

Representation of tensor functions using lower-order structural tensor set: three-dimensional theory

Mohammad Madadi and Pu Zhang*

*Department of Mechanical Engineering, State University of New York at Binghamton,
Binghamton, NY 13902, USA*

Abstract

The representation theory of tensor functions is a powerful mathematical tool for constitutive modeling of anisotropic materials. A major limitation of the traditional theory is that many point groups require fourth- or sixth-order structural tensors, which significantly impedes practical engineering applications. Recent advances have introduced a reformulated representation theory that enables the modeling of anisotropic materials using only lower-order structural tensors (i.e., second-order or lower). Building upon the reformulated theory, this work establishes the representations of tensor functions for three-dimensional centrosymmetric point groups. For each point group, we propose a lower-order structural tensor set and derive the representations of tensor functions explicitly. For scalar-valued and second-order symmetric tensor-valued functions, our theory is indeed applicable to all three-dimensional point groups because their representations are determined by the corresponding centrosymmetric groups. The representation theory presented here is broadly applicable for constitutive modeling of anisotropic materials.

1 Introduction

Constitutive modeling is central to continuum mechanics and materials modeling in engineering and materials science [1]. Constitutive models capture a wide range of mechanical and multiphysical behaviors of materials including stress-strain relationships, yield surfaces, failure criteria, thermal and electrical properties, and mechano-physical behaviors. Constitutive laws are usually described using scalar- or tensor-valued functions with multiple arguments including field and state variables. In addition, material symmetry or anisotropy is incorporated in constitutive laws through structural tensors (i.e., anisotropic tensors) designated for each point group [2].

*Corresponding author, e-mail: pzhang@binghamton.edu

The representation theory of tensor functions [2, 3, 4] is a powerful mathematical tool that provides general forms of constitutive laws consistent with frame-indifference and material symmetry principles. It was established in the mid-20th century by Rivlin [5, 6], Pipkin [7], and Noll [8]. These pioneers developed representations of isotropic tensor functions, primarily for isotropic materials. Thereafter, Wang [9, 10], Smith [11], and Boehler [12] derived isotropic scalar-, vector-, and tensor-valued functions of vectors and 2nd-order tensors. Later on, the representation theory was generalized to anisotropic tensor functions by Boehler and Liu [13, 14], and then Spencer and Betten [15, 16]. Their approach was to transform an anisotropic tensor function into an extended isotropic one by including structural tensor arguments. These structural tensors characterize material symmetry and are invariant under any symmetry operation of the point group [2]. The structural tensors for all two-dimensional (2D) and three-dimensional (3D) point groups are reported by Zheng and Xiao [2, 17]. Despite its theoretical elegance, the practical application of this anisotropic representation theory is rather limited. Firstly, the theory provides only the general mathematical forms, requiring researchers to determine specific functions either empirically or through trial-and-error. Secondly, a major obstacle is that most point groups involve higher-order (i.e., 3rd-order or higher) structural tensors, which complicate and often preclude practical modeling. In practice, constitutive modeling with higher-order structural tensors is rarely feasible. Most crystalline point groups require higher-order structural tensors and their constitutive modeling remains largely unexplored.

To circumvent the obstacle of higher-order structural tensors, Man and Goddard reformulated the representation theory in 2018 [18], enabling the exclusive use of lower-order structural tensors. Unlike the original theory of Boehler and Liu [13, 14], which requires structural tensors to be invariant under all symmetry operations of a point group, the Man-Goddard reformulation relaxes this requirement while imposing additional symmetry constraints afterwards. This reformulation enables the constitutive modeling of anisotropic materials using only lower-order structural tensors. In their work [18], Man and Goddard provided illustrative examples demonstrating the reformulation, but did not fully establish the representations for all point groups. Based on the Man-Goddard reformulation, our recent work [19] introduced a new concept "structural tensor set" and established the representations of tensor functions for all 2D point groups using lower-order structural tensor sets. Besides, our recent work also presented comprehensive review and discussions on the original and reformulated representation theories. Despite the progress for 2D point groups, a critical knowledge gap remains regarding the reformulated representation theory for 3D point groups. The present work aims to fill this knowledge gap by establishing representations of tensor functions for all 3D centrosymmetric point groups, including 11 Laue groups and 3 continuous ones. Our previous work discovered that, for a given point group, the representations of scalar-valued and 2nd-order symmetric tensor-valued functions are determined by its corresponding centrosymmetric

group (e.g., Laue group) [19]. Hence, we limit our theory to centrosymmetric point groups in this work. As long as scalar-valued and 2nd-order symmetric tensor-valued functions are of interest, the presented theory is applicable to all 3D point groups (i.e., 32 crystalline point groups and 7 continuous ones) because one only needs to find their corresponding centrosymmetric groups and the associated representations in this work.

The representation of anisotropic scalar- and tensor-valued functions has broad applications in engineering and materials science [1, 2, 3]. For scalar-valued functions, the theory developed here can be used to model hyperelastic strain energy functions of elastomers, soft composites [20, 21], and biological tissues [22], as well as yield and failure criteria for materials [1, 3]. For tensor-valued functions, the representation theory provides a basis for modeling mechanical, physical, and mechano-physical properties [23], including stress-strain relations, dielectric properties, and conductivity tensors [24]. It should be emphasized that the present work establishes only the general forms of such scalar- and tensor-valued functions. Specific constitutive laws must still be constructed and fitted to experimental or simulation data.

The remainder of this paper is organized as follows. In Sections 2, we revisit the preliminaries of representation theory for tensor functions. Section 3 introduces the proposed lower-order structural tensor sets for all 3D centrosymmetric point groups. The detailed representations of scalar- and 2nd-order symmetric tensor-valued functions are reported in Sections 4–15. Notably, six groups ($\mathcal{C}_i, \mathcal{C}_{2h}, \mathcal{D}_{2h}, \mathcal{C}_{\infty h}, \mathcal{D}_{\infty h}, \mathcal{K}_h$) possess only lower-order structural tensors and can therefore be treated using the original Boehler–Liu formulation. In contrast, eight groups ($\mathcal{C}_{4h}, \mathcal{D}_{4h}, \mathcal{C}_{3i}, \mathcal{D}_{3d}, \mathcal{C}_{6h}, \mathcal{D}_{6h}, \mathcal{T}_h, \mathcal{O}_h$) possess higher-order structural tensors and should employ the Man-Goddard reformulation together with our proposed lower-order structural tensor sets. Throughout this work, we adopt the Schoenflies notation for point groups; for other notation systems, readers may refer to [25]. Finally, the appendix lists functional bases, tensor generators, symmetry operations, and useful matrices for reference.

2 Preliminaries of representation theory

In our previous work [19], we have provided a brief introduction to the representation theory of tensor functions in 2D space. The corresponding theory for 3D is similar. The major formulas are summarized below.

Firstly, we consider the representation of isotropic scalar- and tensor-valued functions. Isotropic tensor functions are useful for the constitutive modeling of isotropic materials. In general, a scalar-valued isotropic tensor function $\psi(\mathbf{v}, \mathbf{A}, \mathbf{W})$ can be expressed as a function of the invariants I_k [26]

of its arguments $\mathbf{v}$, $\mathbf{A}$, and $\mathbf{W}$, as

$$\psi(\mathbf{v}, \mathbf{A}, \mathbf{W}) = \psi(I_k) \quad (1)$$

where $\mathbf{v}$, $\mathbf{A}$, and $\mathbf{W}$ are sets of vectors, 2nd-order symmetric and skew-symmetric tensors, respectively. Herein, the complete set of invariants $I_k (k = 1, 2, \dots, r)$ is called functional basis (or integrity basis). The representation of an isotropic 2nd-order symmetric tensor-valued function $\mathbf{T}(\mathbf{v}, \mathbf{A}, \mathbf{W})$ is expressed as a linear combination of tensor generators $\mathbf{G}_i$, as

$$\mathbf{T}(\mathbf{v}, \mathbf{A}, \mathbf{W}) = \sum \alpha_i \mathbf{G}_i \quad (2)$$

where $\alpha_i = \alpha_i(I_1, I_2, \dots, I_r)$ are scalar coefficient functions of the invariants I_k governed by (1). Once the arguments $\mathbf{v}$, $\mathbf{A}$, and $\mathbf{W}$ are provided, one can find the tensor generators $\mathbf{G}_i$ following methods and formulae presented in [3, 2]. For an isotropic 2nd-order symmetric tensor-valued function $\mathbf{T}(\mathbf{v}, \mathbf{A}, \mathbf{W})$, the functional bases I_k and tensor generators $\mathbf{G}_i$ can be obtained from Table A1 and Table A2 in the Appendix.

Secondly, we consider the representation of anisotropic scalar- and tensor-valued functions, which are needed for constitutive modeling of anisotropic materials. By introducing structural tensors $\mathfrak{M}$, Boehler [13] and Liu [14] introduced isotropic tensor functions $\hat{\psi}(\mathbf{v}, \mathbf{A}, \mathbf{W}, \mathfrak{M})$ and $\hat{\mathbf{T}}(\mathbf{v}, \mathbf{A}, \mathbf{W}, \mathfrak{M})$ for anisotropic materials, which are actually isotropic extension of anisotropic functions. The requirement is that the structural tensors $\mathfrak{M}$ must be invariant under any symmetry operation $\mathbf{Q}$ in the point group $\mathcal{G}$. General forms of the extended isotropic functions $\hat{\psi}$ and $\hat{\mathbf{T}}$ can be derived readily using (1) and (2), respectively. The challenge is that many point groups involve higher-order structural tensors, which hinder the wide applications of the Boehler-Liu formulation.

In order to overcome the challenge of higher-order structural tensors, Man and Goddard [18] reformulated the representation theory of anisotropic tensor functions. In their reformulation, only lower-order structural tensors $\mathfrak{M}$ are needed. The representations are similar to Boehler and Liu above. However, an additional symmetry constraint should be imposed to the tensor functions [18, 19], as

$$\begin{aligned} \hat{\psi}(\mathbf{v}, \mathbf{A}, \mathbf{W}, \mathfrak{M}) &= \hat{\psi}(\mathbf{v}, \mathbf{A}, \mathbf{W}, \langle \mathbf{Q} \rangle \mathfrak{M}) \\ \hat{\mathbf{T}}(\mathbf{v}, \mathbf{A}, \mathbf{W}, \mathfrak{M}) &= \hat{\mathbf{T}}(\mathbf{v}, \mathbf{A}, \mathbf{W}, \langle \mathbf{Q} \rangle \mathfrak{M}) \end{aligned} ; \forall \mathbf{Q} \in \mathcal{G}^* \quad (3)$$

where $\mathcal{G}^*$ denotes the group generators of the point group $\mathcal{G}$, and we [19] have proven that only the group generators need to be considered in (3) rather than the whole point group. The orthogonal transformation operator $\langle \mathbf{Q} \rangle$ is defined after Zheng [2], as

$$\begin{aligned} \langle \mathbf{Q} \rangle \mathbf{v} &= \mathbf{Q} \mathbf{v} = \mathbf{Q}_{ij} \mathbf{v}_j \\ \langle \mathbf{Q} \rangle \mathbf{A} &= \mathbf{Q} \mathbf{A} \mathbf{Q}^T = \mathbf{Q}_{ip} \mathbf{Q}_{jq} \mathbf{A}_{pq} \\ \langle \mathbf{Q} \rangle \mathbb{A} &= \mathbf{Q}_{ip} \mathbf{Q}_{jq} \mathbf{Q}_{kr} \dots \mathbf{Q}_{mt} \mathbb{A}_{pqr\dots t} \end{aligned} \quad (4)$$

where $\mathbf{v}$, $\mathbf{A}$, and $\mathbb{A}$ are first-, second-, and higher-order tensors, respectively.

Using the Man-Goddard reformulation, we have established the representation theory of tensor functions for all 2D point groups in a previous work [19]. The purpose of the present work is to establish the representation theory of tensor functions for all 3D centrosymmetric groups (Figure 1), including 11 Laue groups and 3 continuous groups, which are the most useful groups for constitutive modeling of anisotropic materials.

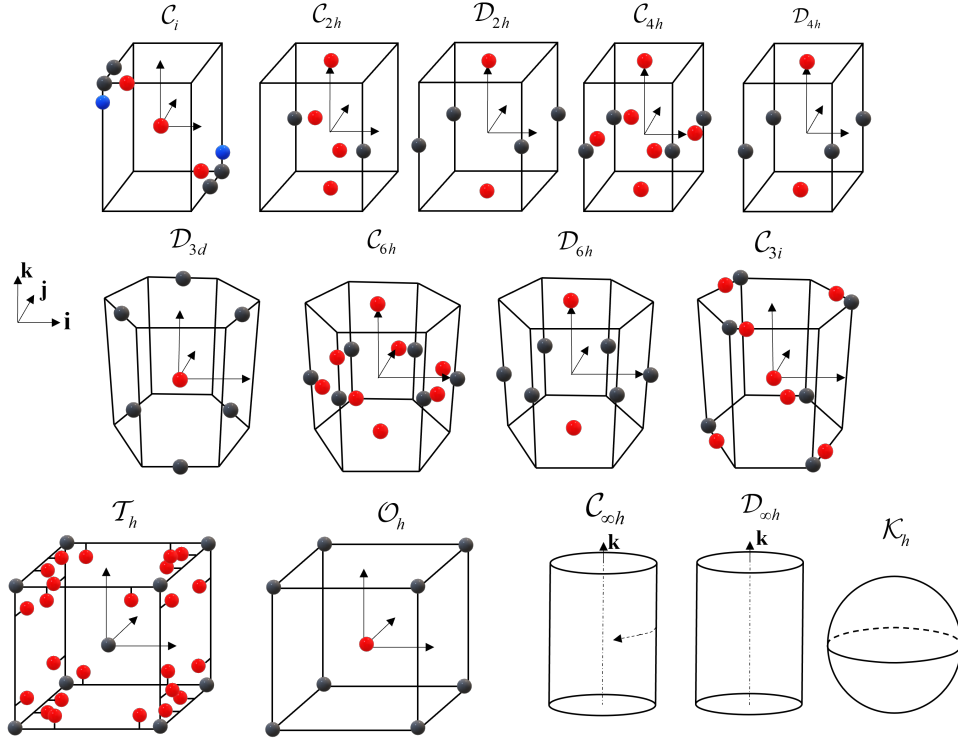


Figure 1: Graphical illustration of 3D centrosymmetric point groups: 11 Laue groups and 3 continuous groups.

3 Lower-order structural tensor set for 3D point groups

In our previous work [19], we proposed the concept "structural tensor set" and provided specific lower-order structural tensors for each 2D point group. The present work generalizes the concept for 3D point groups. Similar to the 2D case, the structural tensor set $\{\mathfrak{M}_i\}$ of a 3D point group $\mathcal{G}$ is defined as

$$\mathcal{G}_s = \{\mathbf{Q} \in \mathcal{O}(3) \mid \{\langle \mathbf{Q} \rangle \mathfrak{M}_i\} = \{\mathfrak{M}_i\}; \quad i = 1, 2, \dots, t\} \quad (5)$$

where $\mathcal{G}_s$ is a subgroup of $\mathcal{G}$ (i.e. $\mathcal{G}_s \leq \mathcal{G}$) and $\mathcal{O}(3)$ denotes the 3D orthogonal group. Herein, we say that the structural tensor set $\{\mathfrak{M}_i\}$ characterizes the group $\mathcal{G}_s$. The traditional definition of structural tensors [2] requires each $\mathfrak{M}_i$ to be invariant $\forall \mathbf{Q} \in \mathcal{G}$. Consequently, higher-order structural

tensors are inevitable for many point groups. In contrast, Eq. (5) only requires the whole structural tensor set to be invariant $\forall \mathbf{Q} \in \mathcal{G}_s$. Hence, it is possible to introduce only lower-order structural tensors. Note that herein we do not mandate $\mathcal{G}_s = \mathcal{G}$, although it is still recommended.

For each point group, the structural tensor set $\mathfrak{M}_i$ is non-unique. One has to devise a structural tensor set that is convenient to use and provides compact mathematical formulae. It usually takes laborious work and a lengthy trial-and-error process to find a complete structural tensor set. Generally, one can choose typical high symmetry directions, lines, and planes to construct the lower-order structural tensors. In what follows, we will take a 3D point group $\mathcal{D}_{4h}$ in Figure 2 as an example and present three different approaches to construct its structural tensor set.

- **Approach I:** Consider a vector $\mathbf{v}_1 = \frac{\sqrt{2}}{2}\mathbf{i} + \frac{\sqrt{2}}{2}\mathbf{j} + \mathbf{k}$ illustrated in Figure 2 (a), which is within a high symmetry plane. We can first define a 2nd-order structural tensor $\mathbf{M}_1 = \mathbf{v}_1 \otimes \mathbf{v}_1$. By applying the point group generators provided in Table A3, the remaining structural tensors are found as $\mathbf{M}_2 = \mathbf{C}_4\mathbf{M}_1\mathbf{C}_4^T$, $\mathbf{M}_3 = \mathbf{C}_4\mathbf{M}_2\mathbf{C}_4^T$, and $\mathbf{M}_4 = \mathbf{C}_{2x}\mathbf{M}_1\mathbf{C}_{2x}^T$. We can further verify that $\{\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_4\}$ form a complete structural tensor set.
- **Approach II:** Consider two orthonormal vectors $\mathbf{v}'_1 = \frac{\sqrt{2}}{2}\mathbf{i} + \frac{\sqrt{2}}{2}\mathbf{j}$ and $\mathbf{v}'_2 = \mathbf{k}$ illustrated in Figure 2 (b). Herein, both vectors are along high symmetry axes. We can start with two structural tensor $\mathbf{M}_1 = \mathbf{v}'_1 \otimes \mathbf{v}'_1$ and $\mathbf{M}_2 = \mathbf{v}'_2 \otimes \mathbf{v}'_2$. By applying the group generators in Table A3, one extra structural tensor $\mathbf{M}_3 = \mathbf{C}_4\mathbf{M}_1\mathbf{C}_4^T$ is found. We can verify that $\{\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3\}$ form a complete structural tensor set.
- **Approach III:** Consider three orthonormal vectors $\mathbf{v}''_1 = \mathbf{i}$, $\mathbf{v}''_2 = \mathbf{j}$, and $\mathbf{v}''_3 = \mathbf{k}$ illustrated in Figure 2 (c). These three vectors are all along high symmetry axes and coincide with the coordinate axes. We can define three structural tensors as $\mathbf{M}_1 = \mathbf{v}''_1 \otimes \mathbf{v}''_1$, $\mathbf{M}_2 = \mathbf{v}''_2 \otimes \mathbf{v}''_2$, and $\mathbf{M}_3 = \mathbf{v}''_3 \otimes \mathbf{v}''_3$. Further, we can verify that $\{\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3\}$ form a complete structural tensor set.

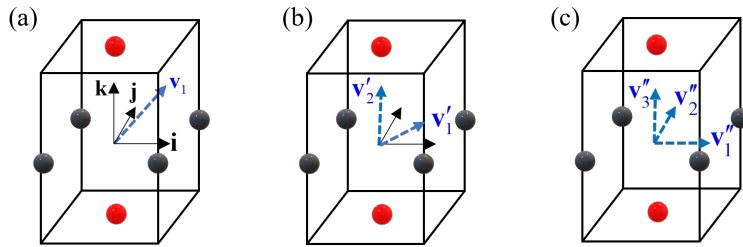


Figure 2: Illustration of various vectors used to define structural tensor set for point group $\mathcal{D}_{4h}$

Remark 3.1. For the convenience of modeling, we strongly suggest choosing a structural tensor

set that characterizes the point group, i.e., $\mathcal{G}_s = \mathcal{G}$. This would ease the burden to impose symmetry constraints (3) afterwards. Unlike 2D point groups [19], the condition $\mathcal{G}_s = \mathcal{G}$ is not easy to fulfill for 3D point groups due to the complexity.

Remark 3.2. The structural tensor set $\{\mathfrak{M}_i\}$ must be complete and invariant $\forall \mathbf{Q} \in \mathcal{G}_s$. This necessary condition needs to be verified for any newly proposed structural tensor sets. In addition, this condition is useful when constructing a structural tensor set. For example, starting with one structural tensor $\mathfrak{M}$, one can find a few other structural tensors by performing symmetry transformation $\langle \mathbf{Q} \rangle \mathfrak{M}$ for $\forall \mathbf{Q} \in \mathcal{G}_s$.

Remark 3.3. It is generally preferable to select a structural tensor set $\{\mathfrak{M}_i\}$ with few members and simple expressions because it would simplify the representations. For example, the Approach III above is strongly recommended for the point group $\mathcal{D}_{4h}$ for its simplicity.

The structural tensors of 3D centrosymmetric point groups are presented in Table 1. For the 6 groups ($\mathcal{C}_i, \mathcal{C}_{2h}, \mathcal{D}_{2h}, \mathcal{C}_{\infty h}, \mathcal{D}_{\infty h}, \mathcal{K}_{\infty}$) with lower-order structural tensors, we simply adopt these tensors provided by Zheng [2]. For these groups, the Boehler-Liu formulation should be used. In contrast, for the 8 point groups ($\mathcal{C}_{4h}, \mathcal{D}_{4h}, \mathcal{C}_{6h}, \mathcal{D}_{6h}, \mathcal{T}_h, \mathcal{O}_h, \mathcal{D}_{3d}, \mathcal{C}_{3i}$) with higher-order structural tensors given by Zheng, we propose lower-order structural tensor sets for them. For these 8 groups, the Man-Goddard reformulation should be used. The representations of scalar- and 2nd-order symmetric tensor-valued functions for all 3D centrosymmetric point groups are presented in Sections 4 to 15.

4 Group $\mathcal{C}_i$ ($\bar{1}$)

For this point group, we simply adopt the 2nd-order structural tensors given by Zheng [2] as follows.

$$\mathbf{K}_1 = \boldsymbol{\varepsilon} \mathbf{i} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}, \mathbf{K}_2 = \boldsymbol{\varepsilon} \mathbf{j} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \mathbf{K}_3 = \boldsymbol{\varepsilon} \mathbf{k} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (6)$$

The Boehler-Liu formulation is used to derive the representations of tensor functions.

The representation of a 2nd-order symmetric tensor-valued function $\mathbf{T}(\mathbf{C}) = \hat{\mathbf{T}}(\mathbf{C}, \mathbf{K}_1, \mathbf{K}_2, \mathbf{K}_3)$ is derived first, where $\mathbf{C}$ is a 2nd-order symmetric tensor (e.g., Cauchy-Green tensor in continuum mechanics). Considering that $\mathbf{K}_i$ are skew-symmetric, the tensor generators and invariants can be obtained using Table A1 and Table A2. Specifically, the tensor generators are

$$\begin{aligned} & \mathbf{I}, \mathbf{C}, \mathbf{C}^2, \mathbf{K}_i^2, \mathbf{C}\mathbf{K}_i - \mathbf{K}_i\mathbf{C}, \mathbf{C}^2\mathbf{K}_i - \mathbf{K}_i\mathbf{C}^2, \mathbf{K}_i\mathbf{C}\mathbf{K}_i, \mathbf{K}_i\mathbf{C}\mathbf{K}_i^2 - \mathbf{K}_i^2\mathbf{C}\mathbf{K}_i, \\ & \mathbf{K}_1\mathbf{K}_2 + \mathbf{K}_2\mathbf{K}_1, \mathbf{K}_1\mathbf{K}_2^2 - \mathbf{K}_2^2\mathbf{K}_1, \mathbf{K}_1^2\mathbf{K}_2 - \mathbf{K}_2\mathbf{K}_1^2, \mathbf{K}_1\mathbf{K}_3 + \mathbf{K}_3\mathbf{K}_1, \mathbf{K}_1\mathbf{K}_3^2 - \mathbf{K}_3^2\mathbf{K}_1, \\ & \mathbf{K}_1^2\mathbf{K}_3 - \mathbf{K}_3\mathbf{K}_1^2, \mathbf{K}_2\mathbf{K}_3 + \mathbf{K}_3\mathbf{K}_2, \mathbf{K}_2\mathbf{K}_3^2 - \mathbf{K}_3^2\mathbf{K}_2, \mathbf{K}_2^2\mathbf{K}_3 - \mathbf{K}_3\mathbf{K}_2^2, \text{ for } i = 1, 2, 3 \end{aligned} \quad (7)$$

Table 1: Structural tensors for 3D centrosymmetric point groups

System (Point group)	Zheng's structural tensors [2]	Proposed structural tensor set
Triclinic ($\mathcal{C}_i$)	$\boldsymbol{\varepsilon}\mathbf{i}, \boldsymbol{\varepsilon}\mathbf{j}, \boldsymbol{\varepsilon}\mathbf{k}$	$\boldsymbol{\varepsilon}\mathbf{i}, \boldsymbol{\varepsilon}\mathbf{j}, \boldsymbol{\varepsilon}\mathbf{k}$
Monoclinic ($\mathcal{C}_{2h}$)	$\mathbf{P}_2, \boldsymbol{\varepsilon}\mathbf{k}$	$\mathbf{P}_2, \boldsymbol{\varepsilon}\mathbf{k}$
Orthorhombic ($\mathcal{D}_{2h}$)	$\mathbf{P}_2$	$\mathbf{P}_2$ (or $\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3$)
Tetragonal ($\mathcal{C}_{4h}$)	$\mathbb{P}_4, \boldsymbol{\varepsilon}\mathbf{k}$	$\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \boldsymbol{\varepsilon}\mathbf{k}$
Tetragonal ($\mathcal{D}_{4h}$)	$\mathbb{P}_4$	$\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3$
Trigonal ($\mathcal{C}_{3i}$)	$\mathbf{k} \otimes \mathbb{P}_3, \boldsymbol{\varepsilon}\mathbf{k}$	$\mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \boldsymbol{\varepsilon}\mathbf{k}$
Trigonal ($\mathcal{D}_{3d}$)	$\mathbf{k} \otimes \mathbb{P}_3$	$\mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3$
Hexagonal ($\mathcal{C}_{6h}$)	$\mathbb{P}_6, \boldsymbol{\varepsilon}\mathbf{k}$	$\mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3, \boldsymbol{\varepsilon}\mathbf{k}$
Hexagonal ($\mathcal{D}_{6h}$)	$\mathbb{P}_6$	$\mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3$
Cubic ($\mathcal{T}_h$)	$\mathbb{T}_h$	$\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3$
Cubic ($\mathcal{O}_h$)	$\mathbb{O}_h$	$\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3$
Cylindrical ($\mathcal{C}_{\infty h}$)	$\boldsymbol{\varepsilon}\mathbf{k}$	$\boldsymbol{\varepsilon}\mathbf{k}$
Cylindrical ($\mathcal{D}_{\infty h}$)	$\mathbf{k} \otimes \mathbf{k}$	$\mathbf{k} \otimes \mathbf{k}$
Spherical ($\mathcal{K}_h$)	$\mathbf{I}$	$\mathbf{I}$

* $\boldsymbol{\varepsilon}$ is the 3rd-order permutation tensor.

The invariants are

$$\begin{aligned}
 &tr\mathbf{C}, tr\mathbf{C}^2, tr\mathbf{C}^3, tr(\mathbf{C}\mathbf{K}_i^2), tr(\mathbf{C}^2\mathbf{K}_i^2), tr(\mathbf{C}^2\mathbf{K}_i^2\mathbf{C}\mathbf{K}_i), \\
 &tr(\mathbf{C}\mathbf{K}_1\mathbf{K}_2), tr(\mathbf{C}\mathbf{K}_1^2\mathbf{K}_2), tr(\mathbf{C}\mathbf{K}_1\mathbf{K}_2^2), tr(\mathbf{C}\mathbf{K}_1\mathbf{K}_3), tr(\mathbf{C}\mathbf{K}_1^2\mathbf{K}_3), \\
 &tr(\mathbf{C}\mathbf{K}_1\mathbf{K}_3^2), tr(\mathbf{C}\mathbf{K}_2\mathbf{K}_3), tr(\mathbf{C}\mathbf{K}_2^2\mathbf{K}_3), tr(\mathbf{C}\mathbf{K}_2\mathbf{K}_3^2), \quad \text{for } i = 1, 2, 3
 \end{aligned} \tag{8}$$

After eliminating the redundant terms in (7) and (8), the representation of $\hat{\mathbf{T}}$ is given as

$$\begin{aligned}
 \hat{\mathbf{T}}(\mathbf{C}, \mathbf{K}_1, \mathbf{K}_2, \mathbf{K}_3) = &\alpha_1\mathbf{K}_1^2 + \alpha_2\mathbf{K}_2^2 + \alpha_3\mathbf{K}_3^2 + \alpha_4(\mathbf{K}_1\mathbf{K}_2 + \mathbf{K}_2\mathbf{K}_1) \\
 &+ \alpha_5(\mathbf{K}_1\mathbf{K}_3 + \mathbf{K}_3\mathbf{K}_1) + \alpha_6(\mathbf{K}_2\mathbf{K}_3 + \mathbf{K}_3\mathbf{K}_2)
 \end{aligned} \tag{9}$$

and

$$\alpha_i = \alpha_i(tr(\mathbf{C}\mathbf{K}_1^2), tr(\mathbf{C}\mathbf{K}_2^2), tr(\mathbf{C}\mathbf{K}_3^2), tr(\mathbf{C}\mathbf{K}_1\mathbf{K}_2), tr(\mathbf{C}\mathbf{K}_1\mathbf{K}_3), tr(\mathbf{C}\mathbf{K}_2\mathbf{K}_3)) \tag{10}$$

The representation of a scalar-valued function $\hat{\psi}(\mathbf{C}, \mathbf{K}_1, \mathbf{K}_2, \mathbf{K}_3)$ follows the same form of (10).

5 Group $\mathcal{D}_{2h}$ (mmm)

For this point group, one may use either one structural tensor $\mathbf{P}_2$ or three structural tensors $\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3$, as shown in Table 1. In both cases, the Boehler-Liu formulation is used. We will

derive the representations using both approaches below.

5.1 Using one structural tensor

Zheng [2] proposed a single structural tensor $\mathbf{P}_2 = \mathbf{i} \otimes \mathbf{i} - \mathbf{j} \otimes \mathbf{j}$ for this point group, a 2nd-order symmetric tensor. The representation $\hat{\mathbf{T}}(\mathbf{C}, \mathbf{P}_2)$ can be obtained using Tables A1-A2, as

$$\begin{aligned} \hat{\mathbf{T}}(\mathbf{C}, \mathbf{P}_2) = & \alpha_0 \mathbf{I} + \alpha_1 \mathbf{C} + \alpha_2 \mathbf{C}^2 + \alpha_3 \mathbf{P}_2 + \alpha_4 \mathbf{P}_2^2 \\ & + \alpha_5 (\mathbf{C} \mathbf{P}_2 + \mathbf{P}_2 \mathbf{C}) + \alpha_6 (\mathbf{C}^2 \mathbf{P}_2 + \mathbf{P}_2 \mathbf{C}^2) + \alpha_7 (\mathbf{C} \mathbf{P}_2^2 + \mathbf{P}_2^2 \mathbf{C}) \end{aligned} \quad (11)$$

where α_i is given by

$$\alpha_i = \alpha_i(\text{tr} \mathbf{C}, \text{tr} \mathbf{C}^2, \text{tr} \mathbf{C}^3, \text{tr}(\mathbf{C} \mathbf{P}_2), \text{tr}(\mathbf{C}^2 \mathbf{P}_2), \text{tr}(\mathbf{C} \mathbf{P}_2^2), \text{tr}(\mathbf{C}^2 \mathbf{P}_2^2)) \quad (12)$$

The representation of a scalar-valued function $\hat{\psi}(\mathbf{C}, \mathbf{P}_2)$ follows the same form of (12).

5.2 Using three structural tensors

For orthotropic materials, a popular set of structural tensors is $\{\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3\}$ with $\mathbf{M}_1 = \mathbf{i} \otimes \mathbf{i}$, $\mathbf{M}_2 = \mathbf{j} \otimes \mathbf{j}$ and $\mathbf{M}_3 = \mathbf{k} \otimes \mathbf{k}$. The representation of a tensor-valued function $\hat{\mathbf{T}}$ was provided by Boehler [12] as

$$\begin{aligned} \hat{\mathbf{T}}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) = & \alpha_1 \mathbf{M}_1 + \alpha_2 \mathbf{M}_2 + \alpha_3 \mathbf{M}_3 + \alpha_4 (\mathbf{M}_1 \mathbf{C} + \mathbf{C} \mathbf{M}_1) \\ & + \alpha_5 (\mathbf{M}_2 \mathbf{C} + \mathbf{C} \mathbf{M}_2) + \alpha_6 (\mathbf{M}_3 \mathbf{C} + \mathbf{C} \mathbf{M}_3) + \alpha_7 \mathbf{C}^2 \end{aligned} \quad (13)$$

where α_i is

$$\begin{aligned} \alpha_i = & \alpha_i(\text{tr}(\mathbf{C} \mathbf{M}_1), \text{tr}(\mathbf{C} \mathbf{M}_2), \text{tr}(\mathbf{C} \mathbf{M}_3), \text{tr}(\mathbf{C}^2 \mathbf{M}_1), \text{tr}(\mathbf{C}^2 \mathbf{M}_2), \text{tr}(\mathbf{C}^2 \mathbf{M}_3), \text{tr} \mathbf{C}^3) \\ = & \tilde{\alpha}_i(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) \end{aligned} \quad (14)$$

The representation of a scalar-valued function $\hat{\psi}$ follows the same form of (14), as

$$\hat{\psi}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) = \hat{\psi}(\text{tr}(\mathbf{C} \mathbf{M}_1), \text{tr}(\mathbf{C} \mathbf{M}_2), \text{tr}(\mathbf{C} \mathbf{M}_3), \text{tr}(\mathbf{C}^2 \mathbf{M}_1), \text{tr}(\mathbf{C}^2 \mathbf{M}_2), \text{tr}(\mathbf{C}^2 \mathbf{M}_3), \text{tr} \mathbf{C}^3) \quad (15)$$

These representation formulae for orthotropic materials are very useful for multiple other point groups including $\mathcal{D}_{4h}$, $\mathcal{T}_h$, and $\mathcal{O}_h$ to be introduced below.

6 Group $\mathcal{D}_{4h}$ ($4/mmm$)

Zheng [2] proposed a 4th-order structural tensor $\mathbb{P}_4$ for this point group. Given the fact that higher-order structural tensors are inconvenient to use, we propose a lower-order structural tensor set $\{\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3\}$ instead, the same as Section 5.2. For this point group, the Man-Goddard reformulation is needed.

The representations of tensor functions have been provided in Eqs. (13)-(15). But additional constraints (3) must be imposed on the representations. The group generators of this point group are $\mathcal{G}^* = \{\mathbf{C}_4, \mathbf{C}_{2x}, \bar{\mathbf{I}}\}$ in Table A3. The operations $\mathbf{C}_{2x}$ and $\bar{\mathbf{I}}$ keep all three structural tensors $\mathbf{M}_i$ invariant. However, the operation $\mathbf{C}_4$ permutes $\mathbf{M}_1$ and $\mathbf{M}_2$, i.e., $\mathbf{C}_4\mathbf{M}_1\mathbf{C}_4^T = \mathbf{M}_2$ and $\mathbf{C}_4\mathbf{M}_2\mathbf{C}_4^T = \mathbf{M}_1$. Thus, $\mathbf{C}_4$ would impose additional constraints based on (3) to the representations, as

$$\begin{aligned}\hat{\mathbf{T}}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \hat{\mathbf{T}}(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_1, \mathbf{M}_3), \\ \hat{\psi}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \hat{\psi}(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_1, \mathbf{M}_3)\end{aligned}\tag{16}$$

Accordingly, the constraints to the coefficients $\tilde{\alpha}_i$ in (14) are

$$\begin{aligned}\tilde{\alpha}_1(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_2(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_1, \mathbf{M}_3), \\ \tilde{\alpha}_4(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_5(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_1, \mathbf{M}_3), \\ \tilde{\alpha}_i(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_i(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_1, \mathbf{M}_3) \quad \text{for } i = 3, 6, 7\end{aligned}\tag{17}$$

Remark 6.1. Some constraints on the scalar coefficient functions $\tilde{\alpha}_i$ are redundant and should be removed. The reason is that not all constraints are independent. For example, in (17), we have removed a constraint $\tilde{\alpha}_2(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) = \tilde{\alpha}_1(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_1, \mathbf{M}_3)$ because it is equivalent to the first equation in (17). Hence, extra efforts are required to remove redundancy of the representations for each group.

7 Group $\mathcal{T}_h$ ($m\bar{3}$)

This point group has a 4th-order structural tensor $\mathbb{T}_h$ [2]. We adopt the lower-order structural tensor set $\{\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3\}$ in Section 5.2. The representations of tensor functions have been shown in (13)-(15). Additional constraints need to be imposed following the Man-Goddard reformulation.

This point group has four generators $\mathcal{G}^* = \{\mathbf{Q}_p^{2\pi/3}, \mathbf{C}_{2x}, \mathbf{C}_{2y}, \bar{\mathbf{I}}\}$ in Table A3. The operations $\mathbf{C}_{2x}$, $\mathbf{C}_{2y}$, and $\bar{\mathbf{I}}$ keep all three structural tensors invariant. In contrast, $\mathbf{Q}_p^{2\pi/3}$ permutes them, as

$$\mathbf{Q}_p^{2\pi/3}\mathbf{M}_1(\mathbf{Q}_p^{2\pi/3})^T = \mathbf{M}_2, \quad \mathbf{Q}_p^{2\pi/3}\mathbf{M}_2(\mathbf{Q}_p^{2\pi/3})^T = \mathbf{M}_3, \quad \mathbf{Q}_p^{2\pi/3}\mathbf{M}_3(\mathbf{Q}_p^{2\pi/3})^T = \mathbf{M}_1\tag{18}$$

Thus, $\mathbf{Q}_p^{2\pi/3}$ will impose an additional constraint to the representations, as $\hat{\mathbf{T}}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) = \hat{\mathbf{T}}(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1)$. Accordingly, the constraints to the coefficient functions $\tilde{\alpha}_i$ in (13) are

$$\begin{aligned}\tilde{\alpha}_1(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_3(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1), \quad \tilde{\alpha}_2(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) = \tilde{\alpha}_1(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1) \\ \tilde{\alpha}_4(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_6(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1), \quad \tilde{\alpha}_5(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) = \tilde{\alpha}_4(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1) \\ \tilde{\alpha}_7(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_7(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1)\end{aligned}\tag{19}$$

Moreover, the additional constraint on (15) requires that $\hat{\psi}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) = \hat{\psi}(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1)$.

8 Group $\mathcal{O}_h$ ($m\bar{3}m$)

Rather than a 4th-order structural tensor $\mathbb{O}_h$ [2], we adopt the structural tensor set $\{\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3\}$ in Section 5.2. The representations of tensor functions have been shown in (13)-(15). Additional constraints need to be imposed following the Man-Goddard reformulation.

This point group has four group generators $\mathcal{G}^* = \{\mathbf{Q}_p^{2\pi/3}, \mathbf{C}_{4x}, \mathbf{C}_{2y}, \bar{\mathbf{I}}\}$ in Table A3. Among the four group generators, $\mathbf{C}_{2y}$ and $\bar{\mathbf{I}}$ keep the structural tensors invariant, whereas $\mathbf{C}_{4x}$ and $\mathbf{Q}_p^{2\pi/3}$ transform them as follows.

$$\begin{aligned} \mathbf{C}_{4x}\mathbf{M}_1\mathbf{C}_{4x}^T &= \mathbf{M}_1, & \mathbf{Q}_p^{2\pi/3}\mathbf{M}_1(\mathbf{Q}_p^{2\pi/3})^T &= \mathbf{M}_2 \\ \mathbf{C}_{4x}\mathbf{M}_2\mathbf{C}_{4x}^T &= \mathbf{M}_3, & \mathbf{Q}_p^{2\pi/3}\mathbf{M}_2(\mathbf{Q}_p^{2\pi/3})^T &= \mathbf{M}_3 \\ \mathbf{C}_{4x}\mathbf{M}_3\mathbf{C}_{4x}^T &= \mathbf{M}_2, & \mathbf{Q}_p^{2\pi/3}\mathbf{M}_3(\mathbf{Q}_p^{2\pi/3})^T &= \mathbf{M}_1 \end{aligned} \quad (20)$$

Hence, we need to impose additional constraints (3) for $\mathbf{C}_{4x}$ and $\mathbf{Q}_p^{2\pi/3}$, respectively. As to the tensor-valued function $\hat{\mathbf{T}}$, the group generator $\mathbf{C}_{4x}$ requires that $\hat{\mathbf{T}}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) = \hat{\mathbf{T}}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_3, \mathbf{M}_2)$, while the group generator $\mathbf{Q}_p^{2\pi/3}$ requires that $\hat{\mathbf{T}}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) = \hat{\mathbf{T}}(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1)$. Accordingly, the additional constraints to the coefficient functions $\tilde{\alpha}_i$ in (13) are as follows.

For the generator $\mathbf{Q}_p^{2\pi/3}$:

$$\begin{aligned} \tilde{\alpha}_1(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_3(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1), & \tilde{\alpha}_2(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_1(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1), \\ \tilde{\alpha}_4(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_6(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1), & \tilde{\alpha}_5(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_4(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1), \\ \tilde{\alpha}_7(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_7(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1) \end{aligned}$$

For the generator $\mathbf{C}_{4x}$:

$$\begin{aligned} \tilde{\alpha}_3(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_2(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_3, \mathbf{M}_2), & \tilde{\alpha}_6(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_5(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_3, \mathbf{M}_2), \\ \tilde{\alpha}_i(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) &= \tilde{\alpha}_i(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_3, \mathbf{M}_2) \quad \text{for } i = 1, 4, 7 \end{aligned} \quad (21)$$

Similarly, $\mathbf{C}_{4x}$ and $\mathbf{Q}_p^{2\pi/3}$ also impose additional constraints to the scalar-valued tensor function $\hat{\psi}$ in (15) as

$$\hat{\psi}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3) = \hat{\psi}(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_3, \mathbf{M}_1) = \hat{\psi}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_3, \mathbf{M}_2) \quad (22)$$

9 Group $\mathcal{C}_{2h}$ ($2/m$)

For this point group, we simply adopt the two 2nd-order structural tensors $\mathbf{P}_2 = \mathbf{i} \otimes \mathbf{i} - \mathbf{j} \otimes \mathbf{j}$ and $\mathbf{K}_3 = \boldsymbol{\varepsilon} \mathbf{k}$ proposed by Zheng [2]. the Boehler-Liu formulation is used to derive the representations. Considering that $\mathbf{P}_2$ is symmetric and $\mathbf{K}_3$ is skew-symmetric, the tensor generators are obtained

from Table A2 as

$$\begin{aligned} & \mathbf{I}, \mathbf{C}, \mathbf{C}^2, \mathbf{P}_2, \mathbf{P}_2^2, \mathbf{CP}_2 + \mathbf{P}_2\mathbf{C}, \mathbf{C}^2\mathbf{P}_2 + \mathbf{P}_2\mathbf{C}^2, \mathbf{CP}_2^2 + \mathbf{P}_2^2\mathbf{C}, \\ & \mathbf{K}_3^2, \mathbf{CK}_3 - \mathbf{K}_3\mathbf{C}, \mathbf{C}^2\mathbf{K}_3 - \mathbf{K}_3\mathbf{C}^2, \mathbf{K}_3\mathbf{CK}_3, \mathbf{K}_3\mathbf{CK}_3^2 - \mathbf{K}_3^2\mathbf{CK}_3, \\ & \mathbf{P}_2\mathbf{K}_3 - \mathbf{K}_3\mathbf{P}_2, \mathbf{P}_2^2\mathbf{K}_3 - \mathbf{K}_3\mathbf{P}_2^2, \mathbf{K}_3\mathbf{P}_2\mathbf{K}_3, \mathbf{K}_3\mathbf{P}_2\mathbf{K}_3^2 - \mathbf{K}_3^2\mathbf{P}_2\mathbf{K}_3 \end{aligned} \quad (23)$$

and the invariants are obtained from Table A1 as

$$\begin{aligned} & tr\mathbf{C}, tr\mathbf{C}^2, tr\mathbf{C}^3, tr(\mathbf{CP}_2), tr(\mathbf{C}^2\mathbf{P}_2), tr(\mathbf{CP}_2^2), tr(\mathbf{C}^2\mathbf{P}_2^2), \\ & tr(\mathbf{CK}_3^2), tr(\mathbf{C}^2\mathbf{K}_3^2), tr(\mathbf{C}^2\mathbf{K}_3^2\mathbf{CK}_3) \end{aligned} \quad (24)$$

There are redundant terms in (23) and (24). After eliminating the redundant terms, we obtain

$$\begin{aligned} \hat{\mathbf{T}}(\mathbf{C}, \mathbf{P}_2, \mathbf{K}_3) = & \alpha_0\mathbf{I} + \alpha_1\mathbf{C} + \alpha_2\mathbf{C}^2 + \alpha_3\mathbf{P}_2 + \alpha_4\mathbf{P}_2^2 + \alpha_5(\mathbf{CP}_2 + \mathbf{P}_2\mathbf{C}) \\ & + \alpha_6(\mathbf{C}^2\mathbf{P}_2 + \mathbf{P}_2\mathbf{C}^2) + \alpha_7(\mathbf{CP}_2^2 + \mathbf{P}_2^2\mathbf{C}) + \alpha_8(\mathbf{CK}_3 - \mathbf{K}_3\mathbf{C}) + \alpha_9(\mathbf{C}^2\mathbf{K}_3 - \mathbf{K}_3\mathbf{C}^2) \\ & + \alpha_{10}\mathbf{K}_3\mathbf{CK}_3 + \alpha_{11}(\mathbf{K}_3\mathbf{CK}_3^2 - \mathbf{K}_3^2\mathbf{CK}_3) + \alpha_{12}(\mathbf{P}_2\mathbf{K}_3 - \mathbf{K}_3\mathbf{P}_2) \end{aligned} \quad (25)$$

and

$$\alpha_i = \alpha_i(tr\mathbf{C}, tr\mathbf{C}^2, tr\mathbf{C}^3, tr(\mathbf{CP}_2), tr(\mathbf{C}^2\mathbf{P}_2), tr(\mathbf{CP}_2^2), tr(\mathbf{C}^2\mathbf{P}_2^2), tr(\mathbf{C}^2\mathbf{K}_3^2\mathbf{CK}_3)) \quad (26)$$

The representation of a scalar-valued function $\hat{\psi}$ follows the same form of (26).

10 Group $\mathcal{C}_{4h}$ ($4/m$)

For this point group, we propose a lower-order structural tensor set $\{\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \mathbf{K}_3\}$, where $\mathbf{M}_i$ are defined in Section 5.2 and $\mathbf{K}_3 = \epsilon\mathbf{k}$. The purpose of $\mathbf{K}_3$ is to break the in-plane reflection symmetry. The Man-Goddard reformulation needs to be used. The group generators are $\mathcal{G}^* = \{\mathbf{C}_4, \bar{\mathbf{I}}\}$. The group generator $\bar{\mathbf{I}}$ keeps all structural tensors invariant. In contrast, the group generator $\mathbf{C}_4$ keeps $\mathbf{M}_3$ and $\mathbf{K}_3$ invariant but permutes $\mathbf{M}_1$ and $\mathbf{M}_2$. Hence, $\mathbf{C}_4$ would impose additional constraints to the representations.

The tensor generators and invariants can be obtained by adding extra terms related to $\mathbf{K}_3$ in (13) and (14). The tensor generators are

$$\begin{aligned} & \mathbf{M}_i, \mathbf{M}_i\mathbf{C} + \mathbf{CM}_i, \mathbf{C}^2, \mathbf{K}_3^2, \mathbf{CK}_3 - \mathbf{K}_3\mathbf{C}, \mathbf{C}^2\mathbf{K}_3 - \mathbf{K}_3\mathbf{C}^2, \mathbf{K}_3\mathbf{CK}_3, \mathbf{K}_3\mathbf{CK}_3^2 - \mathbf{K}_3^2\mathbf{CK}_3, \\ & \mathbf{M}_i\mathbf{K}_3 - \mathbf{K}_3\mathbf{M}_i, \mathbf{M}_i^2\mathbf{K}_3 - \mathbf{K}_3\mathbf{M}_i^2, \mathbf{K}_3\mathbf{M}_i\mathbf{K}_3, \mathbf{K}_3\mathbf{M}_i\mathbf{K}_3^2 - \mathbf{K}_3^2\mathbf{M}_i\mathbf{K}_3, \text{ for } i = 1, 2, 3 \end{aligned} \quad (27)$$

and the invariants are

$$\begin{aligned} & tr(\mathbf{CM}_i), tr(\mathbf{C}^2\mathbf{M}_i), tr\mathbf{C}^3, tr(\mathbf{CK}_3^2), tr(\mathbf{C}^2\mathbf{K}_3^2), tr(\mathbf{C}^2\mathbf{K}_3^2\mathbf{CK}_3), \\ & tr(\mathbf{CM}_i\mathbf{K}_3), tr(\mathbf{C}^2\mathbf{M}_i\mathbf{K}_3), tr(\mathbf{CM}_i^2\mathbf{K}_3), tr(\mathbf{CK}_3^2\mathbf{M}_i\mathbf{K}_3), \text{ for } i = 1, 2, 3 \end{aligned} \quad (28)$$

After eliminating the redundant terms in (27) and (28), the representation of $\hat{\mathbf{T}}$ is obtained as

$$\begin{aligned}\hat{\mathbf{T}}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \mathbf{K}_3) = & \alpha_1 \mathbf{M}_1 + \alpha_2 \mathbf{M}_2 + \alpha_3 \mathbf{M}_3 + \alpha_4 (\mathbf{M}_1 \mathbf{C} + \mathbf{C} \mathbf{M}_1) \\ & + \alpha_5 (\mathbf{M}_2 \mathbf{C} + \mathbf{C} \mathbf{M}_2) + \alpha_6 (\mathbf{M}_3 \mathbf{C} + \mathbf{C} \mathbf{M}_3) + \alpha_7 \mathbf{C}^2 + \alpha_8 (\mathbf{C} \mathbf{K}_3 - \mathbf{K}_3 \mathbf{C}) \\ & + \alpha_9 (\mathbf{C}^2 \mathbf{K}_3 - \mathbf{K}_3 \mathbf{C}^2) + \alpha_{10} \mathbf{K}_3 \mathbf{C} \mathbf{K}_3 + \alpha_{11} (\mathbf{K}_3 \mathbf{C} \mathbf{K}_3^2 - \mathbf{K}_3^2 \mathbf{C} \mathbf{K}_3) \\ & + \alpha_{12} (\mathbf{M}_1 \mathbf{K}_3 - \mathbf{K}_3 \mathbf{M}_1) + \alpha_{13} (\mathbf{M}_2 \mathbf{K}_3 - \mathbf{K}_3 \mathbf{M}_2)\end{aligned}\quad (29)$$

where α_i are

$$\begin{aligned}\alpha_i = & \alpha_i (tr(\mathbf{C} \mathbf{M}_1), tr(\mathbf{C} \mathbf{M}_2), tr(\mathbf{C} \mathbf{M}_3), tr(\mathbf{C}^2 \mathbf{M}_1), tr(\mathbf{C}^2 \mathbf{M}_2), tr(\mathbf{C}^2 \mathbf{M}_3), tr \mathbf{C}^3, \\ & tr(\mathbf{C} \mathbf{M}_1 \mathbf{K}_3), tr(\mathbf{C}^2 \mathbf{M}_1 \mathbf{K}_3), tr(\mathbf{C} \mathbf{M}_2 \mathbf{K}_3), tr(\mathbf{C}^2 \mathbf{M}_2 \mathbf{K}_3)) \\ = & \tilde{\alpha}_i(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \mathbf{K}_3)\end{aligned}\quad (30)$$

Note that the group generator $\mathbf{C}_4$ imposes an additional constraint $\hat{\mathbf{T}}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \mathbf{K}_3) = \hat{\mathbf{T}}(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_1, \mathbf{M}_3, \mathbf{K}_3)$ to the representation. Using (29)-(30), the additional constraints to coefficient functions are as follows.

$$\begin{aligned}\tilde{\alpha}_1(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \mathbf{K}_3) &= \tilde{\alpha}_2(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_1, \mathbf{M}_3, \mathbf{K}_3), \\ \tilde{\alpha}_4(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \mathbf{K}_3) &= \tilde{\alpha}_5(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_1, \mathbf{M}_3, \mathbf{K}_3), \\ \tilde{\alpha}_{12}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \mathbf{K}_3) &= \tilde{\alpha}_{13}(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_1, \mathbf{M}_3, \mathbf{K}_3), \\ \tilde{\alpha}_i(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \mathbf{K}_3) &= \tilde{\alpha}_i(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_1, \mathbf{M}_3, \mathbf{K}_3) \quad \text{for } i = 3, 6, 7, 8, 9, 10, 11\end{aligned}\quad (31)$$

The representation of a scalar-valued function $\hat{\psi}$ follows the same form of (30). Moreover, the group generator $\mathbf{C}_4$ imposes an additional constraint $\hat{\psi}(\mathbf{C}, \mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3, \mathbf{K}_3) = \hat{\psi}(\mathbf{C}, \mathbf{M}_2, \mathbf{M}_1, \mathbf{M}_3, \mathbf{K}_3)$ to the representation.

11 Group $\mathcal{C}_{3i}$ ($\bar{3}$ or $\mathcal{S}_6$)

Since the structural tensors proposed by Zheng [2] include a 4th-order tensor, we need to construct a lower-order structural tensor set for this point group. By defining a vector $\mathbf{u} = \mathbf{i} + \mathbf{k}$ in a high symmetry plane, we propose a structural tensor set $\{\mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3\}$ with detailed tensors given as

$$\mathbf{T}_1 = \mathbf{u} \otimes \mathbf{u}, \quad \mathbf{T}_2 = \mathbf{C}_3 \mathbf{T}_1 \mathbf{C}_3^T, \quad \mathbf{T}_3 = \mathbf{C}_3 \mathbf{T}_2 \mathbf{C}_3^T, \quad \mathbf{K}_3 = \epsilon \mathbf{k} \quad (32)$$

The purpose of $\mathbf{K}_3$ is to break the in-plane reflection symmetry. For this point group, the Man-Goddard reformulation is needed to derive the representations. This point group has two group generators $\mathcal{G}^* = \{\mathbf{C}_3, \bar{\mathbf{I}}\}$. The operation $\bar{\mathbf{I}}$ keeps all four structural tensors invariant. The operation $\mathbf{C}_3$ keeps $\mathbf{K}_3$ invariant but permutes $\mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3$ to each other as shown in (32). Hence, the operation $\mathbf{C}_3$ imposes additional constraints to the representations.

Using Tables A1-A2, the tensor generators are

$$\begin{aligned}
& \mathbf{I}, \mathbf{C}, \mathbf{C}^2, \mathbf{T}_i, \mathbf{T}_i^2, \mathbf{K}_3^2, \mathbf{C}\mathbf{T}_i + \mathbf{T}_i\mathbf{C}, \mathbf{C}^2\mathbf{T}_i + \mathbf{T}_i\mathbf{C}^2, \mathbf{C}\mathbf{T}_i^2 + \mathbf{T}_i^2\mathbf{C}, \\
& \mathbf{T}_1\mathbf{T}_2 + \mathbf{T}_2\mathbf{T}_1, \mathbf{T}_1^2\mathbf{T}_2 + \mathbf{T}_2\mathbf{T}_1^2, \mathbf{T}_1\mathbf{T}_2^2 + \mathbf{T}_2^2\mathbf{T}_1, \mathbf{T}_1\mathbf{T}_3 + \mathbf{T}_3\mathbf{T}_1, \mathbf{T}_1^2\mathbf{T}_3 + \mathbf{T}_3\mathbf{T}_1^2, \\
& \mathbf{T}_1\mathbf{T}_3^2 + \mathbf{T}_3^2\mathbf{T}_1, \mathbf{T}_2\mathbf{T}_3 + \mathbf{T}_3\mathbf{T}_2, \mathbf{T}_2^2\mathbf{T}_3 + \mathbf{T}_3\mathbf{T}_2^2, \mathbf{T}_2\mathbf{T}_3^2 + \mathbf{T}_3^2\mathbf{T}_2, \\
& \mathbf{C}\mathbf{K}_3 - \mathbf{K}_3\mathbf{C}, \mathbf{C}^2\mathbf{K}_3 - \mathbf{K}_3\mathbf{C}^2, \mathbf{K}_3\mathbf{C}\mathbf{K}_3, \mathbf{K}_3\mathbf{C}\mathbf{K}_3^2 - \mathbf{K}_3^2\mathbf{C}\mathbf{K}_3, \\
& \mathbf{T}_i\mathbf{K}_3 - \mathbf{K}_3\mathbf{T}_i, \mathbf{T}_i^2\mathbf{K}_3 - \mathbf{K}_3\mathbf{T}_i^2, \mathbf{K}_3\mathbf{T}_i\mathbf{K}_3, \mathbf{K}_3\mathbf{T}_i\mathbf{K}_3^2 - \mathbf{K}_3^2\mathbf{T}_i\mathbf{K}_3, \text{ for } i = 1, 2, 3
\end{aligned} \tag{33}$$

and the invariants are

$$\begin{aligned}
& tr\mathbf{C}, tr\mathbf{C}^2, tr\mathbf{C}^3, tr(\mathbf{C}\mathbf{T}_i), tr(\mathbf{C}^2\mathbf{T}_i), tr(\mathbf{C}\mathbf{T}_i^2), tr(\mathbf{C}^2\mathbf{T}_i^2), tr(\mathbf{C}\mathbf{K}_3^2), \\
& tr(\mathbf{C}^2\mathbf{K}_3^2), tr(\mathbf{C}^2\mathbf{K}_3^2\mathbf{C}\mathbf{K}_3), tr(\mathbf{C}\mathbf{T}_1\mathbf{T}_2), tr(\mathbf{C}\mathbf{T}_1\mathbf{T}_3), tr(\mathbf{C}\mathbf{T}_2\mathbf{T}_3), \\
& tr(\mathbf{C}\mathbf{T}_i\mathbf{K}_3), tr(\mathbf{C}^2\mathbf{T}_i\mathbf{K}_3), tr(\mathbf{C}\mathbf{T}_i^2\mathbf{K}_3), tr(\mathbf{C}\mathbf{K}_3^2\mathbf{T}_i\mathbf{K}_3), \text{ for } i = 1, 2, 3
\end{aligned} \tag{34}$$

After eliminating the redundant terms in (33) and (34), the representation of $\hat{\mathbf{T}}$ is as follows.

$$\begin{aligned}
\hat{\mathbf{T}}(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = & \alpha_0\mathbf{I} + \alpha_1\mathbf{T}_1 + \alpha_2\mathbf{T}_2 + \alpha_3\mathbf{T}_3 + \alpha_4\mathbf{C} + \alpha_5\mathbf{C}^2 \\
& + \alpha_6(\mathbf{C}\mathbf{T}_1 + \mathbf{T}_1\mathbf{C}) + \alpha_7(\mathbf{C}^2\mathbf{T}_1 + \mathbf{T}_1\mathbf{C}^2) + \alpha_8(\mathbf{C}\mathbf{T}_2 + \mathbf{T}_2\mathbf{C}) \\
& + \alpha_9(\mathbf{C}^2\mathbf{T}_2 + \mathbf{T}_2\mathbf{C}^2) + \alpha_{10}(\mathbf{C}\mathbf{T}_3 + \mathbf{T}_3\mathbf{C}) + \alpha_{11}(\mathbf{C}^2\mathbf{T}_3 + \mathbf{T}_3\mathbf{C}^2) \\
& + \alpha_{12}(\mathbf{T}_1\mathbf{T}_2 + \mathbf{T}_2\mathbf{T}_1) + \alpha_{13}(\mathbf{T}_1\mathbf{T}_3 + \mathbf{T}_3\mathbf{T}_1) + \alpha_{14}(\mathbf{T}_2\mathbf{T}_3 + \mathbf{T}_3\mathbf{T}_2) \\
& + \alpha_{15}(\mathbf{C}\mathbf{K}_3 - \mathbf{K}_3\mathbf{C}) + \alpha_{16}(\mathbf{C}^2\mathbf{K}_3 - \mathbf{K}_3\mathbf{C}^2) + \alpha_{17}\mathbf{K}_3\mathbf{C}\mathbf{K}_3 \\
& + \alpha_{18}(\mathbf{K}_3\mathbf{C}\mathbf{K}_3^2 - \mathbf{K}_3^2\mathbf{C}\mathbf{K}_3) + \alpha_{19}\mathbf{K}_3\mathbf{T}_1\mathbf{K}_3 + \alpha_{20}\mathbf{K}_3\mathbf{T}_2\mathbf{K}_3 + \alpha_{21}\mathbf{K}_3\mathbf{T}_3\mathbf{K}_3
\end{aligned} \tag{35}$$

where

$$\begin{aligned}
\alpha_i = & \alpha_i(tr(\mathbf{C}\mathbf{T}_1), tr(\mathbf{C}\mathbf{T}_2), tr(\mathbf{C}\mathbf{T}_3), tr(\mathbf{C}\mathbf{T}_1\mathbf{T}_2), tr(\mathbf{C}\mathbf{T}_1\mathbf{T}_3), tr(\mathbf{C}\mathbf{T}_2\mathbf{T}_3)) \\
= & \tilde{\alpha}_i(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3)
\end{aligned} \tag{36}$$

Note that the group generator $\mathbf{C}_3$ imposes an additional constraint $\hat{\mathbf{T}}(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = \hat{\mathbf{T}}(\mathbf{C}, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_1, \mathbf{K}_3)$, which requires the coefficient functions to satisfy

$$\begin{aligned}
\tilde{\alpha}_1(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = \tilde{\alpha}_3(\mathbf{C}, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_1, \mathbf{K}_3), \quad \tilde{\alpha}_2(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = \tilde{\alpha}_1(\mathbf{C}, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_1, \mathbf{K}_3), \\
\tilde{\alpha}_6(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = \tilde{\alpha}_{10}(\mathbf{C}, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_1, \mathbf{K}_3), \quad \tilde{\alpha}_7(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = \tilde{\alpha}_{11}(\mathbf{C}, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_1, \mathbf{K}_3) \\
\tilde{\alpha}_8(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = \tilde{\alpha}_6(\mathbf{C}, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_1, \mathbf{K}_3), \quad \tilde{\alpha}_9(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = \tilde{\alpha}_7(\mathbf{C}, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_1, \mathbf{K}_3) \\
\tilde{\alpha}_{12}(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = \tilde{\alpha}_{13}(\mathbf{C}, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_1, \mathbf{K}_3), \quad \tilde{\alpha}_{14}(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = \tilde{\alpha}_{12}(\mathbf{C}, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_1, \mathbf{K}_3), \\
\tilde{\alpha}_{19}(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = \tilde{\alpha}_{21}(\mathbf{C}, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_1, \mathbf{K}_3), \quad \tilde{\alpha}_{20}(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = \tilde{\alpha}_{19}(\mathbf{C}, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_1, \mathbf{K}_3), \\
\tilde{\alpha}_i(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = \tilde{\alpha}_i(\mathbf{C}, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_1, \mathbf{K}_3) \quad \text{for } i = 0, 4, 5, 15, 16, 17, 18
\end{aligned} \tag{37}$$

The representation of a scalar-valued function $\hat{\psi}$ follows the same form of (36). In addition, the group generator $\mathbf{C}_3$ imposes an additional constraint $\hat{\psi}(\mathbf{C}, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \mathbf{K}_3) = \hat{\psi}(\mathbf{C}, \mathbf{T}_2, \mathbf{T}_3, \mathbf{T}_1, \mathbf{K}_3)$ to the representation.

12 Group $\mathcal{D}_{3d} (\bar{3}m)$

Since the structural tensor $\mathbf{k} \otimes \mathbb{P}_3$ given by Zheng [2] is a 4th-order tensor, we propose a lower-order structural tensor set to replace it. Firstly, we define a vector $\mathbf{v} = \mathbf{j} + \mathbf{k}$. The structural tensor set $\{\mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3\}$ is then defined by $\mathbf{D}_1 = \mathbf{v} \otimes \mathbf{v}$, $\mathbf{D}_2 = \mathbf{C}_3 \mathbf{D}_1 \mathbf{C}_3^T$, and $\mathbf{D}_3 = \mathbf{C}_3 \mathbf{D}_2 \mathbf{C}_3^T$. In this case, the Man-Goddard reformulation is used.

This point group has three group generators $\mathcal{G}^* = \{\mathbf{C}_3, \mathbf{C}_{2x}, \bar{\mathbf{I}}\}$. The operation $\bar{\mathbf{I}}$ keeps these structural tensors invariant but $\mathbf{C}_3$ and $\mathbf{C}_{2x}$ transform them in the following way.

$$\begin{aligned} \mathbf{C}_3 \mathbf{D}_1 \mathbf{C}_3^T &= \mathbf{D}_2, & \mathbf{C}_{2x} \mathbf{D}_1 \mathbf{C}_{2x}^T &= \mathbf{D}_1, \\ \mathbf{C}_3 \mathbf{D}_2 \mathbf{C}_3^T &= \mathbf{D}_3, & \mathbf{C}_{2x} \mathbf{D}_2 \mathbf{C}_{2x}^T &= \mathbf{D}_3, \\ \mathbf{C}_3 \mathbf{D}_3 \mathbf{C}_3^T &= \mathbf{D}_1, & \mathbf{C}_{2x} \mathbf{D}_3 \mathbf{C}_{2x}^T &= \mathbf{D}_2 \end{aligned} \quad (38)$$

Therefore, the group generators $\mathbf{C}_3$ and $\mathbf{C}_{2x}$ would impose additional constraints to the representations.

All three $\mathbf{D}_i$ are symmetric. The tensor generators are obtained as

$$\begin{aligned} &\mathbf{I}, \mathbf{C}, \mathbf{C}^2, \mathbf{D}_i, \mathbf{D}_i^2, \mathbf{C} \mathbf{D}_i + \mathbf{D}_i \mathbf{C}, \mathbf{C}^2 \mathbf{D}_i + \mathbf{D}_i \mathbf{C}^2, \mathbf{C} \mathbf{D}_i^2 + \mathbf{D}_i^2 \mathbf{C}, \\ &\mathbf{D}_1 \mathbf{D}_2 + \mathbf{D}_2 \mathbf{D}_1, \mathbf{D}_1^2 \mathbf{D}_2 + \mathbf{D}_2 \mathbf{D}_1^2, \mathbf{D}_1 \mathbf{D}_2^2 + \mathbf{D}_2^2 \mathbf{D}_1, \\ &\mathbf{D}_1 \mathbf{D}_3 + \mathbf{D}_3 \mathbf{D}_1, \mathbf{D}_1^2 \mathbf{D}_3 + \mathbf{D}_3 \mathbf{D}_1^2, \mathbf{D}_1 \mathbf{D}_3^2 + \mathbf{D}_3^2 \mathbf{D}_1, \\ &\mathbf{D}_2 \mathbf{D}_3 + \mathbf{D}_3 \mathbf{D}_2, \mathbf{D}_2^2 \mathbf{D}_3 + \mathbf{D}_3 \mathbf{D}_2^2, \mathbf{D}_2 \mathbf{D}_3^2 + \mathbf{D}_3^2 \mathbf{D}_2, \text{ for } i = 1, 2, 3 \end{aligned} \quad (39)$$

and the invariants are

$$\begin{aligned} &tr \mathbf{C}, tr \mathbf{C}^2, tr \mathbf{C}^3, tr(\mathbf{C} \mathbf{D}_i), tr(\mathbf{C}^2 \mathbf{D}_i), tr(\mathbf{C} \mathbf{D}_i^2), tr(\mathbf{C}^2 \mathbf{D}_i^2), \\ &tr(\mathbf{C} \mathbf{D}_1 \mathbf{D}_2), tr(\mathbf{C} \mathbf{D}_1 \mathbf{D}_3), tr(\mathbf{C} \mathbf{D}_2 \mathbf{D}_3), \text{ for } i = 1, 2, 3 \end{aligned} \quad (40)$$

After eliminating redundant terms in (39) and (40), the representation is given as

$$\begin{aligned} \hat{\mathbf{T}}(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \alpha_0 \mathbf{I} + \alpha_1 \mathbf{D}_1 + \alpha_2 \mathbf{D}_2 + \alpha_3 \mathbf{D}_3 + \alpha_4 \mathbf{C} + \alpha_5 \mathbf{C}^2 \\ &+ \alpha_6 (\mathbf{C} \mathbf{D}_1 + \mathbf{D}_1 \mathbf{C}) + \alpha_7 (\mathbf{C}^2 \mathbf{D}_1 + \mathbf{D}_1 \mathbf{C}^2) + \alpha_8 (\mathbf{C} \mathbf{D}_2 + \mathbf{D}_2 \mathbf{C}) \\ &+ \alpha_9 (\mathbf{C}^2 \mathbf{D}_2 + \mathbf{D}_2 \mathbf{C}^2) + \alpha_{10} (\mathbf{C} \mathbf{D}_3 + \mathbf{D}_3 \mathbf{C}) + \alpha_{11} (\mathbf{C}^2 \mathbf{D}_3 + \mathbf{D}_3 \mathbf{C}^2) \\ &+ \alpha_{12} (\mathbf{D}_1 \mathbf{D}_2 + \mathbf{D}_2 \mathbf{D}_1) + \alpha_{13} (\mathbf{D}_1 \mathbf{D}_3 + \mathbf{D}_3 \mathbf{D}_1) + \alpha_{14} (\mathbf{D}_2 \mathbf{D}_3 + \mathbf{D}_3 \mathbf{D}_2) \end{aligned} \quad (41)$$

and

$$\begin{aligned} \alpha_i &= \alpha_i (tr(\mathbf{C} \mathbf{D}_1), tr(\mathbf{C} \mathbf{D}_2), tr(\mathbf{C} \mathbf{D}_3), tr(\mathbf{C} \mathbf{D}_1 \mathbf{D}_2), tr(\mathbf{C} \mathbf{D}_1 \mathbf{D}_3), tr(\mathbf{C} \mathbf{D}_2 \mathbf{D}_3)) \\ &= \tilde{\alpha}_i(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) \end{aligned} \quad (42)$$

As mentioned earlier, the group generators $\mathbf{C}_3$ and $\mathbf{C}_{2x}$ impose additional constraints $\hat{\mathbf{T}}(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) = \hat{\mathbf{T}}(\mathbf{C}, \mathbf{D}_2, \mathbf{D}_3, \mathbf{D}_1)$ and $\hat{\mathbf{T}}(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) = \hat{\mathbf{T}}(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_3, \mathbf{D}_2)$ to the repre-

sensation, respectively. The corresponding constraints to the coefficient functions $\tilde{\alpha}_i$ are given as

For the generator $\mathbf{C}_3$:

$$\begin{aligned}
\tilde{\alpha}_1(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_3(\mathbf{C}, \mathbf{D}_2, \mathbf{D}_3, \mathbf{D}_1), & \tilde{\alpha}_2(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_1(\mathbf{C}, \mathbf{D}_2, \mathbf{D}_3, \mathbf{D}_1), \\
\tilde{\alpha}_6(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_{10}(\mathbf{C}, \mathbf{D}_2, \mathbf{D}_3, \mathbf{D}_1), & \tilde{\alpha}_7(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_{11}(\mathbf{C}, \mathbf{D}_2, \mathbf{D}_3, \mathbf{D}_1), \\
\tilde{\alpha}_8(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_6(\mathbf{C}, \mathbf{D}_2, \mathbf{D}_3, \mathbf{D}_1), & \tilde{\alpha}_9(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_7(\mathbf{C}, \mathbf{D}_2, \mathbf{D}_3, \mathbf{D}_1), \\
\tilde{\alpha}_{12}(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_{13}(\mathbf{C}, \mathbf{D}_2, \mathbf{D}_3, \mathbf{D}_1), & \tilde{\alpha}_{13}(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_{14}(\mathbf{C}, \mathbf{D}_2, \mathbf{D}_3, \mathbf{D}_1), \\
\tilde{\alpha}_i(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_i(\mathbf{C}, \mathbf{D}_2, \mathbf{D}_3, \mathbf{D}_1) & \text{for } i = 0, 4, 5
\end{aligned} \tag{43}$$

For the generator $\mathbf{C}_{2x}$:

$$\begin{aligned}
\tilde{\alpha}_2(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_3(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_3, \mathbf{D}_2), & \tilde{\alpha}_8(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_{10}(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_3, \mathbf{D}_2), \\
\tilde{\alpha}_9(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_{11}(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_3, \mathbf{D}_2), & \tilde{\alpha}_{12}(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_{13}(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_3, \mathbf{D}_2), \\
\tilde{\alpha}_i(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) &= \tilde{\alpha}_i(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_3, \mathbf{D}_2) & \text{for } i = 0, 1, 4, 5, 6, 7, 14
\end{aligned}$$

The representation of a scalar-valued function $\hat{\psi}$ follows the same form of (42). Moreover, the additional constraints imposed by the group generators $\mathbf{C}_3$ and $\mathbf{C}_{2x}$ are

$$\hat{\psi}(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3) = \hat{\psi}(\mathbf{C}, \mathbf{D}_2, \mathbf{D}_3, \mathbf{D}_1) = \hat{\psi}(\mathbf{C}, \mathbf{D}_1, \mathbf{D}_3, \mathbf{D}_2) \tag{44}$$

13 Group $\mathcal{D}_{6h}$ ($6/mmm$)

The structural tensor $\mathbb{P}_6$ provided by Zheng [2] is a 6th-order one. We propose a lower-order structural tensor set $\{\mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3\}$ to replace it. The three structural tensors are defined as $\mathbf{H}_1 = \mathbf{i} \otimes \mathbf{i}$, $\mathbf{H}_2 = \mathbf{C}_6 \mathbf{H}_1 \mathbf{C}_6^T$ and $\mathbf{H}_3 = \mathbf{C}_6 \mathbf{H}_2 \mathbf{C}_6^T$. In this case, the Man-Goddard reformulation is used. This point group has three group generators $\mathcal{G}^* = \{\mathbf{C}_6, \mathbf{C}_{2x}, \bar{\mathbf{I}}\}$. The generator $\bar{\mathbf{I}}$ keeps all three structural tensors invariant. The other two generators $\mathbf{C}_6$ and $\mathbf{C}_{2x}$ transform them in the following way.

$$\begin{aligned}
\mathbf{C}_6 \mathbf{H}_1 \mathbf{C}_6^T &= \mathbf{H}_2, & \mathbf{C}_{2x} \mathbf{H}_1 \mathbf{C}_{2x}^T &= \mathbf{H}_1, \\
\mathbf{C}_6 \mathbf{H}_2 \mathbf{C}_6^T &= \mathbf{H}_3, & \mathbf{C}_{2x} \mathbf{H}_2 \mathbf{C}_{2x}^T &= \mathbf{H}_3, \\
\mathbf{C}_6 \mathbf{H}_3 \mathbf{C}_6^T &= \mathbf{H}_1, & \mathbf{C}_{2x} \mathbf{H}_3 \mathbf{C}_{2x}^T &= \mathbf{H}_2
\end{aligned} \tag{45}$$

As it is obvious from (45), these two group generators would impose additional constraints to the representations.

All three structural tensors $\mathbf{H}_i$ where $i = 1, 2, 3$ are symmetric. The tensor generators are given as

$$\begin{aligned}
&\mathbf{I}, \mathbf{C}, \mathbf{C}^2, \mathbf{H}_i, \mathbf{H}_i^2, \mathbf{C} \mathbf{H}_i + \mathbf{H}_i \mathbf{C}, \mathbf{C}^2 \mathbf{H}_i + \mathbf{H}_i \mathbf{C}^2, \mathbf{C} \mathbf{H}_i^2 + \mathbf{H}_i^2 \mathbf{C}, \\
&\mathbf{H}_1 \mathbf{H}_2 + \mathbf{H}_2 \mathbf{H}_1, \mathbf{H}_1^2 \mathbf{H}_2 + \mathbf{H}_2 \mathbf{H}_1^2, \mathbf{H}_1 \mathbf{H}_2^2 + \mathbf{H}_2^2 \mathbf{H}_1, \\
&\mathbf{H}_1 \mathbf{H}_3 + \mathbf{H}_3 \mathbf{H}_1, \mathbf{H}_1^2 \mathbf{H}_3 + \mathbf{H}_3 \mathbf{H}_1^2, \mathbf{H}_1 \mathbf{H}_3^2 + \mathbf{H}_3^2 \mathbf{H}_1, \\
&\mathbf{H}_2 \mathbf{H}_3 + \mathbf{H}_3 \mathbf{H}_2, \mathbf{H}_2^2 \mathbf{H}_3 + \mathbf{H}_3 \mathbf{H}_2^2, \mathbf{H}_2 \mathbf{H}_3^2 + \mathbf{H}_3^2 \mathbf{H}_2, \text{ for } i = 1, 2, 3
\end{aligned} \tag{46}$$

and the invariants are

$$\begin{aligned} & tr\mathbf{C}, tr\mathbf{C}^2, tr\mathbf{C}^3, tr(\mathbf{CH}_i), tr(\mathbf{C}^2\mathbf{H}_i), tr(\mathbf{CH}_i^2), tr(\mathbf{C}^2\mathbf{H}_i^2), \\ & tr(\mathbf{CH}_1\mathbf{H}_2), tr(\mathbf{CH}_1\mathbf{H}_3), tr(\mathbf{CH}_2\mathbf{H}_3), \text{ for } i = 1, 2, 3 \end{aligned} \quad (47)$$

After eliminating the redundant terms in (46) and (47), the representation of $\hat{\mathbf{T}}$ is given as

$$\begin{aligned} \hat{\mathbf{T}}(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) = & \alpha_0\mathbf{I} + \alpha_1\mathbf{H}_1 + \alpha_2\mathbf{H}_2 + \alpha_3\mathbf{H}_3 + \alpha_4\mathbf{C} + \alpha_5\mathbf{C}^2 \\ & + \alpha_6(\mathbf{CH}_1 + \mathbf{H}_1\mathbf{C}) + \alpha_7(\mathbf{C}^2\mathbf{H}_1 + \mathbf{H}_1\mathbf{C}^2) + \alpha_8(\mathbf{CH}_2 + \mathbf{H}_2\mathbf{C}) \\ & + \alpha_9(\mathbf{C}^2\mathbf{H}_2 + \mathbf{H}_2\mathbf{C}^2) + \alpha_{10}(\mathbf{CH}_3 + \mathbf{H}_3\mathbf{C}) + \alpha_{11}(\mathbf{C}^2\mathbf{H}_3 + \mathbf{H}_3\mathbf{C}^2) \end{aligned} \quad (48)$$

and

$$\begin{aligned} \alpha_i = & \alpha_i(tr\mathbf{C}, tr\mathbf{C}^2, tr\mathbf{C}^3, tr(\mathbf{CH}_1), tr(\mathbf{C}^2\mathbf{H}_1), tr(\mathbf{CH}_2), tr(\mathbf{C}^2\mathbf{H}_2), tr(\mathbf{CH}_3), tr(\mathbf{C}^2\mathbf{H}_3)) \\ = & \tilde{\alpha}_i(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) \end{aligned} \quad (49)$$

As mentioned earlier, additional constraints are required to be imposed. The group generators $\mathbf{C}_6$ and $\mathbf{C}_{2x}$ require that $\hat{\mathbf{T}}(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) = \hat{\mathbf{T}}(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1)$ and $\hat{\mathbf{T}}(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) = \hat{\mathbf{T}}(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_3, \mathbf{H}_2)$, respectively. Consequently, we can find the constraints to the coefficient functions $\tilde{\alpha}_i$ as

For the generator $\mathbf{C}_6$:

$$\begin{aligned} \tilde{\alpha}_1(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) &= \tilde{\alpha}_3(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1), & \tilde{\alpha}_2(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) &= \tilde{\alpha}_1(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1), \\ \tilde{\alpha}_6(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) &= \tilde{\alpha}_{10}(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1), & \tilde{\alpha}_8(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) &= \tilde{\alpha}_6(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1), \\ \tilde{\alpha}_7(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) &= \tilde{\alpha}_{11}(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1), & \tilde{\alpha}_9(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) &= \tilde{\alpha}_7(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1), \\ \tilde{\alpha}_i(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) &= \tilde{\alpha}_i(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1) & \text{ for } i = 0, 4, 5 \end{aligned} \quad (50)$$

For the generator $\mathbf{C}_{2x}$:

$$\begin{aligned} \tilde{\alpha}_2(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) &= \tilde{\alpha}_3(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_3, \mathbf{H}_2), & \tilde{\alpha}_8(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) &= \tilde{\alpha}_{10}(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_3, \mathbf{H}_2), \\ \tilde{\alpha}_9(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) &= \tilde{\alpha}_{11}(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_3, \mathbf{H}_2), \\ \tilde{\alpha}_i(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) &= \tilde{\alpha}_i(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_3, \mathbf{H}_2) & \text{ for } i = 0, 1, 4, 5, 6, 7 \end{aligned}$$

The representation of a scalar-valued function $\hat{\psi}$ follows the same form of (49). Moreover, the additional constraints imposed by the group generators $\mathbf{C}_6$ and $\mathbf{C}_{2x}$ are

$$\hat{\psi}(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3) = \hat{\psi}(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1) = \hat{\psi}(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_3, \mathbf{H}_2) \quad (51)$$

14 Group $\mathcal{C}_{6h}$ (6/m)

The structural tensors provided by Zheng [2] involve a 6th-order tensor. We propose a lower-order structural tensor set $\{\mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3, \mathbf{K}_3\}$ for this point group. Herein, $\mathbf{H}_i$ are identical to that in Section 13 and $\mathbf{K}_3 = \epsilon\mathbf{k}$ is introduced to break the in-plane reflection symmetry. In this case,

the Man-Goddard reformulation is used. There are only two group generators $\mathcal{G}^* = \{\mathbf{C}_6, \bar{\mathbf{I}}\}$. The generator $\bar{\mathbf{I}}$ keeps all structural tensors invariant; whereas $\mathbf{C}_6$ transform them in the following way.

$$\mathbf{C}_6 \mathbf{H}_1 \mathbf{C}_6^T = \mathbf{H}_2, \quad \mathbf{C}_6 \mathbf{H}_2 \mathbf{C}_6^T = \mathbf{H}_3, \quad \mathbf{C}_6 \mathbf{H}_3 \mathbf{C}_6^T = \mathbf{H}_1, \quad \mathbf{C}_6 \mathbf{K}_3 \mathbf{C}_6^T = \mathbf{K}_3 \quad (52)$$

As it is obvious from (52), $\mathbf{C}_6$ keeps $\mathbf{K}_3$ invariant but permutes $\mathbf{H}_1, \mathbf{H}_2$ and $\mathbf{H}_3$. Hence, the generator $\mathbf{C}_6$ would impose additional constraints to the representations.

The representation of a tensor-valued function $\hat{\mathbf{T}}$ is considered first. We can start with the representations (48) and (49) for the point group $\mathcal{D}_{6h}$ and add additional terms related to $\mathbf{K}_3$. The tensor generators are given as

$$\begin{aligned} & \mathbf{I}, \mathbf{C}, \mathbf{C}^2, \mathbf{H}_i, \mathbf{CH}_i + \mathbf{H}_i \mathbf{C}, \mathbf{C}^2 \mathbf{H}_i + \mathbf{H}_i \mathbf{C}^2, \mathbf{K}_3^2, \\ & \mathbf{CK}_3 - \mathbf{K}_3 \mathbf{C}, \mathbf{C}^2 \mathbf{K}_3 - \mathbf{K}_3 \mathbf{C}^2, \mathbf{K}_3 \mathbf{CK}_3, \mathbf{K}_3 \mathbf{CK}_3^2 - \mathbf{K}_3^2 \mathbf{CK}_3, \\ & \mathbf{H}_i \mathbf{K}_3 - \mathbf{K}_3 \mathbf{H}_i, \mathbf{H}_i^2 \mathbf{K}_3 - \mathbf{K}_3 \mathbf{H}_i^2, \mathbf{K}_3 \mathbf{H}_i \mathbf{K}_3, \mathbf{K}_3 \mathbf{H}_i \mathbf{K}_3^2 - \mathbf{K}_3^2 \mathbf{H}_i \mathbf{K}_3, \text{ for } i = 1, 2, 3 \end{aligned} \quad (53)$$

and the invariants are

$$\begin{aligned} & tr \mathbf{C}, tr \mathbf{C}^2, tr \mathbf{C}^3, tr(\mathbf{CH}_i), tr(\mathbf{C}^2 \mathbf{H}_i), tr(\mathbf{CK}_3^2), tr(\mathbf{C}^2 \mathbf{K}_3^2), tr(\mathbf{C}^2 \mathbf{K}_3^2 \mathbf{CK}_3), \\ & tr(\mathbf{CH}_i \mathbf{K}_3), tr(\mathbf{C}^2 \mathbf{H}_i \mathbf{K}_3), tr(\mathbf{CH}_i^2 \mathbf{K}_3), tr(\mathbf{CK}_3^2 \mathbf{H}_i \mathbf{K}_3), \text{ for } i = 1, 2, 3 \end{aligned} \quad (54)$$

After eliminating redundant terms in (53) and (54), the representation of $\hat{\mathbf{T}}$ is expressed as

$$\begin{aligned} \hat{\mathbf{T}}(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3, \mathbf{K}_3) = & \alpha_0 \mathbf{I} + \alpha_1 \mathbf{H}_1 + \alpha_2 \mathbf{H}_2 + \alpha_3 \mathbf{H}_3 + \alpha_4 \mathbf{C} + \alpha_5 \mathbf{C}^2 \\ & + \alpha_6 (\mathbf{CH}_1 + \mathbf{H}_1 \mathbf{C}) + \alpha_7 (\mathbf{C}^2 \mathbf{H}_1 + \mathbf{H}_1 \mathbf{C}^2) + \alpha_8 (\mathbf{CH}_2 + \mathbf{H}_2 \mathbf{C}) + \alpha_9 (\mathbf{C}^2 \mathbf{H}_2 + \mathbf{H}_2 \mathbf{C}^2) \\ & + \alpha_{10} (\mathbf{CH}_3 + \mathbf{H}_3 \mathbf{C}) + \alpha_{11} (\mathbf{C}^2 \mathbf{H}_3 + \mathbf{H}_3 \mathbf{C}^2) + \alpha_{12} (\mathbf{CK}_3 - \mathbf{K}_3 \mathbf{C}) \\ & + \alpha_{13} (\mathbf{C}^2 \mathbf{K}_3 - \mathbf{K}_3 \mathbf{C}^2) + \alpha_{14} (\mathbf{K}_3 \mathbf{CK}_3) + \alpha_{15} (\mathbf{K}_3 \mathbf{CK}_3^2 - \mathbf{K}_3^2 \mathbf{CK}_3) \end{aligned} \quad (55)$$

and

$$\begin{aligned} \alpha_i = & \alpha_i(tr \mathbf{C}, tr \mathbf{C}^2, tr \mathbf{C}^3, tr(\mathbf{CH}_1), tr(\mathbf{C}^2 \mathbf{H}_1), tr(\mathbf{CH}_2), tr(\mathbf{C}^2 \mathbf{H}_2), tr(\mathbf{CH}_3), tr(\mathbf{C}^2 \mathbf{H}_3)) \\ = & \tilde{\alpha}_i(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3, \mathbf{K}_3) \end{aligned} \quad (56)$$

As mentioned earlier, the group generator $\mathbf{C}_6$ imposes an additional constraint $\hat{\mathbf{T}}(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3, \mathbf{K}_3) = \hat{\mathbf{T}}(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1, \mathbf{K}_3)$ to the representation, which requires the coefficient functions to satisfy the following constraints.

$$\begin{aligned} \tilde{\alpha}_1(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3, \mathbf{K}_3) &= \tilde{\alpha}_3(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1, \mathbf{K}_3), \\ \tilde{\alpha}_2(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3, \mathbf{K}_3) &= \tilde{\alpha}_1(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1, \mathbf{K}_3), \\ \tilde{\alpha}_6(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3, \mathbf{K}_3) &= \tilde{\alpha}_{10}(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1, \mathbf{K}_3), \\ \tilde{\alpha}_8(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3, \mathbf{K}_3) &= \tilde{\alpha}_6(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1, \mathbf{K}_3), \\ \tilde{\alpha}_7(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3, \mathbf{K}_3) &= \tilde{\alpha}_{11}(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1, \mathbf{K}_3), \\ \tilde{\alpha}_9(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3, \mathbf{K}_3) &= \tilde{\alpha}_7(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1, \mathbf{K}_3), \\ \tilde{\alpha}_i(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3, \mathbf{K}_3) &= \tilde{\alpha}_i(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1, \mathbf{K}_3) \text{ for } i = 0, 4, 5, 12, 13, 14, 15 \end{aligned} \quad (57)$$

The representation of a scalar-valued function $\hat{\psi}$ follows the same form of (56). Moreover, the additional constraint imposed by $\mathbf{C}_6$ is

$$\hat{\psi}(\mathbf{C}, \mathbf{H}_1, \mathbf{H}_2, \mathbf{H}_3, \mathbf{K}_3) = \hat{\psi}(\mathbf{C}, \mathbf{H}_2, \mathbf{H}_3, \mathbf{H}_1, \mathbf{K}_3) \quad (58)$$

15 Continuous groups

In this section, we provide the representations of tensor functions for three centrosymmetric continuous groups $\mathcal{C}_{\infty h}$, $\mathcal{D}_{\infty h}$ (transversely isotropic) and $\mathcal{K}_{\infty}$ (isotropic). For simplicity purposes, we only present the final results. Most of the results can be found in the literature.

For the transversely isotropic group $\mathcal{C}_{\infty h}$, Zheng proposed $\mathbf{K}_3 = \boldsymbol{\varepsilon} \mathbf{k}$ as the structural tensor. The representation of $\hat{\mathbf{T}}$ is

$$\begin{aligned} \hat{\mathbf{T}}(\mathbf{C}, \mathbf{K}_3) = & \alpha_0 \mathbf{I} + \alpha_1 \mathbf{C} + \alpha_2 \mathbf{C}^2 + \alpha_3 \mathbf{K}_3^2 + \alpha_4 (\mathbf{C} \mathbf{K}_3 - \mathbf{K}_3 \mathbf{C}) \\ & + \alpha_5 (\mathbf{C}^2 \mathbf{K}_3 - \mathbf{K}_3 \mathbf{C}^2) + \alpha_6 (\mathbf{K}_3 \mathbf{C} \mathbf{K}_3) + \alpha_7 (\mathbf{K}_3 \mathbf{C} \mathbf{K}_3^2 - \mathbf{K}_3^2 \mathbf{C} \mathbf{K}_3) \end{aligned} \quad (59)$$

and

$$\alpha_i = \alpha_i(\text{tr} \mathbf{C}, \text{tr} \mathbf{C}^2, \text{tr} \mathbf{C}^3, \text{tr}(\mathbf{C} \mathbf{K}_3^2), \text{tr}(\mathbf{C}^2 \mathbf{K}_3^2), \text{tr}(\mathbf{C}^2 \mathbf{K}_3^2 \mathbf{C} \mathbf{K}_3)) \quad (60)$$

The representation of a scalar-valued function $\hat{\psi}$ is the same as (60).

For the transversely isotropic group $\mathcal{D}_{\infty h}$, Boehler [3] proposed $\mathbf{M}_3 = \mathbf{k} \otimes \mathbf{k}$ as the structural tensor. The representation of a tensor-valued function $\hat{\mathbf{T}}$ is

$$\hat{\mathbf{T}}(\mathbf{C}, \mathbf{M}_3) = \alpha_0 \mathbf{I} + \alpha_1 \mathbf{C} + \alpha_2 \mathbf{C}^2 + \alpha_3 \mathbf{M}_3 + \alpha_4 (\mathbf{C} \mathbf{M}_3 + \mathbf{M}_3 \mathbf{C}) + \alpha_5 (\mathbf{C}^2 \mathbf{M}_3 + \mathbf{M}_3 \mathbf{C}^2) \quad (61)$$

and

$$\alpha_i = \alpha_i(\text{tr} \mathbf{C}, \text{tr} \mathbf{C}^2, \text{tr} \mathbf{C}^3, \text{tr}(\mathbf{C} \mathbf{M}_3), \text{tr}(\mathbf{C}^2 \mathbf{M}_3)) \quad (62)$$

The representation of a scalar-valued function $\hat{\psi}$ is the same as (62).

Finally, for the isotropic group $\mathcal{K}_{\infty}$, the representations are well known as

$$\mathbf{T}(\mathbf{C}) = \alpha_0 \mathbf{I} + \alpha_1 \mathbf{C} + \alpha_2 \mathbf{C}^2 \quad (63)$$

and

$$\alpha_i = \alpha_i(\text{tr} \mathbf{C}, \text{tr} \mathbf{C}^2, \text{tr} \mathbf{C}^3) \quad (64)$$

The representation of a scalar-valued function ψ is the same as (64).

16 Conclusion

In this work, we present a systematic study on the representation of tensor functions using lower-order structural tensor sets for 3D centrosymmetric point groups. The traditional representation theory by Boehler and Liu involves higher-order structural tensors that are inconvenient to use for constitutive modeling of anisotropic materials. Based on a reformulated representation theory by Man and Goddard, we propose lower-order structural tensor sets for 3D centrosymmetric point groups and derive the representations of scalar- and 2nd-order symmetric tensor-valued functions for each group. Among the 14 centrosymmetric groups in 3D space, six groups ($\mathcal{C}_i, \mathcal{C}_{2h}, \mathcal{D}_{2h}, \mathcal{C}_{\infty h}, \mathcal{D}_{\infty h}$, and $\mathcal{K}_h$) have lower-order structural tensors so the original Boehler-Liu formulation is used. In contrast, for the eight groups ($\mathcal{C}_{4h}, \mathcal{D}_{4h}, \mathcal{C}_{3i}, \mathcal{D}_{3d}, \mathcal{C}_{6h}, \mathcal{D}_{6h}, \mathcal{T}_h$, and $\mathcal{O}_h$) involving higher-order structural tensors, the Man-Goddard reformulation and our proposed lower-order structural tensor sets should be used. The key difference between the Boehler-Liu formulation and Man-Goddard reformulation is that the latter relaxes symmetry constraints to structural tensors but requires additional constraints to the representations afterwards. The representation theory developed in this work provides explicit expressions of tensor functions for constitutive modeling of anisotropic materials. For scalar-valued and 2nd-order symmetric tensor-valued functions, the presented theory is applicable to all 3D point groups because their representations are determined by the corresponding centrosymmetric groups. Certainly, the structural tensor sets are non-unique. Researchers can devise new structural tensor sets and derive the representations following a similar procedure. Future research can be towards developing specific constitutive laws for anisotropic materials and integrating the presented theory with artificial intelligence to enable data-driven constitutive modeling.

Acknowledgments

This work is funded by National Science Foundation through the grant CMMI-2244952.

Declaration of Interest Statement

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

- [1] Niels Saabye Ottosen and Matti Ristinmaa. *The mechanics of constitutive modeling*. Elsevier, Amsterdam, Netherlands, 2005.
- [2] Q.-S. Zheng. Theory of Representations for Tensor Functions—A Unified Invariant Approach to Constitutive Equations. *Applied Mechanics Reviews*, 47(11):545–587, November 1994.
- [3] Jean-Paul Boehler. *Applications of tensor functions in solid mechanics*. Springer, Vienna, 1987.
- [4] Nikolas Apel. *Approaches to the description of anisotropic material behaviour at finite elastic and plastic deformations: theory and numerics*. PhD thesis, Zugl.: Stuttgart, Univ., Diss., 2004.
- [5] Ronald S Rivlin. Large elastic deformations of isotropic materials iv. further developments of the general theory. *Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences*, 241(835):379–397, 1948.
- [6] Ronald S Rivlin. Further remarks on the stress-deformation relations for isotropic materials. In *Collected Papers of RS Rivlin: Volume I and II*, pages 1014–1035. Springer, Berlin, Germany, 1955.
- [7] Allen Compere Pipkin and RS Rivlin. The formulation of constitutive equations in continuum physics. i. In *Collected Papers of RS Rivlin: Volume I and II*, pages 1111–1126. Springer, Berlin, Germany, 1959.
- [8] Walter Noll. Representations of certain isotropic tensor functions. *Archiv der Mathematik*, 21(1):87–90, 1970.
- [9] CC Wang. On representations for isotropic functions: Part i. isotropic functions of symmetric tensors and vectors. *Archive for Rational Mechanics and Analysis*, 33(4):249–267, January 1969.
- [10] CC Wang. On representations for isotropic functions: Part ii. isotropic functions of skew-symmetric tensors, symmetric tensors, and vectors. *Archive for Rational Mechanics and Analysis*, 33:268–287, 1969.
- [11] GF Smith. On isotropic functions of symmetric tensors, skew-symmetric tensors and vectors. *International Journal of Engineering Science*, 9(10):899–916, 1971.

- [12] J. P. Boehler. On irreducible representations for isotropic scalar functions. *ZAMM - Journal of Applied Mathematics and Mechanics / Zeitschrift für Angewandte Mathematik und Mechanik*, 57(6):323–327, 1977.
- [13] Jean-Paul Boehler. A simple derivation of representations for non-polynomial constitutive equations in some cases of anisotropy. *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*, 59(4):157–167, 1979.
- [14] I-Shin Liu et al. On representations of anisotropic invariants. *International Journal of Engineering Science*, 20(10):1099–1109, 1982.
- [15] AJM Spencer. The formulation of constitutive equation for anisotropic solids. In *Mechanical Behavior of Anisotropic Solids/Comportment Mécanique des Solides Anisotropes: Proceedings of the Euromech Colloquium 115 Villard-de-Lans, June 19–22, 1979/Colloque Euromech 115 Villard-de-Lans, 19–22 juin 1979*, pages 3–26. Springer, Dordrecht, 1982.
- [16] Josef Betten. Irreducible invariants of fourth-order tensors. *Mathematical Modelling*, 8:29–33, 1987.
- [17] H. Xiao. On isotropic extension of anisotropic tensor functions. *ZAMM - Journal of Applied Mathematics and Mechanics / Zeitschrift für Angewandte Mathematik und Mechanik*, 76(4):205–214, 1996.
- [18] Chi-Sing Man and Joe D Goddard. Remarks on isotropic extension of anisotropic constitutive functions via structural tensors. *Mathematics and Mechanics of Solids*, 23(4):554–563, 2018.
- [19] Mohammad Madadi, Lin Cheng, and Pu Zhang. Representation of tensor functions using lower-order structural tensor set: Two-dimensional point groups. *Journal of Elasticity*, 157(4):72, 2025.
- [20] Jiexian Ma, Zihan Liu, and Pu Zhang. Precisely patterning liquid metal microfibers through electrohydrodynamic printing for soft conductive composites and electronics. *Advanced Materials*, page 2507646, 2025.
- [21] Aminur Rahman, Mohammad Madadi, Jiexian Ma, and Pu Zhang. Overcoming conductivity–stretchability trade-off in soft conductive composites through liquid metal junctions. *ACS Applied Materials & Interfaces*, 0(0):null, 0. PMID: 40928007.
- [22] Grégory Chagnon, Marie Rebouah, and Denis Favier. Hyperelastic energy densities for soft biological tissues: a review. *Journal of Elasticity*, 120(2):129–160, 2015.

- [23] Mohammad Madadi and Pu Zhang. Finite-size effect on the percolation and electromechanical behaviors of liquid metal particulate composites. *Soft Matter*, 20(5):1061–1069, 2024.
- [24] Quang-Kha Nguyen and Pu Zhang. Modeling electromechanical behaviors of soft conductive composites embedded with liquid metal fibers. *Mechanics of Materials*, 190:104920, 2024.
- [25] Marc De Graef and Michael E. McHenry. *Structure of Materials: An Introduction to Crystallography, Diffraction and Symmetry*. Cambridge University Press, Cambridge, 2 edition, 2012.
- [26] A.J.M. Spencer. Theory of invariants. In A.C. Eringen, editor, *Mathematics*, pages 239–353. Academic Press, 1971.
- [27] Vera Ebbing. *Design of polyconvex energy functions for all anisotropy classes*. Inst. für Mechanik, Abt. Bauwissenschaften, 2010.

Appendix

Table A1: Invariants in the 3D isotropic irreducible functional bases of $\mathbf{A}_i$ and $\mathbf{W}_i$ [2, 11].

Variables	Invariants
$\mathbf{A}$	$tr\mathbf{A}, tr\mathbf{A}^2, tr\mathbf{A}^3$
$\mathbf{A}_1, \mathbf{A}_2$	$tr(\mathbf{A}_1\mathbf{A}_2), tr(\mathbf{A}_1^2\mathbf{A}_2), tr(\mathbf{A}_1\mathbf{A}_2^2), tr(\mathbf{A}_1^2\mathbf{A}_2^2)$
$\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3$	$tr(\mathbf{A}_1\mathbf{A}_2\mathbf{A}_3)$
$\mathbf{W}$	$tr\mathbf{W}^2$
$\mathbf{A}, \mathbf{W}$	$tr(\mathbf{A}\mathbf{W}^2), tr(\mathbf{A}^2\mathbf{W}^2), tr(\mathbf{A}^2\mathbf{W}^2\mathbf{A}\mathbf{W})$
$\mathbf{A}_1, \mathbf{A}_2, \mathbf{W}$	$tr(\mathbf{A}_1\mathbf{A}_2\mathbf{W}), tr(\mathbf{A}_1^2\mathbf{A}_2\mathbf{W}), tr(\mathbf{A}_1\mathbf{A}_2^2\mathbf{W}), tr(\mathbf{A}_1\mathbf{W}^2\mathbf{A}_2\mathbf{W})$
$\mathbf{W}_1, \mathbf{W}_2$	$tr(\mathbf{W}_1\mathbf{W}_2)$
$\mathbf{A}, \mathbf{W}_1, \mathbf{W}_2$	$tr(\mathbf{A}\mathbf{W}_1\mathbf{W}_2), tr(\mathbf{A}\mathbf{W}_1^2\mathbf{W}_2), tr(\mathbf{A}\mathbf{W}_1\mathbf{W}_2^2)$
$\mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3$	$tr(\mathbf{W}_1\mathbf{W}_2\mathbf{W}_3)$

Table A2: Tensor generators in the 3D irreducible representations for isotropic 2nd-order symmetric tensor-valued functions of $\mathbf{A}_i$ and $\mathbf{W}_i$ [2, 11].

Variables	Generators
	$\mathbf{I}$
$\mathbf{A}$	$\mathbf{A}, \mathbf{A}^2$
$\mathbf{W}$	$\mathbf{W}^2$
$\mathbf{A}_1, \mathbf{A}_2$	$\mathbf{A}_1\mathbf{A}_2 + \mathbf{A}_2\mathbf{A}_1, \mathbf{A}_1^2\mathbf{A}_2 + \mathbf{A}_2\mathbf{A}_1^2, \mathbf{A}_1\mathbf{A}_2^2 + \mathbf{A}_2^2\mathbf{A}_1$
$\mathbf{A}, \mathbf{W}$	$\mathbf{A}\mathbf{W} - \mathbf{W}\mathbf{A}, \mathbf{A}^2\mathbf{W} - \mathbf{W}\mathbf{A}^2, \mathbf{W}\mathbf{A}\mathbf{W}, \mathbf{W}\mathbf{A}\mathbf{W}^2 - \mathbf{W}^2\mathbf{A}\mathbf{W}$
$\mathbf{W}_1, \mathbf{W}_2$	$\mathbf{W}_1\mathbf{W}_2 + \mathbf{W}_2\mathbf{W}_1, \mathbf{W}_1\mathbf{W}_2^2 - \mathbf{W}_2^2\mathbf{W}_1, \mathbf{W}_1^2\mathbf{W}_2 - \mathbf{W}_2\mathbf{W}_1^2$

Table A3: Group generators of 3D Laue groups [27].

Laue group	Group generators
$\mathcal{C}_i$	$\bar{\mathbf{I}}$
$\mathcal{C}_{2h}$	$\mathbf{C}_2, \bar{\mathbf{I}}$
$\mathcal{D}_{2h}$	$\mathbf{C}_2, \mathbf{C}_{2x}, \bar{\mathbf{I}}$
$\mathcal{C}_{4h}$	$\mathbf{C}_4, \bar{\mathbf{I}}$
$\mathcal{D}_{4h}$	$\mathbf{C}_4, \mathbf{C}_{2x}, \bar{\mathbf{I}}$
$\mathcal{C}_{3i}$	$\mathbf{C}_3, \bar{\mathbf{I}}$
$\mathcal{D}_{3d}$	$\mathbf{C}_3, \mathbf{C}_{2x}, \bar{\mathbf{I}}$
$\mathcal{C}_{6h}$	$\mathbf{C}_6, \bar{\mathbf{I}}$
$\mathcal{D}_{6h}$	$\mathbf{C}_6, \mathbf{C}_{2x}, \bar{\mathbf{I}}$
$\mathcal{T}_h$	$\mathbf{C}_{2x}, \mathbf{C}_{2y}, \mathbf{Q}_p^{2\pi/3}, \bar{\mathbf{I}}$
$\mathcal{O}_h$	$\mathbf{C}_{4x}, \mathbf{C}_{2y}, \mathbf{Q}_p^{2\pi/3}, \bar{\mathbf{I}}$

Useful matrices for Table A3:

$$\begin{aligned}
 \mathbf{I} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \bar{\mathbf{I}} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \mathbf{C}_2 = \mathbf{Q}_{X_3}^\pi = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \mathbf{C}_{2x} = \mathbf{Q}_{X_1}^\pi = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \\
 \mathbf{C}_4 = \mathbf{Q}_{X_3}^{\pi/2} &= \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \mathbf{C}_3 = \mathbf{Q}_{X_3}^{2\pi/3} = \begin{bmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \mathbf{C}_6 = \mathbf{Q}_{X_3}^{\pi/3} = \begin{bmatrix} 1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \\
 \mathbf{C}_{2y} = \mathbf{Q}_{X_2}^\pi &= \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \mathbf{Q}_p^{2\pi/3} = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \mathbf{C}_{4x} = \mathbf{Q}_{X_1}^{\pi/2} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}
 \end{aligned}$$