	$\bar{3}$m$_{100}$	A$_{2u}$	0	{4}	6mm	6mm	B$_2$	1	{}	6/mm’m’	6/m	B$_u$	0	{2}
$\bar{3}$’m	31m$_{100}$	A$_1$	0	{}	6mm1’	6mm	A$_1$	0	{}	6/m’m’m’	622	A$_1$	0	{}
$\bar{3}$’m	31m$_{100}$	A$_2$	2	{2}	6mm1’	6mm	A$_2$	**1+5**	{}	6/m’m’m’	622	B$_2$	0	{}
$\bar{3}$’m’	32$_{100}$1	A$_1$	0	{}	6mm1’	6mm	B$_1$	1	{}	6/m’m’m’	622	B$_1$	0	{}
$\bar{3}$’m’	32$_{100}$1	A$_2$	0	{}	6mm1’	6mm	B$_2$	1	{}	6/m’m’m’	622	A$_2$	0	{}
$\bar{3}$m’	$\bar{3}$	A$_g$	0	{}	6’mm’	31m$_{100}$	A$_1$	0	{}	23	23	A	0	{}
$\bar{3}$m’	$\bar{3}$	^{2}E$_g$	0	{}	6’mm’	31m$_{100}$	A$_2$	3	{}	23	23	^{2}E	0	{}
$\bar{3}$m’	$\bar{3}$	^{1}E$_g$	0	{}	6m’m’	6	A	0	{}	23	23	^{1}E	0	{}
$\bar{3}$m’	$\bar{3}$	A$_u$	1	{2}	6m’m’	6	^{1}E$_2$	0	{}	231’	23	A	**1+2**	{}
$\bar{3}$m’	$\bar{3}$	^{2}E$_u$	1	{2}	6m’m’	6	^{2}E$_2$	0	{}	m$\bar{3}$	m$\bar{3}$	A$_g$	0	{}
$\bar{3}$m’	$\bar{3}$	^{1}E$_u$	1	{2}	6m’m’	6	^{2}E$_1$	0	{}	m$\bar{3}$	m$\bar{3}$	A$_u$	1	{2}
6	6	A	0	{}	6m’m’	6	^{1}E$_1$	0	{}	m$\bar{3}$	m$\bar{3}$	^{2}E$_g$	0	{}
6	6	^{1}E$_2$	0	{}	6m’m’	6	B	0	{}	m$\bar{3}$	m$\bar{3}$	^{2}E$_u$	1	{2}
6	6	^{2}E$_2$	0	{}	$\bar{6}$m2	$\bar{6}$2$_{210}$m$_{100}$	A’$_1$	0	{}	m$\bar{3}$	m$\bar{3}$	^{1}E$_g$	0	{}
6	6	^{2}E$_1$	0	{}	$\bar{6}$m2	$\bar{6}$2$_{210}$m$_{100}$	A”$_1$	2	{2}	m$\bar{3}$	m$\bar{3}$	^{1}E$_u$	1	{2}
6	6	^{1}E$_1$	0	{}	$\bar{6}$m2	$\bar{6}$2$_{210}$m$_{100}$	A”$_2$	1	{}	m$\bar{3}$1’	m$\bar{3}$	A$_g$	0	{}
6	6	B	0	{}	$\bar{6}$m2	$\bar{6}$2$_{210}$m$_{100}$	A’$_2$	1	{}	m$\bar{3}$1’	m$\bar{3}$	A$_u$	**1+3**	{}
61’	6	A	**1+3**	{}	$\bar{6}$m21’	$\bar{6}$2$_{210}$m$_{100}$	A’$_1$	0	{}	m’$\bar{3}$′	23	A	0	{}
61’	6	B	0	{2}	$\bar{6}$m21’	$\bar{6}$2$_{210}$m$_{100}$	A”$_1$	**1+4**	{}	432	432	A$_1$	0	{}
6’	3	A	2	{}	$\bar{6}$m21’	$\bar{6}$2$_{210}$m$_{100}$	A”$_2$	1	{}	432	432	A$_2$	0	{}
$\bar{6}$	$\bar{6}$	A’	0	{}	$\bar{6}$m21’	$\bar{6}$2$_{210}$m$_{100}$	A’$_2$	1	{}	4321’	432	A$_1$	**1+4**	{}
$\bar{6}$	$\bar{6}$	^{2}E’	0	{}	$\bar{6}$’m’2	312$_{120}$	A$_1$	0	{}	4321’	432	A$_2$	0	{2}
$\bar{6}$	$\bar{6}$	^{1}E’	0	{}	$\bar{6}$’m’2	312$_{120}$	A$_2$	0	{}	4’32’	23	A	2	{}
$\bar{6}$	$\bar{6}$	A”	1	{}	$\bar{6}$’m2’	31m$_{100}$	A$_1$	0	{}	4’32’	23	^{2}E	2	{}
$\bar{6}$	$\bar{6}$	^{2}E”	1	{}	$\bar{6}$’m2’	31m$_{100}$	A$_2$	2	{2}	4’32’	23	^{1}E	2	{}
$\bar{6}$	$\bar{6}$	^{1}E”	1	{}	$\bar{6}$m’2’	$\bar{6}$	A’	0	{}	$\bar{4}$3m	$\bar{4}$3m	A$_1$	0	{}
$\bar{6}$1’	$\bar{6}$	A’	0	{}	$\bar{6}$m’2’	$\bar{6}$	^{2}E’	0	{}	$\bar{4}$3m	$\bar{4}$3m	A$_2$	1	{2, 2}
$\bar{6}$1’	$\bar{6}$	A”	**1+2**	{}	$\bar{6}$m’2’	$\bar{6}$	^{1}E’	0	{}	$\bar{4}$3m1’	$\bar{4}$3m	A$_1$	0	{}
$\bar{6}$′	3	A	0	{}	$\bar{6}$m’2’	$\bar{6}$	A”	2	{}	$\bar{4}$3m1’	$\bar{4}$3m	A$_2$	**1+3**	{}
6/m	6/m	A$_g$	0	{}	$\bar{6}$m’2’	$\bar{6}$	^{2}E”	2	{}	$\bar{4}$’3m’	23	A	0	{}

Table D8. Continued

MPG	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor	*MPG*	G_u	Irrep	Free	Tor
6/m	6/m	${}^{1}E_{2g}$	0	{}	$\bar{6}m'2'$	$\bar{6}$	${}^{1}E''$	2	{}	$\bar{4}'3m'$	23	${}^{2}E$	0	{}
6/m	6/m	${}^{2}E_{2g}$	0	{}	6/mmm	6/mmm	A_{1g}	0	{}	$\bar{4}'3m'$	23	${}^{1}E$	0	{}
6/m	6/m	A_u	1	{2}	6/mmm	6/mmm	A_{1u}	3	{2, 2, 2}	$m\bar{3}m$	$m\bar{3}m$	A_{1g}	0	{}
6/m	6/m	${}^{1}E_{2u}$	1	{2}	6/mmm	6/mmm	B_{2g}	2	{}	$m\bar{3}m$	$m\bar{3}m$	A_{1u}	2	{2, 2, 2}
6/m	6/m	${}^{2}E_{2u}$	1	{2}	6/mmm	6/mmm	B_{2u}	1	{2}	$m\bar{3}m$	$m\bar{3}m$	A_{2g}	1	{}
6/m	6/m	${}^{2}E_{1g}$	1	{}	6/mmm	6/mmm	B_{1g}	2	{}	$m\bar{3}m$	$m\bar{3}m$	A_{2u}	1	{}
6/m	6/m	${}^{1}E_{1g}$	1	{}	6/mmm	6/mmm	B_{1u}	1	{2}	$m\bar{3}m1'$	$m\bar{3}m$	A_{1g}	0	{}
6/m	6/m	B_g	1	{}	6/mmm	6/mmm	A_{2g}	2	{}	$m\bar{3}m1'$	$m\bar{3}m$	A_{1u}	**1+6**	{}
6/m	6/m	${}^{2}E_{1u}$	0	{2}	6/mmm	6/mmm	A_{2u}	1	{2}	$m\bar{3}m1'$	$m\bar{3}m$	A_{2g}	1	{}
6/m	6/m	${}^{1}E_{1u}$	0	{2}	6/mmm1'	6/mmm	A_{1g}	0	{}	$m\bar{3}m1'$	$m\bar{3}m$	A_{2u}	1	{}
6/m	6/m	B_u	0	{2}	6/mmm1'	6/mmm	A_{1u}	**1+8**	{}	$m'\bar{3}'m$	$\bar{4}3m$	A_1	0	{}
6/m1'	6/m	A_g	0	{}	6/mmm1'	6/mmm	B_{2g}	2	{}	$m'\bar{3}'m$	$\bar{4}3m$	A_2	3	{2}
6/m1'	6/m	A_u	**1+4**	{2}	6/mmm1'	6/mmm	B_{2u}	1	{2}	$m\bar{3}m'$	$m\bar{3}$	A_g	0	{}
6/m1'	6/m	B_g	1	{}	6/mmm1'	6/mmm	B_{1g}	2	{}	$m\bar{3}m'$	$m\bar{3}$	A_u	3	{}
6/m1'	6/m	B_u	0	{4}	6/mmm1'	6/mmm	B_{1u}	1	{2}	$m\bar{3}m'$	$m\bar{3}$	${}^{2}E_g$	0	{}
6'/m	$\bar{6}$	A'	0	{}	6/mmm1'	6/mmm	A_{2g}	2	{}	$m\bar{3}m'$	$m\bar{3}$	${}^{2}E_u$	3	{}
6'/m	$\bar{6}$	A''	3	{}	6/mmm1'	6/mmm	A_{2u}	1	{2}	$m\bar{3}m'$	$m\bar{3}$	${}^{1}E_g$	0	{}
6/m'	6	A	0	{}	6/m'mm	6mm	A_1	0	{}	$m\bar{3}m'$	$m\bar{3}$	${}^{1}E_u$	3	{}
6/m'	6	B	0	{}	6/m'mm	6mm	A_2	4	{2, 2}	$m'\bar{3}'m'$	432	A_1	0	{}
										$m'\bar{3}'m'$	432	A_2	0	{}

Table D9. Character tables of 1D representations of the crystallographic point groups.

1	1
A	1

211	1	2_{100}
A	1	1
B	1	−1

121	1	2_{010}
A	1	1
B	1	−1

112	1	2_{001}
A	1	1
B	1	−1

$\bar{1}$	1	$\bar{1}$
A_g	1	1
A_u	1	−1

m11	1	m_{100}
A’	1	1
A”	1	−1

1m1	1	m_{010}
A’	1	1
A”	1	−1

11m	1	m_{001}
A’	1	1
A”	1	−1

3	1	3^+_{001}	3^-_{001}
A	1	1	1
^{2}E	1	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$
^{1}E	1	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$

222	1	2_{100}	2_{010}	2_{001}
A_1	1	1	1	1
B_3	1	1	−1	−1
B_2	1	−1	1	−1
B_1	1	−1	−1	1

2/m11	1	2_{100}	$\bar{1}$	m_{100}
A_g	1	1	1	1
A_u	1	1	−1	−1
B_g	1	−1	1	−1
B_u	1	−1	−1	1

2mm	1	2_{100}	m_{010}	m_{001}
A_1	1	1	1	1
A_2	1	1	−1	−1
B_2	1	−1	1	−1
B_1	1	−1	−1	1

12/m1	1	2_{010}	$\bar{1}$	m_{010}
A_g	1	1	1	1
A_u	1	1	−1	−1
B_g	1	−1	1	−1
B_u	1	−1	−1	1

m2m	1	2_{010}	m_{100}	m_{001}
A_1	1	1	1	1
A_2	1	1	−1	−1
B_1	1	−1	1	−1
B_2	1	−1	−1	1

$2_{110}2_{1\bar{1}0}2$	1	2_{001}	$2_{1\bar{1}0}$	2_{110}
A_1	1	1	1	1
B_1	1	1	−1	−1

4	1	2_{001}	4^+_{001}	4^-_{001}
A	1	1	1	1
B	1	1	−1	−1
^{2}E	1	−1	i	$-i$
^{1}E	1	−1	$-i$	i

112/m	1	2_{001}	$\bar{1}$	m_{001}
A_g	1	1	1	1
A_u	1	1	−1	−1
B_g	1	−1	1	−1
B_u	1	−1	−1	1

mm2	1	2_{001}	m_{100}	m_{010}
A_1	1	1	1	1
A_2	1	1	−1	−1
B_2	1	−1	1	−1
B_1	1	−1	−1	1

$m_{110}m_{1-10}2$	1	2_{001}	$m_{1\bar{1}0}$	m_{110}
A_1	1	1	1	1
A_2	1	1	−1	−1

$\bar{4}$	1	2_{001}	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$
A	1	1	1	1
B	1	1	−1	−1
^{2}E	1	−1	i	$-i$
^{1}E	1	−1	$-i$	i

$32_{100}1$	1	2_{100}	3^+_{001}	3^-_{001}	2_{110}	2_{010}
A_1	1	1	1	1	1	1
A_2	1	−1	1	1	−1	−1

312_{120}	1	2_{120}	3^+_{001}	3^-_{001}	2_{210}	$2_{1\bar{1}0}$
A_1	1	1	1	1	1	1
A_2	1	−1	1	1	−1	−1

6	1	2_{001}	6^+_{001}	3^+_{001}	3^-_{001}	6^-_{001}
A	1	1	1	1	1	1
${}^1E_2$	1	1	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$
${}^2E_2$	1	1	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$
${}^2E_1$	1	−1	$e^{\frac{\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$
${}^1E_1$	1	−1	$e^{-\frac{\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{\pi i}{3}}$
B	1	−1	−1	1	1	−1

$\bar{3}$	1	$\bar{1}$	3^+_{001}	3^-_{001}	$\bar{3}^+_{001}$	$\bar{3}^-_{001}$
A_g	1	1	1	1	1	1
${}^2E_g$	1	1	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$
${}^1E_g$	1	1	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$
A_u	1	−1	1	1	−1	−1
${}^2E_u$	1	−1	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$
${}^1E_u$	1	−1	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$

Table D9. Continued

$31m_{100}$	1	m_{100}	3^{+}_{001}	3^{-}_{001}	m_{110}	m_{010}
A_1	1	1	1	1	1	1
A_2	1	−1	1	1	−1	−1

$3m_{120}1$	1	m_{120}	3^{+}_{001}	3^{-}_{001}	m_{210}	$m_{1\bar{1}0}$
A_1	1	1	1	1	1	1
A_2	1	−1	1	1	−1	−1

$\bar{6}$	1	m_{001}	3^{+}_{001}	3^{-}_{001}	$\bar{6}^{+}_{001}$	$\bar{6}^{-}_{001}$
A'	1	1	1	1	1	1
^{2}E'	1	1	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$
^{1}E'	1	1	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$
A"	1	−1	1	1	−1	−1
^{2}E"	1	−1	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$
^{1}E"	1	−1	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$

422	1	2_{100}	2_{010}	2_{001}	$2_{1\bar{1}0}$	4^{+}_{001}	4^{-}_{001}	2_{110}
A_1	1	1	1	1	1	1	1	1
B_1	1	1	1	1	−1	−1	−1	−1
B_2	1	−1	−1	1	1	−1	−1	1
A_2	1	−1	−1	1	−1	1	1	−1

mmm	1	2_{100}	2_{010}	2_{001}	$\bar{1}$	m_{100}	m_{010}	m_{001}
A_g	1	1	1	1	1	1	1	1
A_u	1	1	1	1	−1	−1	−1	−1
B_{3g}	1	1	−1	−1	1	1	−1	−1
B_{3u}	1	1	−1	−1	−1	−1	1	1
B_{2g}	1	−1	1	−1	1	−1	1	−1
B_{2u}	1	−1	1	−1	−1	1	−1	1
B_{1g}	1	−1	−1	1	1	−1	−1	1
B_{1u}	1	−1	−1	1	−1	1	1	−1

$\bar{4}2m_{110}$	1	2_{100}	2_{010}	2_{001}	$m_{1\bar{1}0}$	$\bar{4}^{+}_{001}$	$\bar{4}^{-}_{001}$	m_{110}
A_1	1	1	1	1	1	1	1	1
B_1	1	1	1	1	−1	−1	−1	−1
B_2	1	−1	−1	1	1	−1	−1	1
A_2	1	−1	−1	1	−1	1	1	−1

$m_{110}m_{1-10}m$	1	2_{001}	$2_{1\bar{1}0}$	2_{110}	$\bar{1}$	m_{001}	$m_{1\bar{1}0}$	m_{110}
A_g	1	1	1	1	1	1	1	1
A_u	1	1	1	1	−1	−1	−1	−1
B_{1g}	1	1	−1	−1	1	1	−1	−1
B_{1u}	1	1	−1	−1	−1	−1	1	1

$\bar{4}2m_{100}$	1	2_{001}	$2_{1\bar{1}0}$	2_{110}	m_{100}	m_{010}	$\bar{4}^{+}_{001}$	$\bar{4}^{-}_{001}$
A_1	1	1	1	1	1	1	1	1
B_1	1	1	1	1	−1	−1	−1	−1
B_2	1	1	−1	−1	1	1	−1	−1
A_2	1	1	−1	−1	−1	−1	1	1

Table D9. Continued

4/m	1	2_{001}	4^+_{001}	4^-_{001}	$\bar{1}$	m_{001}	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$
A_g	1	1	1	1	1	1	1	1
A_u	1	1	1	1	−1	−1	−1	−1
B_g	1	1	−1	−1	1	1	−1	−1
B_u	1	1	−1	−1	−1	−1	1	1
^2E_g	1	−1	i	$-i$	1	−1	i	$-i$
^2E_u	1	−1	i	$-i$	−1	1	$-i$	i
^1E_g	1	−1	$-i$	i	1	−1	$-i$	i
^1E_u	1	−1	$-i$	i	−1	1	i	$-i$

4mm	1	2_{001}	4^+_{001}	4^-_{001}	m_{100}	m_{010}	$m_{1\bar{1}0}$	m_{110}
A_1	1	1	1	1	1	1	1	1
A_2	1	1	1	1	−1	−1	−1	−1
B_1	1	1	−1	−1	1	1	−1	−1
B_2	1	1	−1	−1	−1	−1	1	1

23	1	2_{100}	2_{010}	2_{001}	3^-_{111}	$3^-_{\bar{1}\bar{1}1}$	$3^-_{1\bar{1}\bar{1}}$	$3^-_{\bar{1}1\bar{1}}$	3^+_{111}	$3^+_{\bar{1}1\bar{1}}$	$3^+_{\bar{1}\bar{1}1}$	$3^+_{1\bar{1}\bar{1}}$
A	1	1	1	1	1	1	1	1	1	1	1	1
^2E	1	1	1	1	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$
^1E	1	1	1	1	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$

622	1	2_{100}	2_{120}	2_{001}	6^+_{001}	3^+_{001}	3^-_{001}	6^-_{001}	2_{210}	2_{110}	2_{010}	$2_{1\bar{1}0}$
A_1	1	1	1	1	1	1	1	1	1	1	1	1
B_2	1	1	−1	−1	−1	1	1	−1	−1	1	1	−1
B_1	1	−1	1	−1	−1	1	1	−1	1	−1	−1	1
A_2	1	−1	−1	1	1	1	1	1	−1	−1	−1	−1

$\bar{3}m_{100}$	1	2_{100}	$\bar{1}$	m_{100}	3^+_{001}	3^-_{001}	2_{110}	2_{010}	$\bar{3}^+_{001}$	$\bar{3}^-_{001}$	m_{110}	m_{010}
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1
A_{1u}	1	1	−1	−1	1	1	1	1	−1	−1	−1	−1
A_{2g}	1	−1	1	−1	1	1	−1	−1	1	1	−1	−1
A_{2u}	1	−1	−1	1	1	1	−1	−1	−1	−1	1	1

$\bar{6}2_{100}m_{210}$	1	2_{100}	m_{120}	m_{001}	3^+_{001}	3^-_{001}	2_{110}	2_{010}	$\bar{6}^+_{001}$	$\bar{6}^-_{001}$	m_{210}	$m_{1\bar{1}0}$
A’$_1$	1	1	1	1	1	1	1	1	1	1	1	1
A”$_1$	1	1	−1	−1	1	1	1	1	−1	−1	−1	−1
A”$_2$	1	−1	1	−1	1	1	−1	−1	−1	−1	1	1
A’$_2$	1	−1	−1	1	1	1	−1	−1	1	1	−1	−1

Table D9. Continued

$\bar{3}m_{210}$	1	2_{120}	$\bar{1}$	m_{120}	3^+_{001}	3^-_{001}	2_{210}	$2_{1\bar{1}0}$	$\bar{3}^+_{001}$	$\bar{3}^-_{001}$	m_{210}	$m_{1\bar{1}0}$
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1
A_{1u}	1	1	−1	−1	1	1	1	1	−1	−1	−1	−1
A_{2g}	1	−1	1	−1	1	1	−1	−1	1	1	−1	−1
A_{2u}	1	−1	−1	1	1	1	−1	−1	−1	−1	1	1

$\bar{6}2_{210}m_{100}$	1	2_{120}	m_{100}	m_{001}	3^+_{001}	3^-_{001}	2_{210}	$2_{1\bar{1}0}$	$\bar{6}^+_{001}$	$\bar{6}^-_{001}$	m_{110}	m_{010}
A'_1	1	1	1	1	1	1	1	1	1	1	1	1
A''_1	1	1	−1	−1	1	1	1	1	−1	−1	−1	−1
A''_2	1	−1	1	−1	1	1	−1	−1	−1	−1	1	1
A'_2	1	−1	−1	1	1	1	−1	−1	1	1	−1	−1

432	1	2_{100}	2_{010}	2_{001}	3^-_{111}	$3^-_{\bar{1}\bar{1}1}$	$3^-_{1\bar{1}\bar{1}}$	$3^-_{\bar{1}1\bar{1}}$	3^+_{111}	$3^+_{\bar{1}1\bar{1}}$	$3^+_{\bar{1}\bar{1}1}$	$3^+_{1\bar{1}\bar{1}}$	$2_{1\bar{1}0}$	4^+_{001}	4^-_{001}	2_{110}	$2_{01\bar{1}}$	2_{011}	4^+_{100}	4^-_{100}	$2_{\bar{1}01}$	4^-_{010}	2_{101}	4^+_{010}
A_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
A_2	1	1	1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1

6/m	1	2_{001}	$\bar{1}$	m_{001}	6^+_{001}	3^+_{001}	3^-_{001}	6^-_{001}	$\bar{6}^+_{001}$	$\bar{3}^+_{001}$	$\bar{3}^-_{001}$	$\bar{6}^-_{001}$
A_g	1	1	1	1	1	1	1	1	1	1	1	1
$^1E_{2g}$	1	1	1	1	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$
$^2E_{2g}$	1	1	1	1	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$
A_u	1	1	−1	−1	1	1	1	1	−1	−1	−1	−1
$^1E_{2u}$	1	1	−1	−1	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$
$^2E_{2u}$	1	1	−1	−1	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$
$^2E_{1g}$	1	−1	1	−1	$e^{\frac{\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$
$^1E_{1g}$	1	−1	1	−1	$e^{-\frac{\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{\pi i}{3}}$
B_g	1	−1	1	−1	−1	1	1	−1	−1	1	1	−1
$^2E_{1u}$	1	−1	−1	1	$e^{\frac{\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$
$^1E_{1u}$	1	−1	−1	1	$e^{-\frac{\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$
B_u	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1

Table D9. Continued

6mm	1	2_{001}	m_{100}	m_{120}	6^+_{001}	3^+_{001}	3^-_{001}	6^-_{001}	m_{210}	m_{110}	m_{010}	$m_{1\bar{1}0}$
A_1	1	1	1	1	1	1	1	1	1	1	1	1
A_2	1	1	−1	−1	1	1	1	1	−1	−1	−1	−1
B_1	1	−1	1	−1	−1	1	1	−1	−1	1	1	−1
B_2	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1

4/mmm	1	2_{100}	2_{010}	2_{001}	$2_{1\bar{1}0}$	4^+_{001}	4^-_{001}	2_{110}	$\bar{1}$	m_{100}	m_{010}	m_{001}	$m_{1\bar{1}0}$	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$	m_{110}
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
A_{1u}	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1
B_{1g}	1	1	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1
B_{1u}	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1
B_{2g}	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1
B_{2u}	1	−1	−1	1	1	−1	−1	1	−1	1	1	−1	−1	1	1	−1
A_{2g}	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1	−1	1	1	−1
A_{2u}	1	−1	−1	1	−1	1	1	−1	−1	1	1	−1	1	−1	−1	1

$m\bar{3}$	1	2_{100}	2_{010}	2_{001}	3^-_{111}	$3^-_{\bar{1}\bar{1}1}$	$3^-_{1\bar{1}\bar{1}}$	$3^-_{\bar{1}1\bar{1}}$	3^+_{111}	$3^+_{\bar{1}1\bar{1}}$	$3^+_{\bar{1}\bar{1}1}$	$3^+_{1\bar{1}\bar{1}}$	$\bar{1}$	m_{100}	m_{010}	m_{001}	$\bar{3}^-_{111}$	$\bar{3}^-_{\bar{1}\bar{1}1}$	$\bar{3}^-_{1\bar{1}\bar{1}}$	$\bar{3}^-_{\bar{1}1\bar{1}}$	$\bar{3}^+_{111}$	$\bar{3}^+_{\bar{1}1\bar{1}}$	$\bar{3}^+_{\bar{1}\bar{1}1}$	$\bar{3}^+_{1\bar{1}\bar{1}}$
A_g	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
A_u	1	1	1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1
^2E_g	1	1	1	1	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	1	1	1	1	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$
^2E_u	1	1	1	1	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	−1	−1	−1	−1	$e^{-\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$
^1E_g	1	1	1	1	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	1	1	1	1	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$
^1E_u	1	1	1	1	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	−1	−1	−1	−1	$e^{\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$	$e^{-\frac{\pi i}{3}}$

$\bar{4}3m$	1	2_{100}	2_{010}	2_{001}	3^-_{111}	$3^-_{\bar{1}\bar{1}1}$	$3^-_{1\bar{1}\bar{1}}$	$3^-_{\bar{1}1\bar{1}}$	3^+_{111}	$3^+_{\bar{1}1\bar{1}}$	$3^+_{\bar{1}\bar{1}1}$	$3^+_{1\bar{1}\bar{1}}$	$m_{1\bar{1}0}$	$\bar{4}^+_{001}$	$\bar{4}^-_{001}$	m_{110}	$m_{01\bar{1}}$	m_{011}	$\bar{4}^+_{100}$	$\bar{4}^-_{100}$	$m_{\bar{1}01}$	$\bar{4}^-_{010}$	m_{101}	$\bar{4}^+_{010}$
A_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
A_2	1	1	1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1

Table D9. Continued

6/mmm	1	2_{100}	2_{120}	2_{001}	$\bar{1}$	m_{100}	m_{120}	m_{001}	6^+_{001}	3^+_{001}	3^-_{001}	6^-_{001}	2_{210}	2_{110}	2_{010}	$2_{1\bar{1}0}$	$\bar{6}^+_{001}$	$\bar{3}^+_{001}$	$\bar{3}^-_{001}$	$\bar{6}^-_{001}$	m_{210}	m_{110}	m_{010}	$m_{1\bar{1}0}$
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
A_{1u}	1	1	1	1	−1	−1	−1	−1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1
B_{2g}	1	1	−1	−1	1	1	−1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1
B_{2u}	1	1	−1	−1	−1	−1	1	1	−1	1	1	−1	−1	1	1	−1	1	−1	−1	1	1	−1	−1	1
B_{1g}	1	−1	1	−1	1	−1	1	−1	−1	1	1	−1	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1
B_{1u}	1	−1	1	−1	−1	1	−1	1	−1	1	1	−1	1	−1	−1	1	1	−1	−1	1	−1	1	1	−1
A_{2g}	1	−1	−1	1	1	−1	−1	1	1	1	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1
A_{2u}	1	−1	−1	1	−1	1	1	−1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1

$m\bar{3}m$	{1}	$\{2_{100}, 2_{010}, 2_{001}\}$	$\{3^-_{111}, 3^-_{\bar{1}\bar{1}1}, 3^-_{1\bar{1}\bar{1}}, 3^-_{\bar{1}1\bar{1}}, 3^+_{111}, 3^+_{\bar{1}1\bar{1}}, 3^+_{\bar{1}\bar{1}1}, 3^+_{1\bar{1}\bar{1}}\}$	$\{2_{1\bar{1}0}, 2_{110}, 2_{01\bar{1}}, 2_{011}, 2_{\bar{1}01}, 2_{101}\}$	$\{4^+_{001}, 4^-_{001}, 4^+_{100}, 4^-_{100}, 4^-_{010}, 4^+_{010}\}$	$\{\bar{1}\}$	$\{m_{100}, m_{010}, m_{001}\}$	$\{\bar{3}^-_{111}, \bar{3}^-_{\bar{1}\bar{1}1}, \bar{3}^-_{1\bar{1}\bar{1}}, \bar{3}^-_{\bar{1}1\bar{1}}, \bar{3}^+_{111}, \bar{3}^+_{\bar{1}1\bar{1}}, \bar{3}^+_{\bar{1}\bar{1}1}, \bar{3}^+_{1\bar{1}\bar{1}}\}$	$\{m_{1\bar{1}0}, m_{110}, m_{01\bar{1}}, m_{011}, m_{\bar{1}01}, m_{101}\}$	$\{\bar{4}^+_{001}, \bar{4}^-_{001}, \bar{4}^+_{100}, \bar{4}^-_{100}, \bar{4}^-_{010}, \bar{4}^+_{010}\}$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1
A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1

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